MULTISCALE METHODS AND ANALYSIS FOR THE NONLINEAR SCHRÖDINGER EQUATION WITH WAVE OPERATOR

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MULTISCALE METHODS AND ANALYSIS FOR THE NONLINEAR SCHRÖDINGER EQUATION WITH WAVE OPERATOR

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Declaration

I hereby declare that this thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in the thesis.

This thesis has also not been submitted for any degree in any university previously.

郭怡辰

Guo Yichen

13 August 2021

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Contents

Summary

The Schrödinger equation is a fundamental partial differential equation that describes the wave function of particles in quantum mechanics. The nonlinear Schrödinger equation with wave operator (NLSW) arises from the nonrelativistic limit of Klein-Gordon equation, and plays an important part in many physics applications such as plasma and light bullets. Depending on the parameters, the solution can be highly oscillatory, and it is worthwhile to design multiscale methods to study the equation numerically.

The aim of this thesis is to propose different multiscale methods to solve the NLSW and related equations, and establish uniform error estimates. Rigorous proofs are presented, and numerical results are reported to verify the theoretical error bounds. The thesis mainly consists of the following three parts:

In the first part, the system of ordinary differential equations (ODEs) arises from finite difference spatial discretization of the NLSW is discussed. The equation system involving a parameter $0 < \varepsilon \leq 1$, and the solution of this system propagates wave with $O(\varepsilon^2)$ wavelength. The amplitude of the leading oscillation of the solution is $O(\varepsilon^4)$ for well-prepared initial data, and $O(\varepsilon^2)$ for ill-prepared initial data. Based on the nested Picard iteration and the exponential integrator, a uniformly second order accurate numerical scheme is developed. The uniform error bound $O(\tau^2)$ is rigorously established w.r.t $\varepsilon \in (0, 1]$ and for fixed ε, the method converges with third order accuracy as $\tau \to 0$. Numerical results are presented to confirm the error estimates and show the optimality.

The second part is devoted to studying a uniformly accurate numerical method for the NLSW. The parameter $0 < \varepsilon \leq 1$ controls the strength of the wave operator, and the NLSW converges to the nonlinear Schrödinger equation (NLS) as $\varepsilon \to 0^+$. The solution of the NLSW differs from the solution of the NLS with a highly oscillation function in time with $O(\varepsilon^2)$ wavelength. To overcome the difficulties from the rapid oscillations, we propose a nested Picard iterative integrator sine pseudospectral (NPI-SP) method for the NLSW. The optimal uniform error bound $O(\tau^2)$ in time and spectral accuracy in space for both well-prepared and ill-prepared initial data in H^1 norms is rigorously proved, which significantly improves the existing results. Numerical studies confirm the error estimates and show that they are sharp.

The last part is to study the long-time dynamics of the NLSW with weak nonlinearities. The nonlinearity strength is characterized by ε^2 with $\varepsilon \in (0, 1]$ and with $O(1)$ initial data, and the long-time dynamics is up to time at $O(\varepsilon^{-\beta})$ and with $0 \le \beta \le 2$. An exponential wave integrator Fourier spectral pseudospectral (EWI-SP) method is applied to the NLSW to numerically solve the equation in the long-time regime. The error bound of the EWI-SP method is carried out, which is uniform $O(\varepsilon^{2-\beta}\tau^2)$ in time and spectral accuracy in space up to time at $O(\varepsilon^{-\beta})$. Extensive numerical results are reported to support the theoretical long-time error estimates, and suggest they are optimal. The method is also efficient for high dimensional problems, with dynamics presented as examples.

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List of Symbols and Abbreviations

i	imaginary unit
t	time variable
$\boldsymbol{x}$	spatial variable
c	speed of light
$\hbar$	reduced Planck constant
τ	time step size
h	space mesh size
∇	gradient
$\Delta = \nabla \cdot \nabla$	Laplacian
$\mathbb{R}^d$	d-dimensional Euclidean space
$\mathbb{C}^d$	d-dimensional complex space
$\mathbb{T}^d$	d-dimensional torus
$\mathrm{Re}(f)$	the real part of f
$\mathrm{Im}(f)$	the imaginary part of f
$\overline{f}$	the conjugate part of f
$\boldsymbol{y}^T$	the transpose part of vector $\boldsymbol{y}$
$\boldsymbol{y}^*$	the conjugate transpose of vector $\boldsymbol{y}$
∂_t	the partial derivative of t
$A \lesssim B$	$A \leq C \cdot B$ for some generic constant $C > 0$

1D	one dimension
2D	two dimension
3D	three dimension
ODE	ordinary differential equation
PDE	partial differential equation
NLS	nonlinear Schrödinger equation
NLSW	nonlinear Schrödinger equation with wave operator
NKGE	nonlinear Klein-Gordon equation
NPI	nested Picard integrator
NPI-SP	nested Picard integrator sine pseudospectral
EWI	exponential wave integrator
EWI-FP	exponential wave integrator Fourier pseudospectral

Chapter 1

Introduction

This chapter serves as an introduction of the thesis. In the first section, a brief overview of the Schrödinger equation and the Klein-Gordon equation is presented. In the second section, an introduction of the nonlinear Schrödinger equation with wave operator (NLSW) is provided. In the third section, the existing results of the NLSW and related equations are reviewed. The problems to study and the scope of the thesis are shown in the last two sections.

1.1 Background

The Schrödinger equation is a linear partial differential dispersive equation that plays the important role in quantum mechanics, as the Newton's second law in classical mechanics [20, 87, 92, 96]. Denote complex scalar function $\psi := \psi(\boldsymbol{x}, t)$ as the wave function, describing the distribution of the particles. The Schrödinger equation is

$$i\hbar\partial_t\psi(\boldsymbol{x}, t) = -\frac{\hbar^2}{m}\nabla^2\psi(\boldsymbol{x}, t) + V(\boldsymbol{x}, t)\psi(\boldsymbol{x}, t), \quad \boldsymbol{x} \in \mathbb{R}^d, \tag{1.1.1}$$

where t is time, $\boldsymbol{x}$ is the spatial coordinate, ∇^2 is the Laplace operator and $V(\boldsymbol{x}, t)$ stands for the potential. The constants involved are m the mass, $\hbar$ the reduced Plank constant and $i = \sqrt{-1}$ the imaginary unit.

The Schrödinger equation, as a dispersive equation [63, 67, 98], could describe the evolution of a quantum system. However, it would no longer be valid when the velocity of the particle is so high that special relativity should be applied with quantum mechanics together. In 1926, the Klein-Gordon equation was proposed to describe the motion of high velocity particles [17, 23, 32, 80, 109]. The Klein-Gordon equation is

$$\frac{\hbar^2}{mc^2}\partial_{tt}\psi(\boldsymbol{x},t) - \frac{\hbar^2}{m}\nabla^2\psi(\boldsymbol{x},t) + mc^2\psi(\boldsymbol{x},t) = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, \tag{1.1.2}$$

where c is the speed of light. The Klein-Gordon equation can be seen as the form of a Schrödinger equation system which includes two coupled first order differential equations in time.

The nonlinear version of the Klein-Gordon equation (NKGE) [46, 49, 76, 90, 93, 99] is as follows:

$$\frac{\hbar^2}{mc^2}\partial_{tt}\psi(\boldsymbol{x},t) - \frac{\hbar^2}{m}\nabla^2\psi(\boldsymbol{x},t) + mc^2\psi(\boldsymbol{x},t) + f(\psi(\boldsymbol{x},t)) = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, \tag{1.1.3}$$

where $f : \mathbb{C} \to \mathbb{C}$ is a given nonlinear function. In most previous studies and applications [7, 37, 49, 87, 95], the nonlinearity $f(\psi)$ is often taken as the power nonlinearity, which is

$$f(\psi) = \lambda|\psi|^{2p}\psi, \tag{1.1.4}$$

where $\lambda \in \mathbb{R}$ and p is a positive integer. The nonlinear Klein-Gordon equation has various physical applications [22, 108, 112] and many numerical methods [38, 39, 51, 84] have been developed to solve it.

By rescaling $t, \boldsymbol{x}, \psi, \lambda$ and c in (1.1.3), we can normalize the other constants, and consider the modulated function $\phi(\boldsymbol{x},t) = e^{-ic^2t}\psi(\boldsymbol{x},t)$, we have the following modulated equation:

$$i\partial_t\phi(\boldsymbol{x},t) - \frac{1}{c^2}\partial_{tt}\phi(\boldsymbol{x},t) + \nabla^2\phi(\boldsymbol{x},t) + f(\phi(\boldsymbol{x},t)) = 0, \quad \boldsymbol{x} \in \mathbb{R}^d. \tag{1.1.5}$$

Taking the non-relativistic limit of the nonlinear Klein-Gordon equation, i.e. $c \to \infty$, the NKGE will converge to the following nonlinear Schrödinger equation with wave operator (NLSW) [72, 73, 75, 91, 100]

$$i\partial_t\phi(\boldsymbol{x},t) - \varepsilon^2\partial_{tt}\phi(\boldsymbol{x},t) + \nabla^2\phi(\boldsymbol{x},t) + f(\phi(\boldsymbol{x},t)) = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, \tag{1.1.6}$$

if we denote the parameter ε by $\varepsilon = \frac{1}{c}$. As $c \to \infty$, $0 < \varepsilon \le 1$ and $\varepsilon \to 0$.

1.2 The nonlinear Schrödinger equation with wave operator (NLSW)

In this thesis we discuss the nonlinear Schrödinger equation with wave operator (NLSW) in d, ($d = 1, 2, 3$) dimensions as [3, 6, 30, 73, 91] (denote the wave function $\psi := \psi(\boldsymbol{x}, t)$)

$$\begin{cases} i\partial_t\psi - \varepsilon^2\partial_{tt}\psi + \nabla^2\psi + F(|\psi|^2)\psi = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, \quad t > 0 \\ \psi(\boldsymbol{x}, 0) = \psi_0(\boldsymbol{x}), \quad \partial_t\psi(\boldsymbol{x}, 0) = \psi_1^\varepsilon(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d, \end{cases} \tag{1.2.1}$$

x is the space variable and t is the time variable. $F(|\psi|^2) = |\psi|^{2p}$ (p is a positive integer) is the power nonlinearity. $0 < \varepsilon \leq 1$ is the aforementioned parameter introduced by the light speed c controlling the perturbation operator. This equation (1.2.1) has many different physical applications, for instance the Langmuir wave envelope approximation in plasma [18, 30], and the modulated planar pulse approximation of the sine-Gordon equation for light bullets [10, 108].

The NLSW has the two following conserved quantities, the energy $E^\varepsilon(t)$ which is defined by

$$E^\varepsilon(t) := \int_{\mathbb{R}^d} \varepsilon^2|\partial_t\psi(\boldsymbol{x}, t)|^2 + |\nabla\psi(\boldsymbol{x}, t)|^2 - \tilde{F}(|\psi(\boldsymbol{x}, s)|^2)d\boldsymbol{x} \equiv E^\varepsilon(0), \quad t \geq 0, \tag{1.2.2}$$

where $\tilde{F}$ is the primitive function of F defined by

$$\tilde{F}(s) = \int_0^s F(\rho)d\rho,$$

and the mass $N^\varepsilon(t)$ which is defined by

$$N^\varepsilon(t) := \int_{\mathbb{R}^d} |\psi(\boldsymbol{x}, t)|^2 d\boldsymbol{x} - 2\varepsilon^2 \int_{\mathbb{R}^d} \mathrm{Im}\Big(\overline{\psi(\boldsymbol{x}, t)}\partial_t\psi(\boldsymbol{x}, t)\Big)d\boldsymbol{x} \equiv N^\varepsilon(0), \quad t \geq 0, \tag{1.2.3}$$

where $\overline{c}$ and $\mathrm{Im}(c)$ are the conjugate and the imaginary part of c if $c \in \mathbb{C}$.

As proven in [3, 18, 78, 91], when $\varepsilon \to 0^+$ the solution of equation (1.2.1) will collapse to the following limit equation, which is the nonlinear Schrödinger equation (NLS):

$$\begin{cases} i\partial_t\psi(\boldsymbol{x}, t) + \nabla^2\psi(\boldsymbol{x}, t) + F(|\psi(\boldsymbol{x}, t)|^2)\psi(\boldsymbol{x}, t) = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, \quad t > 0, \\ \psi(\boldsymbol{x}, 0) = \psi_0(\boldsymbol{x}), \quad x \in \mathbb{R}^d. \end{cases} \tag{1.2.4}$$

As proved in [18], if the initial data of the NLSW (1.2.1) $(\psi_0, \psi_1^\varepsilon) \in H^2 \times H^2$, $\|\psi_1^\varepsilon\|_{H^2}$ is uniformly bounded w.r.t. ε, then there exists a constant $T > 0$ independent of ε, such that the solution ψ^ε of the NLSW (1.2.1) with parameter ε and the solution ψ^s of the NLS (1.2.4) exists on $[0, T]$. The convergence speed can be bounded by:

$$\|\psi^\varepsilon - \psi^s\|_{L^\infty([0,T];H^2)} \leq C\varepsilon^2. \tag{1.2.5}$$

By analytical results [18, 78, 91], the solution of (1.2.1) differs from the solution of (1.2.4) with a oscillating function with $O(\varepsilon^2)$ wavelength because of the second order differential term. To measure the difference from the solution of equation (1.2.1) to the solution of equation (1.2.4), we can assume the initial velocity ψ_1^ε to be:

$$\psi_1^\varepsilon(\boldsymbol{x}) = i(\nabla^2\psi_0(\boldsymbol{x}) + F(|\psi_0(\boldsymbol{x})|^2\psi_0(\boldsymbol{x}))) + \varepsilon^\alpha\omega^\varepsilon(\boldsymbol{x}), \quad \alpha \geq 0, \tag{1.2.6}$$

where $i(\nabla^2\psi_0(x) + F(|\psi_0(x)|^2\psi_0(x)))$ is the initial velocity for the NLS (1.2.4), and $\omega^\varepsilon(\boldsymbol{x})$ the initial perturbation. Then we have the following asymptotic expansion for the solution $\psi^\varepsilon(x, t)$ of NLSW (denote $\psi^s(x, t)$ to be the solution of NLS) [3]:

$$\begin{aligned} \psi^\varepsilon(\boldsymbol{x}, t) =& \psi^s(\boldsymbol{x}, t) + \varepsilon^2\{\text{no oscillation terms}\} \\ &+ \varepsilon^{2+\min\{\alpha,2\}}\phi(\boldsymbol{x}, \frac{t}{\varepsilon^2}) + \{\text{higher order oscillations}\}, \end{aligned} \tag{1.2.7}$$

where $\phi(\boldsymbol{x}, t)$ is a non-oscillatory function.

Based on this asymptotic expansion, we can identify two cases for the imposed initial data (1.2.6). α is a parameter describing how close the initial value is compared with NLS case. When $\alpha \geq 2$ the initial data is called the well-prepared case, as $\partial_{tt}\psi(x, t)|_{t=0}$ is bounded, and $0 \leq \alpha < 2$ is called ill-prepared case correspondingly, where $\partial_{tt}\psi(x, t)|_{t=0}$ is no longer bounded. The asymptotic expansion also shows a uniform method w.r.t. ε is required to study the limit $\varepsilon \to 0^+$, which means the choice of the time and space step size to achieve the same accuracy should be independent of ε. Otherwise, if time step τ depends on ε, when $\varepsilon \ll 1$, the number of time steps $N = T/\tau$ will be too large, and the computation is too expensive.

The unboundedness of $\partial_{tt}\psi(x, t)$ prevents the previous exponential wave integrator (EWI) method [7] to achieve uniform second order accuracy in time. To improve

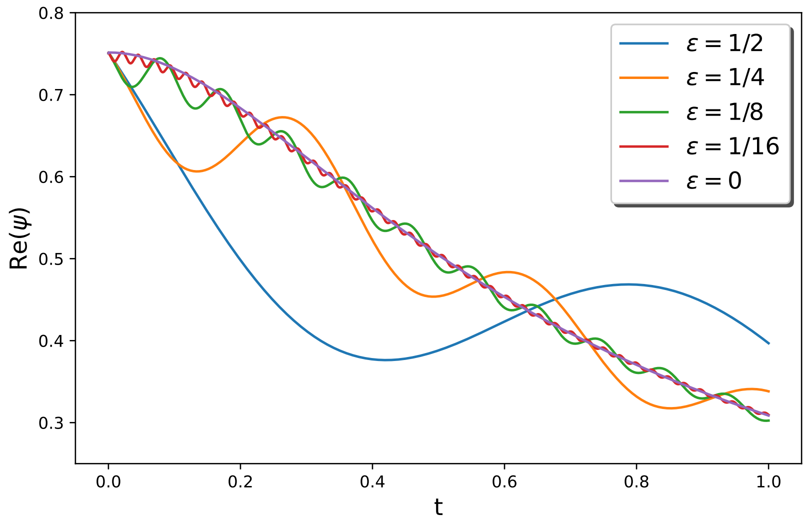

Figure 1.1: The real part of equation (1.2.1) solution at $x = 0$ with $F(|\psi(x,t)|^2) = -|\psi(x,t)|^2$, $\psi_0(x) = \pi^{-1/4}e^{-x^2/2}$, $\omega^\varepsilon(x) = e^{-x^2/2}$, $\alpha = 2$ for different ε.

this integrator method, we are to apply the idea of Picard iteration. The Picard iteration, given differential equation $\frac{dy}{dt} = f(x,y)$, $y(x_0) = y_0$, constructs a sequence $\{y_n(x)\}$ that will converge to the solution $y(x)$. The iteration from $y_n(t)$ to $y_{n+1}(x)$ is $y_{n+1}(x) = y_0 + \int_{x_0}^{x} f(t, y_n(t))dt$. It can be proved that the nested Picard integrator no longer requires the boundedness of $\partial_{tt}\psi(x,t)$ to stay uniform second order in time.

To illustrate the solution behavior for equation (1.2.1) and the limit equation (1.2.4), Figure 1.1 and 1.2 shows how the real part of the solution changes with time at the point $x = 0$, with $F(|\psi(x,t)|^2) = -|\psi(x,t)|^2$, $\psi_0(x) = \pi^{-1/4}e^{-x^2/2}$, $\omega^\varepsilon(x) = e^{-x^2/2}$. Figure 1.1 shows different solutions with different ε (where $\varepsilon = 0$ is the graph of the solution of limit equation (1.2.4)) for a well-prepared case $\alpha = 2$, and Figure 1.1 shows solutions for an ill-prepared case $\alpha = 0$. The spatial distribution of the solution at time $T = 1$ with $\varepsilon = 1/4$ is also shown in figure 1.3.

It can be seen from these graphs that although the solution shows no oscillation in space, it is oscillatory in time with wave length $O(\varepsilon^2)$ for both well-prepared and ill-prepared initial data, and the ill-prepared initial data will lead to larger oscillation. As ε goes to 0, those solutions will converge to the solution of equation 1.2.4.

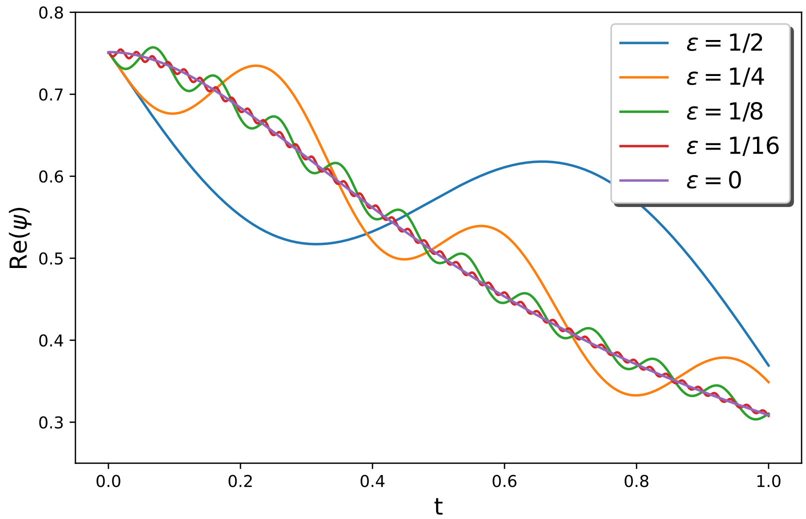

Figure 1.2: The real part of equation (1.2.1) solution at $x = 0$ with $F(|\psi(x,t)|^2) = -|\psi(x,t)|^2$, $\psi_0(x) = \pi^{-1/4}e^{-x^2/2}$, $\omega^\varepsilon(x) = e^{-x^2/2}$, $\alpha = 0$ for different ε.

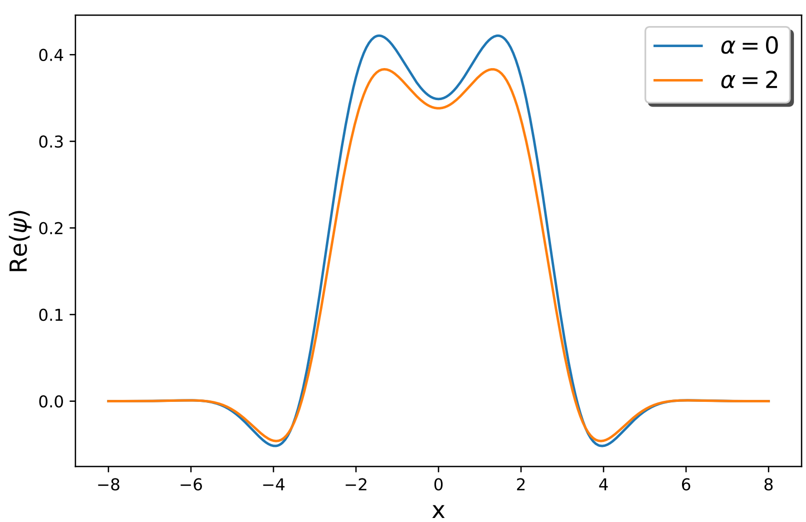

Figure 1.3: The real part of equation (1.2.1) solution at $T = 1$ with $F(|\psi(x,t)|^2) = -|\psi(x,t)|^2$, $\psi_0(x) = \pi^{-1/4}e^{-x^2/2}$, $\omega^\varepsilon(x) = e^{-x^2/2}$, $\varepsilon = 1/4$ for $\alpha = 0$ and $\alpha = 2$.

1.3 Literature review

Various researches have been devoted to the nonlinear Schrödinger equation with wave operator and related equations, both analytically and numerically. In this section we are going to review the existing results.

The nonlinear Schrödinger equation (NLS) has drawn much attentions [2, 35, 45, 55–58, 68, 79, 88]. Numerous numerical methods have been proposed in the previous work to solve the NLS, including the finite difference method [1, 5, 27, 34, 47, 102] or the time-splitting method [15, 21, 33, 43, 54, 70, 71, 74, 77, 78, 86, 97, 106].

As stated in the previous section, the solution of the nonlinear Schrödinger equation with wave operator differs from the solution of the NLS by a highly oscillatory function. There have been various work on solving highly oscillatory ordinary differential equations [8, 29, 31, 42, 48, 52, 59, 69, 85, 89, 101, 116] and partial differential equations [16, 28, 36, 64, 83, 103, 107, 110].

For the NLSW, several numerical methods have been developed in previous works [3, 6, 65, 104, 111]. The conservative Crank-Nicolson finite difference scheme and the semi-implicit finite difference scheme have been proposed [3], and the error estimates shows these two schemes are at order $O(h^2 + \tau)$ and $O(h^2 + \tau^{2/3})$ for well-prepared and ill-prepared case.

However, for the finite difference method, the uniform convergence rates are not uniform in τ. Exponential wave integrator (EWI) applying to the NLSW can greatly improve the uniform convergence rates in τ. EWI has been widely applied in solving highly oscillatory ODE [44, 53, 59–61] and PDE [6, 7, 9, 11, 66, 105, 113, 114] problems. An exponential wave integrator sine pseudospectral (EWI-SP) method for NLSW has been proposed [6], and the method has spectral accuracy in space, and the optimal uniform temporal error bounds $O(\tau^2)$ for well-prepared initial data and $O(\tau)$ for ill-prepared initial data. In order to overcome the difficulties when solving the NLSW under ill-prepared initial data and achieve uniform temporal accuracy, we are to apply nested Picard integrators (NPI) [24, 26] to solve the NLSW in this thesis.

1.4 Problems to study

As is pointed out in the previous sections, although much effort has been devoted to solving the nonlinear Schrödinger equation with wave operator, the current methods cannot achieve uniform second order accuracy for ill-prepared initial data. This motivates us to design new accurate and uniform numerical method to solve the NLSW equation for both well-prepared and ill-prepared cases. Specifically, the purpose of the thesis are:

- Design a proper method for the NLSW and related equations that can achieve second order for temporal errors. The method need to achieve uniform accuracy for both well-prepared and ill-prepared initial data.

- Give rigorously proof for the error bounds, and validate them through numerical examples.

- For the NLSW with a weak nonlinearity, design a method that is second order accurate in time up to the long-time, then compute and analyzed the dynamics.

1.5 Structure and scope of the thesis

The thesis is organized as follows.

Chapter 2 focused on construction a uniformly second order scheme of an ordinary equation system. This ODE system arises from finite difference spatial discretization of the NLSW. Based on the nested Picard iteration and the exponential integrator, the uniformly second order method is developed and analyzed. The uniform error bound $O(\tau^2)$ is rigorously established w.r.t. $\varepsilon \in (0, 1]$ for both well-prepared and ill-prepared initial data. For fixed ε, the method converges with third order accuracy as $\tau \to 0$. Numerical results are presented to confirm the error estimates and show the optimality.

In Chapter 3, a uniformly accurate numerical method for the NLSW is presented.

The scheme, based on the nested Picard iteration and sine pseudospectral method, solves the NLSW truncated on bounded domain. The method overcomes the difficulties from the rapid oscillations in ill-prepared initial data case, and the optimal uniform error bound $O(\tau^2)$ in time and spectral accuracy in space for both well-prepared and ill-prepared initial data in H^1 norms is rigorously proved. Numerical studies confirms the error estimates and show that they are optimal.

Chapter 4 is devoted to study the long-time dynamics of the NLSW with weak nonlinearities. The nonlinearity strength is characterized by ε^2 with $\varepsilon \in (0, 1]$ with $O(1)$ initial data, and the long-time dynamics is up to time at $O(\varepsilon^{-\beta})$ with $0 \leq \beta \leq 2$. An exponential wave integrator Fourier spectral pseudospectral (EWI-FP) method is applied to the NLSW to numerically solve the equation in the long-time regime. The error bound of the EWI-FP method up to time at $O(\varepsilon^{-\beta})$ is carried out, which is uniform $O(\varepsilon^{2-\beta}\tau^2)$ in time and spectral accuracy in space up to time at $O(\varepsilon^{-\beta})$. Extensive numerical results are reported to support the theoretical long-time error estimates, and 2D dynamics presented as examples.

Finally, conclusions are drawn in Chapter 5. Several possible future topics are also discussed.

Research in this thesis mainly focuses on the multiscale methods for the nonlinear Schrödinger equation with wave operator and other related equations. These methods may improve the accuracy for a wide variety of initial data comparing with previous methods, and are very useful for practical computations.

Throughout the thesis, we will use the notation $A \lesssim B$ to mean that there exists a generic constant C independent of ε and time step size τ such that $|A| \leq CB$. C will denote a constant independent of ε and τ that may change from line to line.

Chapter 2

Nested Picard Integrators for Oscillatory ODEs

In this chapter, the ordinary equation system arises from finite difference spatial discretization of the NLSW is discussed. A uniformly second order accurate numerical scheme based on the nested Picard iteration and the exponential integrator is developed, and the error bound is rigorously proved.

2.1 A system of oscillatory ordinary differential equations (ODEs)

In this chapter, we consider the following system of oscillatory ordinary differential equations:

$$\begin{cases} i\dot{\boldsymbol{y}}(t) - \varepsilon^2\ddot{\boldsymbol{y}}(t) - A\boldsymbol{y}(t) - F(\boldsymbol{y}(t))\boldsymbol{y}(t) = 0, \quad t > 0, \\ \boldsymbol{y}(0) = \boldsymbol{y}_0, \qquad \dot{\boldsymbol{y}}(0) = \boldsymbol{y}_1^\varepsilon, \end{cases} \tag{2.1.1}$$

where $\boldsymbol{y} := \boldsymbol{y}(t) = (y_1(t), y_2(t), \cdots, y_d(t))^T \in \mathbb{C}^d$, $|\boldsymbol{y}|^2 = \boldsymbol{y}^*\boldsymbol{y}$ ($\boldsymbol{y}^*$ is the conjugate transpose $\boldsymbol{y}^* = \overline{\boldsymbol{y}}^T$), $\varepsilon \in (0, 1]$ is a parameter, $A \in \mathbb{C}^{d\times d}$ is a positive definite Hermitian matrix, $\boldsymbol{y}_0, \boldsymbol{y}_1^\varepsilon \in \mathbb{C}^d$. The nonlinear term $F : \mathbb{C}^d \to \mathbb{C}^{d\times d}$ is assumed to be locally Lipschitz, e.g. $F(\boldsymbol{y}) = \mathrm{diag}(\boldsymbol{y}\boldsymbol{y}^*)$. We shall consider the case that initial value $\boldsymbol{y}_0$ is fixed and the initial velocity $\boldsymbol{y}_1^\varepsilon = O(1)$ w.r.t. ε.

The ODE system arises from a spatial discretization of the nonlinear Schrödinger equation with wave operator (NLSW) (denote $\psi := \psi(\boldsymbol{x}, t)$):

$$\begin{cases} i\partial_t\psi - \varepsilon^2\partial_{tt}\psi + \nabla^2\psi - F(|\psi|^2)\psi = 0, \quad \boldsymbol{x} \in \mathbb{R}^n, \quad t > 0, \\ \psi(\boldsymbol{x}, 0) = \psi_0(\boldsymbol{x}), \quad \partial_t\psi(\boldsymbol{x}, 0) = \psi_1(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^n, \end{cases} \tag{2.1.2}$$

where $\psi = \psi(\boldsymbol{x}, t)$ is a complex-valued wave function, $F : [0, +\infty) \to \mathbb{R}$ is the nonlinear term and one common nonlinearity reads $F(|\psi(\boldsymbol{x}, t)|^2) = \pm|\psi(\boldsymbol{x}, t)|^2$. After applying suitable spatial discretization such as finite difference, ODE system (2.1.1) could be derived with $F(\boldsymbol{y}) = \pm\text{diag}(\boldsymbol{y}\boldsymbol{y}^*)$.

As shown in [18, 73, 91, 100], when $\varepsilon \to 0^+$, the solution of equation (2.1.1) will converge to the following system of first order nonlinear ordinary equations:

$$\begin{cases} i\dot{\boldsymbol{y}}(t) - A\boldsymbol{y}(t) - F(\boldsymbol{y}(t))\boldsymbol{y}(t) = 0, \quad t > 0, \\ \boldsymbol{y}(0) = \boldsymbol{y}_0. \end{cases} \tag{2.1.3}$$

To characterize the convergence and the asymptotic behavior of equation (2.1.1) for $\varepsilon \ll 1$, we assume the initial velocity can be decomposed as [3, 6, 42, 48]

$$\boldsymbol{y}_1^\varepsilon = i(-A\boldsymbol{y}_0 - F(\boldsymbol{y}_0)\boldsymbol{y}_0) + \varepsilon^\alpha\boldsymbol{\omega}, \tag{2.1.4}$$

$\boldsymbol{\omega}$ is a constant vector and parameter $\alpha \geq 0$ describes the consistency of the initial value and initial velocity for $\boldsymbol{y}(t)$ in equation (2.1.1) ($\boldsymbol{\omega}$ can be dependent on ε, but here we fix $\boldsymbol{\omega}$ for simplicity).

Following [3, 6], we can derive the following asymptotic expansion for the solution $\boldsymbol{y}(t)$ of Eq. (2.1.1):

$$\begin{aligned} \boldsymbol{y}(t) =& \boldsymbol{y}^s(t) + \varepsilon^2\{\text{terms without oscillation}\} \\ &+ \varepsilon^{2+\min\{\alpha,2\}}\boldsymbol{Y}\Big(\frac{t}{\varepsilon^2}\Big) + \text{higher order terms with oscillation}, \end{aligned} \tag{2.1.5}$$

where $\boldsymbol{y}^s(t)$ is the solution of the limit equation (2.1.3), and $\boldsymbol{Y}(t)$ is a smooth function representing the leading oscillation.

For the well-prepared initial data case, i.e. $\alpha \geq 2$, the leading oscillation is of $O(\varepsilon^4)$ amplitude and attributes to the perturbation term $\varepsilon^2\ddot{\boldsymbol{y}}(t)$ in equation (2.1.1). For the ill-prepared case, i.e. $0 \le \alpha < 2$, the leading oscillation is of $O(\varepsilon^2)$ amplitude and comes from the incompatibility of the initial data.

For well-prepared case, uniformly second order methods have been already proposed in [6] but it can not achieve second order for ill-prepared initial data because of the unboundedness of $\ddot{\boldsymbol{y}}(t) = O(\varepsilon^{\alpha-2})$ when $\varepsilon \ll 1$. In this work, we are going to propose a uniformly second order (w.r.t. $\varepsilon \in (0,1]$) method that works for both well-prepared and ill-prepared case in this chapter.

To illustrate the solution behavior for equation (2.1.1) and the limit (2.1.3), Figure 2.1 shows the real part of the solutions for $d = 1$, $A = 1$, $F(y) = |y|^2$, $y_0 = 0.5$, $\omega = 2$ and $\alpha = 2$ with different ε. The $\varepsilon = 0$ is the graph for the solution of equation (2.1.3). It can be seen from Figure 2.1 that the solution of equation (2.1.1) oscillates with wavelength at $O(\varepsilon^2)$, and converges to the the solution of equation (2.1.3).

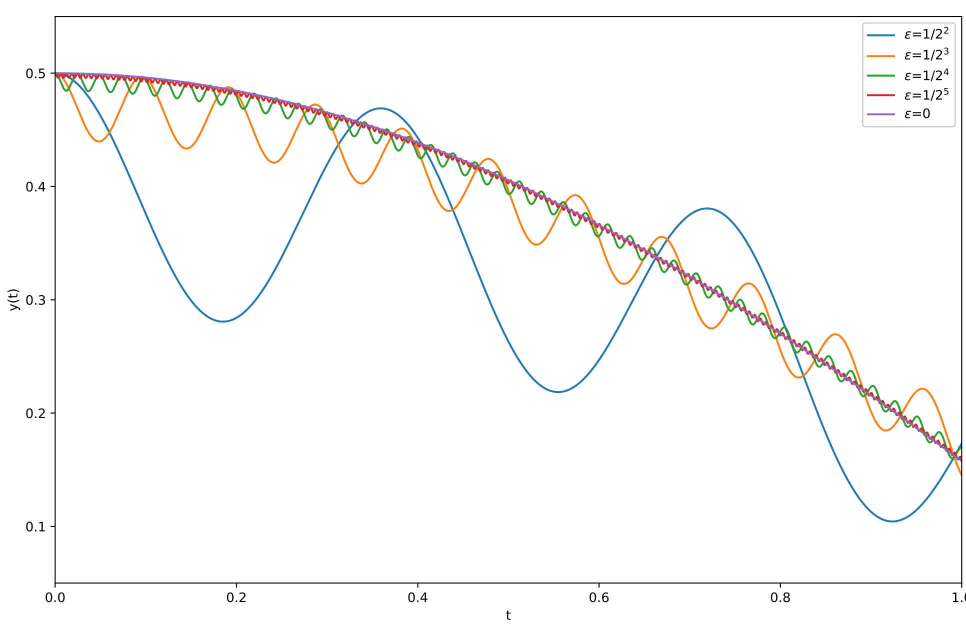

Figure 2.1: $\mathrm{Re}(y(t))$ for different parameter ε.

2.2 Nested Picard integrator (NPI)

2.2.1 The general idea of NPI

In this section we present the details of our uniform second order nested Picard integrator (NPI) for equation (2.1.1). For simplicity, we assume $F(\boldsymbol{y}) = \mathrm{diag}(\boldsymbol{y}\boldsymbol{y}^*)$ in the subsequent discussions, and the method can be easily generalized to more general nonlinearity $F(\cdot)$, e.g. polynomial type function $F(\boldsymbol{y})$. As Hermitian matrix is unitarily diagonalizable, we can write $A = U^*DU$, where $U = (u_{ij})_{d\times d} \in \mathbb{C}^{d\times d}$ is a unitary matrix and $D = \mathrm{diag}(d_{11}, d_{22}, \cdots, d_{dd}) \in \mathbb{C}^{d\times d}$ ($d_{ll} > 0$, $l = 1, \cdots, d$) is diagonal. After the variable change $\tilde{\boldsymbol{y}}(t) = U\boldsymbol{y}(t)$, equation (2.1.1) becomes:

$$\begin{cases} i\dot{\tilde{\boldsymbol{y}}}(t) - \varepsilon^2\ddot{\tilde{\boldsymbol{y}}}(t) - D\tilde{\boldsymbol{y}}(t) - \tilde{F}(\tilde{\boldsymbol{y}}(t))\tilde{\boldsymbol{y}}(t) = 0, \quad t > 0, \\ \tilde{\boldsymbol{y}}(0) = U\boldsymbol{y}_0, \qquad \dot{\tilde{\boldsymbol{y}}}(0) = U\boldsymbol{y}_1^\varepsilon, \end{cases} \tag{2.2.1}$$

where $\tilde{F}(\tilde{\boldsymbol{y}}(t)) = U\mathrm{diag}(U^*\tilde{\boldsymbol{y}}\tilde{\boldsymbol{y}}^*U)U^*$.

Choose the time step size $\Delta t = \tau > 0$ and denote the time steps as $t_n = n\tau$ ($n = 0, 1, \cdots$). In each time interval $t \in [t_n, t_{n+1}]$, we have the variation of constants formula for $\tilde{\boldsymbol{y}}(t_n + s)$:

$$\begin{aligned} \tilde{\boldsymbol{y}}(t_n + s) = &- e^{i\beta^+ s}\beta^{-1}(\beta^-\tilde{\boldsymbol{y}}(t_n) + i\dot{\tilde{\boldsymbol{y}}}(t_n)) + e^{i\beta^- s}\beta^{-1}(\beta^+\tilde{\boldsymbol{y}}(t_n) + i\dot{\tilde{\boldsymbol{y}}}(t_n)) \\ &+ i\gamma\int_0^s \kappa(s-w)\tilde{F}(\tilde{\boldsymbol{y}}(t_n+w))\tilde{\boldsymbol{y}}(t_n+w)\mathrm{d}w, \quad 0 \le s \le \tau, \end{aligned} \tag{2.2.2}$$

where $\beta^+ = \mathrm{diag}(\beta_1^+, \beta_2^+, \cdots, \beta_d^+)$ and $\beta^- = \mathrm{diag}(\beta_1^-, \beta_2^-, \cdots, \beta_d^-)$ are two diagonal matrices with entries given by:

$$\begin{aligned} \beta_l^+ &= \frac{1+\sqrt{1+4\varepsilon^2 d_{ll}}}{2\varepsilon^2} = O\left(\frac{1}{\varepsilon^2}\right), \\ \beta_l^- &= \frac{1-\sqrt{1+4\varepsilon^2 d_{ll}}}{2\varepsilon^2} = \frac{-2d_{ll}}{1+\sqrt{1+4\varepsilon^2 d_{ll}}} = O(1), \end{aligned} \tag{2.2.3}$$

and $\beta = \beta^+ - \beta^- = \mathrm{diag}(\beta_1, \beta_2, \cdots, \beta_d) = O(\varepsilon^{-2})$, $\gamma = \frac{1}{\varepsilon^2}\beta^{-1} = \mathrm{diag}(\gamma_1, \gamma_2, \cdots, \gamma_d) = O(1)$. The kernel $\kappa(t)$ reads

$$\kappa(t) = e^{i\beta^+ t} - e^{i\beta^- t} = \mathrm{diag}(\kappa_1(t), \kappa_2(t), \cdots, \kappa_d(t)). \tag{2.2.4}$$

Therefore, the solution $\boldsymbol{y}(t)$ to (2.1.1) satisfies:

$$\begin{aligned}\boldsymbol{y}(t_n+s) = &- U^* e^{i\beta^+ s}\beta^{-1}(\beta^- U\boldsymbol{y}(t_n) \\ &+ iU\dot{\boldsymbol{y}}(t_n)) + U^* e^{i\beta^- s}\beta^{-1}(\beta^+ U\boldsymbol{y}(t_n) + iU\dot{\boldsymbol{y}}(t_n)) \\ &+ iU^*\gamma\int_0^s \kappa(s-w)UF(\boldsymbol{y}(t_n+w))\boldsymbol{y}(t_n+w)\mathrm{d}w, \quad 0\le s\le\tau,\end{aligned} \tag{2.2.5}$$

where for each component $y_l(t_n+s)$, $l=1,2,\cdots,d$, for $0\le s\le\tau$,

$$\begin{aligned}y_l(t_n+s) = \quad &- \sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\beta_j^{-1}(\beta_j^- y_k(t_n) + i\dot{y}_k(t_n))e^{i\beta_j^+ s} \\ &+ \sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\beta_j^{-1}(\beta_j^+ y_k(t_n) + i\dot{y}_k(t_n))e^{i\beta_j^- s} \\ &+ i\sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\gamma_j\int_0^s \kappa_j(s-w)|y_k(t_n+w)|^2 y_k(t_n+w)\mathrm{d}w,\end{aligned} \tag{2.2.6}$$

From the above integral form (2.2.5), it is not difficult to derive that there exists $T>0$ independent of $\varepsilon\in(0,1]$, such that (2.1.1) with initial data satisfying (2.1.4) admits solution $\boldsymbol{y}(t)\in C([0,T];\mathbb{C}^d)$, and $\dot{\boldsymbol{y}}(t)=O(1)$, $\ddot{\boldsymbol{y}}(t)=O(\varepsilon^{\min\{\alpha-2,0\}})$. To overcome the difficulty induced by the oscillation which results in the unbounded derivatives $\frac{d^k\boldsymbol{y}(t)}{dt^k}$ ($k\ge 2$) for $\varepsilon\to 0^+$, we propose the following nested Picard integrators [26], i.e. we construct approximations of $\boldsymbol{y}(t)$ as

$$\boldsymbol{y}^{n,m}(s) = (y_1^{n,m}(s), y_2^{n,m}(s),\cdots, y_d^{n,m}(s))^T, \quad m=0,1,\cdots,d,$$

to $\boldsymbol{y}(t_n+s)$ for $s\in[0,\tau]$ based on integral equation (2.2.6) via the following nested Picard iteration: $y_l^{n,0}(s)=y_l(t_n)$, for $0\le s\le\tau$,

$$\begin{aligned}y_l^{n,m+1}(s) = \quad &- \sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\beta_j^{-1}(\beta_j^- y_k(t_n) + i\dot{y}_k(t_n))e^{i\beta_j^+ s} \\ &+ \sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\beta_j^{-1}(\beta_j^+ y_k(t_n) + i\dot{y}_k(t_n))e^{i\beta_j^- s} \\ &+ i\sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\gamma_j\int_0^s \kappa_j(s-w)|y_k^{n,m}(w)|^2 y_k^{n,m}(w)\mathrm{d}w,\end{aligned} \tag{2.2.7}$$

where m stands for the number of Picard integration. The $(m+1)$-th Picard iteration $\boldsymbol{y}^{n,m+1}$ is therefore computed by submitting the m-th iteration $\boldsymbol{y}^{n,m}$ into the integral of nonlinear terms in (2.2.6). Based on the aforementioned properties of $\boldsymbol{y}(t)$, we have $\boldsymbol{y}^{n,0}(s) - \boldsymbol{y}(t_n + s) = O(s)$ as $\dot{\boldsymbol{y}}(t) = O(1)$, and then $\boldsymbol{y}^{n,1}(s) - \boldsymbol{y}(t_n + s) = O(s^2)$. Recursively, we would obtain the local error as

$$y_l(t_n + s) - y_l^{n,m}(s) = O(\tau^{m+1}),$$

and the global error would be $O(\tau^m)$.

In order to update NPI approximations from formula (2.2.7), $\dot{\boldsymbol{y}}(t)$ is also required. By taking the derivative of equation (2.2.6), we have for $l = 1, 2, \cdots d$, $0 \leq s \leq \tau$,

$$\begin{aligned} \dot{y}_l(t_n + s) = \quad & -i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^+ \beta_j^{-1} (\beta_j^- y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^+ s} \\ & + i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^- \beta_j^{-1} (\beta_j^+ y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^- s} \\ & + i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j \int_0^s \dot{\kappa}_j(s-w) |y_k(t_n+w)|^2 y_k(t_n+w) \mathrm{d}w, \end{aligned} \tag{2.2.8}$$

and the corresponding approximations $\dot{\boldsymbol{y}}^{n,m+1}(s)$ in the NPI are given by $\dot{y}_l^{n,0}(s) = \dot{y}_l(t_n)$, $0 \leq s \leq \tau$,

$$\begin{aligned} \dot{y}_l^{n,m+1}(s) = \quad & -i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^+ \beta_j^{-1} (\beta_j^- y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^+ s} \\ & + i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^- \beta_j^{-1} (\beta_j^+ y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^- s} \\ & + i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j \int_0^s \dot{\kappa}_j(s-w) |y_k^{n,m}(w)|^2 y_k^{n,m}(w) \mathrm{d}w. \end{aligned} \tag{2.2.9}$$

Similarly, we would have:

$$\varepsilon^2(\dot{y}_l(t_n + s) - \dot{y}_l^{n,m}(s)) = O(\tau^{m+1}).$$

Therefore, (2.2.7) and (2.2.9) form a complete numerical scheme for solving the system (2.1.1) from t_n to t_{n+1} by setting $s = \tau$ at m-th iterates with m-th order accuracy.

2.2.2 Detailed formulas for a uniform second order NPI

Here, we construct a second order NPI for solving (2.1.1) with (2.1.4). Ideally we can directly compute $\boldsymbol{y}^{n,2}(s)$ and $\dot{\boldsymbol{y}}^{n,2}(s)$ from (2.2.7) and (2.2.9), which would be computationally expensive. In practice, for numerical convenience, certain approximations should be done for evaluating $\boldsymbol{y}^{n,m}(s)$ and $\dot{\boldsymbol{y}}^{n,m}(s)$, e.g. when computing the integral (nonlinear) terms in (2.2.7) and (2.2.9). Thus, we introduce numerical approximations in (2.2.7) and (2.2.9) with residual functions $\boldsymbol{R}^n_{m+1}(s), \dot{\boldsymbol{R}}^n_{m+1}(s)$ $(m = 1, 2, \cdots)$ such that $y_l^{n,0}(s) = y_l(t_n)$, $\dot{y}_l^{n,0}(s) = \dot{y}_l(t_n)$, and

$$\begin{aligned} y_l^{n,m+1}(s) :=& -\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^{-1} (\beta_j^- y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^+ s} \\ &+ \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^{-1} (\beta_j^+ y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^- s} \\ &+ i\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j \int_0^s \kappa_j(s-w) |y_k^{n,m}(w)|^2 y_k^{n,m}(w) \mathrm{d}w \\ &- R^n_{m+1,l}(s), \quad 0 \le s \le \tau, \end{aligned} \tag{2.2.10}$$

$$\begin{aligned} \dot{y}_l^{n,m+1}(s) :=& -i\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^+ \beta_j^{-1} (\beta_j^- y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^+ s} \\ &+ i\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \beta_j^- \beta_j^{-1} (\beta_j^+ y_k(t_n) + i\dot{y}_k(t_n)) e^{i\beta_j^- s} \\ &+ i\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j \int_0^s \dot{\kappa}_j(s-w) |y_k^{n,m}(w)|^2 y_k^{n,m}(w) \mathrm{d}w \\ &- \dot{R}^n_{m+1,l}(s), \quad 0 \le s \le \tau, \end{aligned} \tag{2.2.11}$$

where the residual functions $\boldsymbol{R}^n_{m+1}(s) = O(s^{m+1})$, $\varepsilon^2 \dot{\boldsymbol{R}}^n_{m+1}(s) = O(s^{m+1})$ and the accuracy of NPI is preserved, i.e.

$$y_l(t_n + s) - y_l^{n,m}(s) = O(\tau^{m+1}), \quad \varepsilon^2(\dot{y}_l(t_n + s) - \dot{y}_l^{n,m}(s)) = O(\tau^{m+1}).$$

The way we choose the residue functions or the numerical approximations of the integral terms in (2.2.10) and (2.2.11) is such that we only need specify the approximations for (2.2.10) ((2.2.11) can be obtained by taking the derivative of (2.2.10)).

In order to maintain the ε-dependent accuracy, we find that the highly oscillatory factors in (2.2.10) and (2.2.11) have to be treated properly. Here, we adopt Gautschi-type quadrature, and separate the highly oscillatory part and the slow varying part, then integrate the oscillatory part exactly and approximate the non-oscillatory part by high order quadrature. The key observation is that the rapid oscillations are induced by $e^{i\beta^+ t}$, which can be decomposed as

$$e^{i\beta^+ t} = e^{i\frac{1}{\varepsilon^2}t} e^{-i\beta^- t}, \quad \beta^- = O(1).$$

Thus, it is clear that the first term $e^{i\frac{1}{\varepsilon^2}t}$ is the leading frequency of the rapid oscillation and the second term $e^{-i\beta^- t}$ is slow varying.

Below, we detail the construction of practical NPIs up to second order. For simplicity, we introduce two families of functions $h^k_{+,j} : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C}$ and $h^k_{-,j} : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C}$ for $j, k = 1, 2, \cdots, d$ to denote the coefficients of highly oscillatory terms and slow varying terms in the linear part of (2.2.10) as

$$h^k_{+,j}(\boldsymbol{u}, \boldsymbol{v}) = -\beta_j^{-1}(\beta_j^- u_k + iv_k), \quad h^k_{-,j}(\boldsymbol{u}, \boldsymbol{v}) = \beta_j^{-1}(\beta_j^+ u_k + iv_k), \tag{2.2.12}$$

and let $h^{n,k}_{+,j} = h^k_{+,j}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))$, $h^{n,k}_{-,j} = h^k_{-,j}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))$.

First order NPI. Starting with $\boldsymbol{y}^{n,0}(s) = \boldsymbol{y}(t_n)$, we have from (2.2.10) for $l = 1, 2, \cdots, d$,

$$\begin{aligned} y_l^{n,1}(s) =& e^{is/\varepsilon^2} \sum_{j,k=1}^d \overline{u_{jl}} u_{jk} h^{n,k}_{+,j} e^{-i\beta_j^- s} + \sum_{j,k=1}^d \overline{u_{jl}} u_{jk} h^{n,k}_{-,j} e^{i\beta_j^- s} \\ &+ i \sum_{j,k=1}^d \overline{u_{jl}} u_{jk} \gamma_j \Bigg(e^{is/\varepsilon^2} \int_0^s e^{-iw/\varepsilon^2} e^{-i\beta_j^-(s-w)} |y_k(t_n)|^2 y_k(t_n) dw \\ &\qquad - \int_0^s e^{i\beta_j^-(s-w)} |y_k(t_n)|^2 y_k(t_n) dw \Bigg) + O(s^2). \end{aligned}$$

For the integrals, using expansion $e^{i\beta_j^-(w-s)} = e^{i\beta_j^-(s-s)} + O(s) = 1 + O(s)$ $(w \in [0, s])$, we would obtain $y_l^{n,1}$(s). More precisely, introducing coefficients $p_k(s)$ for $k = 0, \pm 1, \pm 2$ as

$$p_k(s) = \int_0^s e^{ikw/\varepsilon^2} dw = O(s), \quad 0 \le s \le \tau, \tag{2.2.13}$$

and denoting $f^n_{+,l,j} = f_{+,l,j}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))$, $f^n_{-,l,j} = f_{-,l,j}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))$, $f^n_l = f_l(\boldsymbol{y}(t_n)))$ for $l, j = 1, 2, \cdots, d$:

$$\begin{aligned} &f^n_{+,l,j} = \sum_{k=1}^d \overline{u_{jl}} u_{jk} h^{n,k}_{+,j}, \quad f^n_{-,l,j} = \sum_{k=1}^d \overline{u_{jl}} u_{jk} h^{n,k}_{-,j}, \\ &f^n_l = \sum_{j,k=1}^d i\overline{u_{jl}} u_{jk} \gamma_j |y_k(t_n)|^2 y_k(t_n), \end{aligned} \tag{2.2.14}$$

we have the following expression for $\boldsymbol{y}^{n,1}(s)$:

$$y_l^{n,1}(s) = e^{is/\varepsilon^2}(\sum_{j=1}^{d} f_{+,l,j}^n e^{-i\beta_j^- s} + f_l^n p_{-1}(s)) + (\sum_{j=1}^{d} f_{-,l,j}^n e^{i\beta_j^- s} - f_l^n s), \quad 0 \le s \le \tau. \quad (2.2.15)$$

Taking the derivative of $y_l^{n,1}(s)$, we would get $\dot{y}_l^{n,1}(s)$, which could be also derived from (2.2.11) via the same approximations $e^{i\beta_j^-(w-s)} = 1 + O(s)$. However, the detailed form of $\dot{y}_l^{n,1}(s)$ does not appear in the constructions of higher order NPIs.

Second order NPI. Continue iteration with $\boldsymbol{y}^{n,1}(s)$, we would have to identify the leading oscillations in the nonlinear integral term. Noticing (2.2.15), we have

$$\begin{aligned} |y_l^{n,1}(s)|^2 =& F_{0,l}^n(s) + sF_{1,l}^n(s) + p_{-1}(s)F_{-2,l}^n(s) + p_1(s)F_{2,l}^n(s) \\ &+ e^{-is/\varepsilon^2}(F_{-3,l}^n(s) + sF_{-4,l}^n(s) + p_1(s)F_{5,l}^n(s)) \\ &+ e^{is/\varepsilon^2}(F_{3,l}^n(s) + sF_{4,l}^n(s) + p_{-1}(s)F_{-5,l}^n(s)), \end{aligned} \quad (2.2.16)$$

where $F_{k,l}^n(s) := F_{k,l}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n), s), k = -5, -4, \cdots, 4, 5$ are given as

$$\begin{aligned} F_{0,l}^n(s) =& |f_{+,l}^n(s)|^2 + |f_{-,l}^n(s)|^2, \quad F_{1,l}^n(s) = 2\,\mathrm{Re}(-\overline{f_l^n} f_{-,l}^n(s)), \\ F_{2,l}^n(s) =& \overline{f_l^n} f_{+,l}^n(s), \quad F_{3,l}^n(s) = f_{+,l}^n(s)\overline{f_{-,l}^n(s)}, \\ F_{4,l}^n(s) =& -\overline{f_l^n} f_{-,l}^n(s), \quad F_{5,l}^n(s) = \overline{f_l^n} f_{-,l}^n(s), \\ F_{-k,l}^n(s) =& \overline{F_{k,l}^n(s)}, \end{aligned} \quad (2.2.17)$$

if we denote

$$f_{+,l}^n(s) = \sum_{j=1}^{d} f_{+,l,j}^n e^{-i\beta_j^- s}, \quad f_{-,l}^n(s) = \sum_{j=1}^{d} f_{-,l,j}^n e^{i\beta_j^- s}.$$

The following expression for $|y_l^{n,1}(s)|^2 y_l^{n,1}(s)$ is then obtained:

$$\begin{aligned} |y_l^{n,1}(s)|^2 y_l^{n,1}(s) =& g_{0,l}^n(s) + sg_{1,l}^n(s) + p_1(s)g_{2,l}^n(s) + p_{-1}(s)g_{3,l}^n(s) \\ &+ e^{-is/\varepsilon^2}(g_{4,l}^n(s) + sg_{5,l}^n(s) + p_1(s)g_{6,l}^n(s)) \\ &+ e^{is/\varepsilon^2}(g_{7,l}^n(s) + sg_{8,l}^n(s) + p_1(s)g_{9,l}^n(s) + p_{-1}(s)g_{10,l}^n(s)) \\ &+ e^{i2s/\varepsilon^2}(g_{11,l}^n(s) + sg_{12,l}^n(s) + p_{-1}(s)g_{13,l}^n(s)), \end{aligned} \quad (2.2.18)$$

where $g_{k,l}^n(s) = g_{k,l}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n), s)$ $(k = 0, 1, \cdots, 13)$ are given in (2.2.19) as

$$
\begin{aligned}
g_{0,l}^n(s) =& F_{-3,l}^n(s) f_{+,l}^n(s) + F_{0,l}^n(s) f_{-,l}^n(s),\\
g_{1,l}^n(s) =& F_{-4,l}^n(s) f_{+,l}^n(s) + F_{1,l}^n(s) f_{-,l}^n(s) - F_{0,l}^n(s) f_l^n,\\
g_{2,l}^n(s) =& F_{-5,l}^n(s) f_{+,l}^n(s) + F_{2,l}^n(s) f_{-,l}^n(s),\\
g_{3,l}^n(s) =& F_{-2,l}^n(s) f_{-,l}^n(s) + F_{-3,l}^n(s) f_l^n, \quad g_{4,l}^n(s) = F_{-3,l}^n(s) f_{-,l}^n(s)\\
g_{5,l}^n(s) =& F_{-4,l}^n(s) f_{+,l}^n(s) + F_{-3,l}^n(s)(-f_l^n), \quad g_{6,l}^n(s) = F_{-5,l}^n(s) f_{-,l}^n(s),\\
g_{7,l}^n(s) =& F_{0,l}^n(s) f_{+,l}^n(s) + F_{3,l}^n(s) f_{-,l}^n(s),\\
g_{8,l}^n(s) =& F_{1,l}^n(s) f_{+,l}^n(s) + F_{4,l}^n(s) f_{-,l}^n(s) + F_{3,l}^n(s)(-f_l^n),\\
g_{9,l}^n(s) =& F_{2,l}^n(s) f_{+,l}^n(s), \quad g_{11,l}^n(s) = F_{3,l}^n(s) f_{+,l}^n(s)\\
g_{10,l}^n(s) =& F_{-2,l}^n(s) f_{+,l}^n(s) + F_{5,l}^n(s) f_{-,l}^n(s) + F_{0,l}^n(s) f_l^n,\\
g_{12,l}^n(s) =& F_{4,l}^n(s) f_{+,l}^n(s), \quad g_{13,l}^n(s) = F_{5,l}^n(s) f_{+,l}^n(s) + F_{3,l}^n(s) f_l^n.
\end{aligned}
\tag{2.2.19}
$$

Making use of the expansion (2.2.18), we can now numerically compute $\boldsymbol{y}^{n,2}(s)$ for $0 \le s \le \tau$, $l = 1, 2, \cdots, d$,

$$
\begin{aligned}
y_l^{n,2}(s) :=& \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} h_{+,j}^{n,k} e^{i\beta_j^+ s} + \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} h_{-,j}^{n,k} e^{i\beta_j^- s}\\
&+ i \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j \Big(\int_0^s e^{i\frac{s-w}{\varepsilon^2} - i\beta_j^-(s-w)} |y_k^{n,1}(t_n+w)|^2 y_k^{n,1}(t_n+w) dw\\
&- \int_0^s e^{i\beta_j^-(s-w)} |y_k^{n,1}(t_n+w)|^2 y_k^{n,1}(t_n+w) dw \Big) + O(s^3).
\end{aligned}
\tag{2.2.20}
$$

To numerically approximate the integrals, we find there are three types of terms to be considered.

Type 1. Terms without ε-dependent rapid oscillation, such as

$$\int_0^s e^{i\beta_j^-(s-w)} w g_{1,k}^n(w) dw.$$

The midpoint rule is adopted to approximate the integral as

$$\int_0^s e^{i\beta_j^-(s-w)} w g_{1,k}^n(w) dw = e^{i\beta_j^- s/2} \frac{s^2}{2} g_{1,k}^n(\frac{s}{2}) + O(s^3).$$

Type 2. Oscillatory terms (ε dependent) with $O(\tau)$ amplitudes, such as

$$\int_0^s e^{-\frac{i}{\varepsilon^2}w}e^{-i\beta_j^-(s-w)}p_1(w)g_{2,k}^n(w)dw.$$

Expanding $e^{-i\beta_j^-(s-w)}g_{2,k}^n(w) = g_{2,k}^n(0) + O(s)$, and integrating the leading part exactly, we have

$$\begin{aligned}\int_0^s e^{-\frac{i}{\varepsilon^2}w}p_1(w)e^{-i\beta_j^-(s-w)}g_{2,k}^n(w)dw &= \int_0^s e^{-\frac{i}{\varepsilon^2}w}p_1(w)g_{2,k}^n(0)dw + O(s^3)\\ &= q_{-1,1}(s)g_{2,k}^n(0) + O(s^3),\end{aligned}$$

where the coefficients $q_{k,l}(s),\ k = 0, \pm1, \pm2,\ l = 0, \pm1$ are defined as

$$q_{k,l}(s) := \int_0^s \int_0^{s_1} e^{iks_1/\varepsilon^2}e^{ils_2/\varepsilon^2}ds_2ds_1 = O(s^2). \tag{2.2.21}$$

Type 3. Oscillatory terms (ε-dependent) with $O(1)$ amplitudes, such as

$$\int_0^s e^{-\frac{i}{\varepsilon^2}w}e^{-i\beta_j^-(s-w)}g_{0,k}^n(w)dw.$$

Recalling Taylor expansion

$$e^{i\beta_j^- w g_{0,k}^n(w)} = g_{0,k}^n(0) + w(i\beta_j^- g_{0,k}^n(0) + \dot{g}_{0,k}^n(0)) + O(\tau^2),$$

and integrating the leading terms exactly, we have

$$\begin{aligned}&\int_0^s e^{-i\beta_j^-(s-w)}e^{-\frac{i}{\varepsilon^2}w}g_{0,k}^n(w)dw\\ =&e^{-i\beta_j^- s}\int_0^s e^{-\frac{i}{\varepsilon^2}w}(g_{0,k}^n(0) + w(i\beta_j^- g_{0,k}^n(0) + \dot{g}_{0,k}^n(0)))dw + O(\tau^3)\\ =&e^{-i\beta_j^- s}\int_0^s e^{-\frac{i}{\varepsilon^2}w}(g_{0,k}^n(0) + p_0(w)(i\beta_j^- g_{0,k}^n(0) + \dot{g}_{0,k}^n(0)))dw + O(\tau^3)\\ =&e^{-i\beta_j^- s}(p_{-1}(s)g_{0,k}^n(0) + q_{-1,0}(s)(i\beta_j^- g_0^n(0) + \dot{g}_{0,k}^n(0))) + O(\tau^3).\end{aligned}$$

Under the aforementioned approximations, we obtain for $s \in [0, \tau]$ and $l = 1, 2, \cdots, d$,

$$\begin{aligned}y_l^{n,2}(s) = &\sum_{j,k=1}^d \overline{u_{jl}}u_{jk}h_{+,j}^{n,k}e^{i\beta_j^+ s} + \sum_{j,k=1}^d \overline{u_{jl}}u_{jk}h_{-,j}^{n,k}e^{i\beta_j^- s}\\ &+ \sum_{j,k=1}^d i\overline{u_{jl}}u_{jk}\gamma_j(G_{+,0,k}^n(s) + e^{-i\beta_j^- s/2}G_{+,1,k}^n(s)\\ &+ e^{-i\beta_j^- s}G_{+,2,k}^n(s) + i\beta_j^- e^{-i\beta_j^- s}G_{+,3,k}^n(s)\\ &+ G_{-,0,k}^n(s) + e^{i\beta_j^- s/2}G_{-,1,k}^n(s)\\ &+ e^{i\beta_j^- s}G_{-,2,k}^n(s) - i\beta_j^- e^{i\beta_j^- s}G_{-,3,k}^n(s)),\ 0 \le s \le \tau,\end{aligned} \tag{2.2.22}$$

where the expressions of $G_{\pm,j,k}$ $(j=0,\pm1,\pm2,\pm3; k=1,2,\cdots,d)$ are given in (2.2.23) as

$$
\begin{aligned}
G^n_{+,0,k}(s) =& G_{+,0,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)\\
=& e^{is/\varepsilon^2}(q_{-1,0}(s)g^n_{1,k}(0)+q_{-1,1}(s)g^n_{2,k}(0)+q_{-1,-1}(s)g^n_{3,k}(0)\\
&+q_{-2,0}(s)g^n_{5,k}(0)+q_{-2,1}(s)g^n_{6,k}(0)+q_{0,1}(s)g^n_{9,k}(0)\\
&+q_{0,-1}(s)g^n_{10,k}(0)+q_{1,0}(s)g^n_{12,k}(0)+q_{1,1}(s)g^n_{13,k}(0)),\\
G^n_{+,1,k}(s) =& G_{+,1,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)=e^{is/\varepsilon^2}(sg^n_{7,k}(s/2)+s^2/2g^n_{8,k}(s/2)),\\
G^n_{+,2,k}(s) =& G_{+,2,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)=e^{is/\varepsilon^2}(p_{-1}(s)g^n_{0,k}(0)+q_{-1,0}(s)\dot{g}^n_{0,k}(0)\\
&+p_{-2}(s)g^n_{4,k}(0)+q_{-2,0}(s)\dot{g}^n_{4,k}(0)\\
&+p_1(s)g^n_{11,k}(0)+q_{1,0}(s)\dot{g}^n_{11,k}(0)),\\
G_{+,3,k}(s) =& G_{+,3,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)\\
=& e^{is/\varepsilon^2}(q_{-1,0}(s)g^n_{0,k}(0)+q_{-2,0}(s)g^n_{4,k}(0)+q_{1,0}(s)g^n_{11,k}(0)),\\
G^n_{-,0,k}(s) =& G_{-,0,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)=q_{0,1}(s)g^n_{2,k}(0)+q_{0,-1}(s)g^n_{3,k}(0)\\
&+q_{-1,0}(s)g^n_{5,k}(0)\\
&+q_{-1,1}(s)g^n_{6,k}(0)+q_{-1,-1}(s)g^n_{8,k}(0)+q_{1,1}(s)g^n_{9,k}(0)\\
&+q_{1,-1}(s)g^n_{10,k}(0)+q_{2,0}(s)g^n_{12,k}(0)+q_{2,-1}(s)g^n_{13,k}(0),\\
G^n_{-,1,k}(s) =& G_{-,1,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)=sg^n_{0,k}(s/2)+s^2/2g^n_{1,k}(s/2),\\
G^n_{-,2,k}(s) =& G_{-,2,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)=p_{-1}(s)g^n_{4,k}(0)+q_{-1,0}(s)\dot{g}^n_{4,k}(0)\\
&+p_1(s)g^n_{7,k}(0)+q_{1,0}(s)\dot{g}^n_{7,k}(0)\\
&+p_2(s)g^n_{11,k}(0)+q_{2,0}(s)\dot{g}^n_{11,k}(0),\\
G_{-,3,k}(s) =& G_{-,3,k}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n);s)=q_{-1,0}(s)g^n_{4,k}(0)+q_{-2,0}(s)g^n_{7,k}(0)\\
&+q_{1,0}(s)g^n_{11,k}(0).
\end{aligned}
\tag{2.2.23}
$$

Applying the same approximation procedure to (2.2.9), we have for $\dot{\boldsymbol{y}}^{n,2}(s)$ $(s \in [0,\tau])$

$$\begin{aligned}\dot{y}_l^{n,2}(s) = & \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\beta_j^+ h_{+,j}^{n,k} e^{i\beta_j^+ s} + \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\beta_j^- h_{-,j}^{n,k} e^{i\beta_j^- s} \\ & - \sum_{j,k=1}^{d} \overline{u_{jl}}u_{jk}\gamma_j(\beta_j^+(G_{+,0,k}^n(s) + e^{-i\beta_j^- s/2}G_{+,1,k}^n(s) \\ & + e^{-i\beta_j^- s}G_{+,2,k}^n(s) + i\beta_j^- e^{-i\beta_j^- s}G_{+,3,k}^n(s)) \\ & + \beta_j^-(G_{-,0,k}^n(s) + e^{i\beta_j^- s/2}G_{-,1,k}^n(s) \\ & + e^{i\beta_j^- s}G_{-,2,k}^n(s) - i\beta_j^- e^{i\beta_j^- s}G_{-,3,k}^n(s))).\end{aligned} \tag{2.2.24}$$

Setting $s = \tau$ in (2.2.20) and (2.2.24), we can update numerical approximations $(\boldsymbol{y}^{n+1}, \dot{\boldsymbol{y}}^{n+1})$ of $\boldsymbol{y}(t), d\boldsymbol{y}(t)/dt$ at time $t = t_{n+1}$ by $(\boldsymbol{y}^{n+1}, \dot{\boldsymbol{y}}^{n+1}) = (\boldsymbol{y}^{n,2}(\tau), \dot{\boldsymbol{y}}^{n,2}(\tau))$.

Below, we present the implementation of the proposed second order NPI scheme. Let $\boldsymbol{y}^n \in \mathbb{C}^d$ and $\dot{y}^n \in \mathbb{C}^d$ to be the numerical approximation of $\boldsymbol{y}(t_n)$ and $\dot{\boldsymbol{y}}(t_n)$. Choose $\boldsymbol{y}^0 = \boldsymbol{y}_0$, $\dot{\boldsymbol{y}}^0 = \boldsymbol{y}_1^\varepsilon$. From t_n to t_{n+1}, for given $\boldsymbol{y}^n$ and $\dot{\boldsymbol{y}}^n$, the proposed second order NPI computes $\boldsymbol{y}^{n+1}$ and $\dot{\boldsymbol{y}}^{n+1}$ by the following steps:

1. For all $j,k = 1,2,\cdots,d$, compute $h_{+,j}^{[n],k} = h_{+,j}^k(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n)$, $h_{-,j}^{[n],k} = h_{-,j}^k(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n)$ by formula (2.2.12).

2. For all $l,j = 1,2,\cdots,d$, compute $f_{+,l,j}^{[n]} = f_{+,l,j}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n)$, $f_{-,l,j}^{[n]} = f_{-,l,j}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n)$, $f_l^{[n]} = f_l(\boldsymbol{y}^n)$ by formula (2.2.14).

3. For all $l,k = 1,2,\cdots,d$, compute $F_{k,l}^{[n]}(0) := F_{k,l}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n, 0)$, $F_{k,l}^{[n]}(\tau/2)$ for $k = -5,-4,\cdots,4,5$ by (2.2.17) .

4. Compute $g_{k,l}^{[n]}(0)$ for $k = 0,1,\cdots,13$, $g_{k,l}^{[n]}(\tau/2)$ for $k = 0,1,2,3,7,8,9,10$ by (2.2.19).

5. Compute $G_{+,k,l}^{[n]}(\tau)$ and $G_{-,k,l}^{[n]}(\tau)$, $k = 0,1,2,3$ by formula (2.2.23).

5. Update $\boldsymbol{y}^{n+1}$ and $\dot{\boldsymbol{y}}^{n+1}$ by

$$
\begin{aligned}
y_l^{n+1} = &\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} h_{+,j}^{[n],k} e^{i\beta_j^+\tau} + \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} h_{-,j}^{[n],k} e^{i\beta_j^-\tau} \\
&+ \sum_{j,k=1}^{d} i\overline{u_{jl}} u_{jk} \gamma_j (G_{+,0,k}^{[n]}(\tau) + e^{-i\beta_j^-\tau/2} G_{+,1,k}^{[n]}(\tau) \\
&+ e^{-i\beta_j^-\tau} G_{+,2,k}^{[n]}(\tau) + i\beta_j^- e^{-i\beta_j^-\tau} G_{+,3,k}^{[n]}(\tau) \\
&+ G_{-,0,k}^{[n]}(\tau) + e^{i\beta_j^-\tau/2} G_{-,1,k}^{[n]}(\tau) + e^{i\beta_j^-\tau} G_{-,2,k}^{[n]}(\tau) - i\beta_j^- e^{i\beta_j^-\tau} G_{-,3,k}^{[n]}(\tau)), \\
\dot{y}_l^{n+1} = &\sum_{j,k=1}^{d} i\overline{u_{jl}} u_{jk} \beta_j^+ h_{+,j}^{[n],k} e^{i\beta_j^+\tau} + \sum_{j,k=1}^{d} i\overline{u_{jl}} u_{jk} \beta_j^- h_{-,j}^{[n],k} e^{i\beta_j^-\tau} \\
&- \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j ((\beta_j^+ (G_{+,0,k}^{[n]}(\tau) + e^{-i\beta_j^-\tau/2} G_{+,1,k}^{[n]}(\tau) \\
&+ e^{-i\beta_j^-\tau} G_{+,2,k}^{[n]}(\tau) + i\beta_j^- e^{-i\beta_j^-\tau} G_{+,3,k}^{[n]}(\tau)) \\
&+ \beta_j^- (G_{-,0,k}^{[n]}(\tau) + e^{i\beta_j^-\tau/2} G_{-,1,k}^{[n]}(\tau) + e^{i\beta_j^-\tau} G_{-,2,k}^{[n]}(\tau) - i\beta_j^- e^{i\beta_j^-\tau} G_{-,3,k}^{[n]}(\tau))).
\end{aligned}
\tag{2.2.25}
$$

2.3 Uniform and optimal error estimates

2.3.1 Main results

For $\boldsymbol{y} = (y_1, y_2, \cdots, y_d)^T \in \mathbb{C}^d$, we consider the following vector norms

$$\|\boldsymbol{y}\|_2^2 := \sum_{l=1}^{d} |y_l|^2, \quad \|\boldsymbol{y}\|_\infty := \max_{l=1,2,\cdots,d} \{|y_l|\}.$$

Based on the theoretical results and the asymptotic expansion (2.1.5), we make the following assumptions on the initial data and exact solution to (2.1.1) with (2.1.4): there exists $T > 0$, such that for $\varepsilon \in (0, 1]$, the solution $\boldsymbol{y}(t)$ to (2.1.1) exists and

$$\|\boldsymbol{\omega}\|_2 \lesssim 1, \quad \sup_{\varepsilon\in(0,1]} \sup_{t\in[0,T]} \|\boldsymbol{y}(t)\|_\infty \lesssim 1, \quad \sup_{\varepsilon\in(0,1]} \sup_{t\in[0,T]} \|\dot{\boldsymbol{y}}(t)\|_\infty \lesssim 1, \tag{2.3.1}$$

where we denote $M = \sup_{\varepsilon\in(0,1]} \sup_{t\in[0,T]} \|\boldsymbol{y}(t)\|_\infty + \varepsilon^2 \sup\limits_{\varepsilon\in(0,1]} \sup_{t\in[0,T]} \|\dot{\boldsymbol{y}}(t)\|_\infty$.

Theorem 2.1. *Let* $\boldsymbol{y}^n$ *and* $\dot{\boldsymbol{y}}^n$ *be the numerical approximation of* $\boldsymbol{y}(t_n)$ *and* $\dot{\boldsymbol{y}}(t_n)$ *from NPI* (2.2.25)*. Under assumption* (2.3.1)*,* $\exists \tau_0 > 0$*, such that* $\forall 0 < \tau < \tau_0$*,*

$$\begin{aligned} &\|\boldsymbol{y}(t_n) - \boldsymbol{y}^n\|_2 + \varepsilon^2 \|\dot{\boldsymbol{y}}(t_n) - \dot{\boldsymbol{y}}^n\|_2 \le C\tau^2, \\ &\|\boldsymbol{y}^n\|_\infty + \varepsilon^2 \|\dot{\boldsymbol{y}}^n\|_\infty \le M + 1, \quad 0 \le n \le \frac{T}{\tau}, \end{aligned} \tag{2.3.2}$$

where C *is independent of* ε*.*

2.3.2 Proof for the NPI

Local truncation error estimates. Denote the second order NPI (2.2.25) flow $\boldsymbol{S} : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C}^d$ and $\dot{\boldsymbol{S}} : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C}^d$ by $\boldsymbol{y}^{n+1} = \boldsymbol{S}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n)$ and $\dot{\boldsymbol{y}}^{n+1} = \dot{\boldsymbol{S}}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n)$, which can be expressed in the component-wise form:

$$y_l^{n+1} = S_l(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n), \qquad \dot{y}_l^{n+1} = \dot{S}_l(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n), \quad l = 1, 2, \cdots, d. \tag{2.3.3}$$

From the construction of the NPI scheme, it is not difficult to derive the following estimates.

Lemma 2.1. *Under the assumption of Theorem 2.1,*

$$\begin{aligned} &\|\boldsymbol{y}(t_{n+1}) - \boldsymbol{S}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))\|_2 \le C\tau^3, \\ &\varepsilon^2 \|\dot{\boldsymbol{y}}(t_{n+1}) - \dot{\boldsymbol{S}}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))\|_2 \le C\tau^3, \end{aligned}$$

where $\boldsymbol{S}(\cdot,\cdot)$ *and* $\dot{\boldsymbol{S}}(\cdot,\cdot)$ *are defined in* (2.3.3)*,* C *is independent of* ε*.*

Proof. Denote local truncation error by $\boldsymbol{\xi}^n := \boldsymbol{y}(t_{n+1}) - \boldsymbol{S}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))$, $\dot{\boldsymbol{\xi}}^n := \dot{\boldsymbol{y}}(t_{n+1}) - \dot{\boldsymbol{S}}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))$. The local error can be easily verified by following the iterations for designing the scheme (2.2.25).

By the construction of NPI (2.2.25), we will first estimate the first order NPI approximation $\boldsymbol{y}^{n,1}(s)$. Noticing function $F(\boldsymbol{y})\boldsymbol{y}$ (here $\mathrm{diag}(\boldsymbol{y}\boldsymbol{y}^H)\boldsymbol{y}$) is Lipschitz on bounded interval $[-(M+1), (M+1)]^d$ with some Lipschitz constant L_M, which means:

$$||a_l|^2 a_l - |b_l|^2 b_l| \le L_M \|\boldsymbol{a} - \boldsymbol{b}\|_2, \quad \forall 1 \le l \le d.$$

For the integration kernel $\kappa(t)$, we have $|\kappa_l(t)| \le 2, \forall 0 \le t \le \tau$. Therefore, we have

$$\begin{aligned}
&|y_l(t_n+s) - y_l^{n,1}(s)| \\
&\le \sum_{j,k=1}^{d} |\overline{u_{jl}} u_{jk}\gamma_j| \int_0^s |\kappa_j(s-w)| \left| |y_k(t_n)|^2 y_k(t_n) - |y_k(t_n+w)|^2 y_k(t_n+w) \right| dw \\
&\quad + \sum_{j,k=1}^{d} |\overline{u_{jl}} u_{jk}\gamma_j| \Bigg(\Bigg| \int_0^s e^{-iw/\varepsilon^2} e^{-i\beta_j^-(s-w)} |y_k(t_n+w)|^2 y_k(t_n+w) dw \\
&\quad - p_{-1}(s)|y_k(t_n+w)|^2 y_k(t_n+w) \Bigg| \\
&\quad + \left| \int_0^s e^{i\beta_j^-(s-w)} |y_k(t_n+w)|^2 y_k(t_n+w) dw - s|y_k(t_n+w)|^2 y_k(t_n+w) \right| \Bigg) \\
&\lesssim \int_0^s L\|\boldsymbol{y}(t_n+w) - \boldsymbol{y}(t_n)\|_2 dw + \sum_{j,k=1}^{d} \int_0^s |e^{i\beta_j^-(s-w)} - 1| |y_k(t_n+w)|^3 dw \\
&\lesssim \int_0^s Lw \max_{t\in[0,\tau]} \|\dot{\boldsymbol{y}}(t_n+t)\|_2 dw + \sum_{j,k=1}^{d} \int_0^s |\beta_j^-(s-w)| |y_k(t_n+w)|^3 dw \\
&\lesssim s^2, \quad \forall 0 \le s \le \tau, 1 \le l \le d.
\end{aligned}$$

Thus, we know that there exists $\tau_0 > 0$ such that for $0 < s \le \tau < \tau_0$,

$$\|\boldsymbol{y}^{n,1}(s)\|_\infty \le \|\boldsymbol{y}(t_n+s)\|_\infty + 1 \le M+1.$$

Continue with the second NPI approximation,

$$\begin{aligned}
&|y_l(t_n+s) - y_l^{n,2}(s)| \\
&\le \sum_{j,k=1}^{d} |\overline{u_{jl}} u_{jk}\gamma_j| \int_0^s |\kappa_j(s-w)| \Big| |y_k^{n,1}(w)|^2 y_k^{n,1}(w) \\
&\quad - |y_k(t_n+w)|^2 y_k(t_n+w) \Big| dw + |R_{2,l}^n(s)| \\
&\le C \int_0^s L\|\boldsymbol{y}(t_n+w) - \boldsymbol{y}^{n,1}(w)\|_2 dw + |R_{2,l}^n(s)| \\
&\lesssim s^3 + |R_{2,l}^n(s)|, \quad \forall 1 \le l \le d.
\end{aligned}$$

where $\boldsymbol{R}_2^n(s) = (R_{2,1}^n(s), \cdots, R_{2,d}^n(s))^T$ is the error for approximating the integrals in (2.2.20). By construction, we write $\boldsymbol{R}_2^n(s) = \boldsymbol{D}_2^n(s) + \boldsymbol{Q}_2^n(s)$, where $\boldsymbol{D}_2^n(s)$ is the error introduced by discarded term in formula (2.2.16) and (2.2.18), $\boldsymbol{Q}_2^n(s)$ is the error introduced by numerical quadrature.

To estimate $\boldsymbol{D}_2^n(s)$, we write

$$
\begin{aligned}
&D_{2,l}^n(s)\\
&= \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j \int_0^s \kappa_j(s-w)\left(e^{3iw/\varepsilon^2}(\sum_{m=1}^{d} f_{+,k,m}^n e^{-i\beta_m^- w})\left(p_{-1}^2(w)|f_k^n|^2\right)\right)dw\\
&\quad + \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j \int_0^s \kappa_j(s-w)\left(-e^{3iw/\varepsilon^2}(\sum_{m=1}^{d} f_{+,k,m}^n e^{-i\beta_m^- w})\left(p_{-1}(w)w|f_k^n|^2\right)\right)dw\\
&\quad + \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j \int_0^s \kappa_j(s-w)\left(e^{2iw/\varepsilon^2}(\sum_{m=1}^{d} f_{-,k,m}^n e^{i\beta_m^- w})\left(p_{-1}^2(w)|f_k^n|^2\right)\right)dw\\
&\quad + \cdots,
\end{aligned}
$$

where other similar terms are omitted for simplicity. Noticing $p_0(w) = w$, $\boldsymbol{D}_2^n(s)$ includes every term containing integrated product of more than one $p_k(w), k = -1, 0, 1$. We estimate one of these terms, and the others can be proved similarly. Since $\gamma_j = (1 + 4\varepsilon^2 d_{jj})^{-1/2}$ and $\kappa_j(t) = e^{i\beta_j^+ t} - e^{i\beta_j^- t}$ are bounded for $j = 1, 2, \cdots, d$, there holds

$$
\begin{aligned}
&\left|\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j \int_0^s \kappa_j(s-w)\left(e^{3iw/\varepsilon^2}(\sum_{m=1}^{d} f_{+,k,m}^n e^{-i\beta_m^- w})\left(p_{-1}^2(w)|f_k^n|^2\right)\right)dw\right|\\
&\le C\int_0^s \sum_{m=1}^{d}\left(|y_m(t_n)| + \varepsilon^2|\dot{y}_m(t_n)|\right)\left(\sum_{k=1}^{d} w^2|y_k^n|^6\right)dw \lesssim \int_0^s w^2 dw \lesssim s^3.
\end{aligned}
$$

Then we can derive $|D_{2,l}^n(s)| \lesssim s^3, l = 1, 2, \cdots, d$.

To estimate $\boldsymbol{Q}_2^n(s)$, we write

$$
\begin{aligned}
Q_{2,l}^n(s) = &\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(\int_0^s e^{i\beta_j^-(s-w)} w g_{1,k}^n(w)dw - e^{i\beta_j^- s/2}\frac{s^2}{2}g_{1,k}^n(\frac{s}{2})\right)\\
&+ \cdots (\text{error of other type 1 error terms})\\
&+ \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(\int_0^s e^{-\frac{i}{\varepsilon^2}w}e^{-i\beta_j^-(s-w)}p_1(w)g_{2,k}^n(w)dw - q_{-1,1}(s)g_{2,k}^n(0)\right)\\
&+ \cdots (\text{error of other type 2 error terms})\\
&+ \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\Bigg(\int_0^s e^{-\frac{i}{\varepsilon^2}w}e^{-i\beta_j^-(s-w)}g_{0,k}^n(w)dw\\
&- e^{-i\beta_j^- s}(p_{-1}(s)g_{0,k}^n(0) + q_{-1,0}(s)(i\beta_l^- g_{0,k}^n(0) + \dot{g}_{0,k}^n(0)))\Bigg)\\
&+ \cdots (\text{error of other type 3 error terms}),
\end{aligned}
$$

where classification of type 1, 2, 3 terms are introduced for numerical quadrature to calculate expression (2.2.20). For simplicity, we prove the estimates for one of each type of terms, and the proof can be easily extended to the other terms.

First we prove the boundedness of $g^n_{m,k}(t)$, $\dot{g}^n_{m,k}(t)$ and $\ddot{g}^n_{m,k}(t)$, $m = 1, 2, \cdots, 13$, $k = 1, 2, \cdots, d$ for $\forall 0 < t < \tau$. Notice all $g^n_{m,k}(t)$ share a similar structure, here we only prove for $g^n_{4,k}(t)$.

$$
\begin{aligned}
g^n_{4,k}(t) &= \left(\sum_{j=1}^{d} \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} f^n_{-,k,j} e^{i\beta_j^- t}\right)^2, \\
\dot{g}^n_{4,k}(t) &= \left(\sum_{j=1}^{d} i\beta_j^- \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} f^n_{-,k,j} e^{i\beta_j^- t}\right)^2 \\
&\quad + 2\left(\sum_{j=1}^{d} \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} i\beta_j^- f^n_{-,k,j} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} f^n_{-,k,j} e^{i\beta_j^- t}\right), \\
\ddot{g}^n_{4,k}(t) &= \left(\sum_{j=1}^{d} -(\beta_j^-)^2 \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} f^n_{-,k,j} e^{i\beta_j^- t}\right)^2 \\
&\quad + 4\left(\sum_{j=1}^{d} i\beta_j^- \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} i\beta_j^- f^n_{-,k,j} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} f^n_{-,k,j} e^{i\beta_j^- t}\right) \\
&\quad + 2\left(\sum_{j=1}^{d} \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} -(\beta_j^-)^2 f^n_{-,k,j} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} f^n_{-,k,j} e^{i\beta_j^- t}\right) \\
&\quad + 2\left(\sum_{j=1}^{d} \overline{f^n_{+,k,j}} e^{i\beta_j^- t}\right)\left(\sum_{j=1}^{d} i\beta_j^- f^n_{-,k,j} e^{i\beta_j^- t}\right)^2.
\end{aligned}
$$

Since β_j^- are bounded $\forall j = 1, 2, \cdots, d$, and $|f^n_{+,k,j}| \lesssim |y_k(t_n)| + \varepsilon^2 |\dot{y}_k(t_n)|$, $|f^n_{-,k,j}| \lesssim |y_k(t_n)| + \varepsilon^2 |\dot{y}_k(t_n)|$, $|f^n_k| \le |y_k(t_n)|^3$ are also bounded by the assumption of the exact solution, we have

$$
g^n_{k,l}(t) \lesssim 1,\ \dot{g}^n_{k,l}(t) \lesssim 1,\ \ddot{g}^n_{k,l}(t) \lesssim 1, \forall k = 1, 2, \cdots, 13,\ l = 1, 2, \cdots d.
$$

Then we estimate $Q^n_{2,l}(s)$.

Type 1. We have

$$
\begin{aligned}
&\left|\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(\int_0^s e^{i\beta_j^-(s-w)}wg_{1,k}^n(w)dw - e^{i\beta_j^- s/2}\frac{s^2}{2}g_{1,k}^n(\frac{s}{2})\right)\right| \\
&\lesssim \sum_{j,k=1}^{d}\int_0^s ((w-s/2)|\dot{\Theta}_k^j(s/2)| + (w-s/2)^2|\ddot{\Theta}_k^j(\xi_k^j(w))|)dw \\
&\le \sum_{j,k=1}^{d}\int_0^s (w-s/2)^2|\ddot{\Theta}_k^j(\xi_k^j(w))|dw
\end{aligned}
$$

where $\Theta_k^j(t) = e^{i\beta_j^-(s-t)}tg_{2,k}^n(t)$ and $0 < \xi_k^j(w) < w$. For derivatives, we get

$$
\begin{aligned}
\dot{\Theta}_k^j(t) &= i\beta_j^- e^{i\beta_j^-(s-t)}tg_{2,k}^n(t) + e^{i\beta_j^-(s-t)}g_{2,k}^n(t) + e^{i\beta_j^-(s-t)}t\dot{g}_{2,k}^n(t), \\
\ddot{\Theta}_k^j(t) &= -(\beta_j^-)^2 e^{i\beta_j^-(s-t)}tg_{2,k}^n(t) + e^{i\beta_j^-(s-t)}t\ddot{g}_{2,k}^n(t) \\
&\quad + 2(i\beta_j^- e^{i\beta_j^-(s-t)}g_{2,k}^n(t) + i\beta_j^- e^{i\beta_j^-(s-t)}t\dot{g}_{2,k}^n(t) + e^{i\beta_j^-(s-t)}\dot{g}_{2,k}^n(t)),
\end{aligned}
$$

and $\ddot{\Theta}_k^j(t) \lesssim 1$ for $\forall 0 \le t \le \tau$ by the boundedness of $g_{2,k}^n(t)$, $\dot{g}_{2,k}^n(t)$ and $\ddot{g}_{2,k}^n(t)$. Thus,

$$
\begin{aligned}
&\left|\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(\int_0^s e^{i\beta_j^-(s-w)}wg_{1,k}^n(w)dw - e^{i\beta_j^- s/2}\frac{s^2}{2}g_{1,k}^n(\frac{s}{2})\right)\right| \\
&\lesssim \sum_{j,k=1}^{d}\int_0^s (w-s/2)^2 dw \\
&\lesssim s^3.
\end{aligned}
$$

Type 2. In view of the boundedness of β_j^-, $g_{2,k}^n(t)$ and $\dot{g}_{2,k}^n(t)$, we derive that

$$
\begin{aligned}
&\left|\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(\int_0^s e^{-\frac{i}{\varepsilon^2}w}e^{-i\beta_j^-(s-w)}p_1(w)g_{2,k}^n(w)dw - q_{-1,1}(s)g_{2,k}^n(0)\right)\right| \\
&\lesssim \sum_{j,k=1}^{d}\int_0^s |e^{-\frac{i}{\varepsilon^2}w}p_1(w)|(|(e^{-i\beta_j^-(s-w)}-1)g_{2,k}^n(w)| + |g_{2,k}^n(w) - g_{2,k}^n(0)|)dw \\
&\lesssim \sum_{j,k=1}^{d}\int_0^s w^2\left(\left|i\beta_j^-(s-w)e^{-i\beta_j^-(s-\xi_1^j(w))}g_{2,k}^n(w)\right| + w|\dot{g}_{2,l}^n(\xi_{2,k}(w))|\right)dw \\
&\lesssim \int_0^s w^2 s dw \\
&\lesssim s^3,
\end{aligned}
$$

where $0 < \xi_1^j(w) < w, 0 < \xi_{2,k}(w) < w$.

Type 3. We can obtain

$$\begin{aligned}
&\Bigg|\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\Bigg(\int_0^s e^{-\frac{i}{\varepsilon^2}w}e^{-i\beta_j^-(s-w)}g_{0,k}^n(w)dw \\
&\quad - e^{-i\beta_j^- s}(p_{-1}(s)g_{0,k}^n(0) + q_{-1,0}(s)(i\beta_l^- g_{0,k}^n(0) + \dot{g}_{0,k}^n(0)))\Bigg)\Bigg| \\
&\lesssim \sum_{j,k=1}^{d} |e^{-i\beta_j^- s}| \int_0^s |e^{-\frac{i}{\varepsilon^2}w}| \left|e^{i\beta_j^- w}g_{0,k}^n(w) - \left(g_{0,k}^n(0) + w(i\beta_j^- g_{0,k}^n(0) + \dot{g}_{0,k}^n(0))\right)\right| dw \\
&\le \sum_{j,k=1}^{d} \int_0^s w^2 \Bigg| - (\beta_j^-)^2 e^{i\beta_j^-\xi_k^j(w)} g_{0,k}^n(\xi_k^j(w)) + i\beta_j^- e^{i\beta_j^-\xi_k^j(w)}\dot{g}_{0,k}^n(\xi_k^j(w)) \\
&\quad + e^{i\beta_j^-\xi_k^j(w)}\ddot{g}_{0,k}^n(\xi_k^j(w))\Bigg| dw \\
&\lesssim \int_0^s w^2 dw \\
&\lesssim s^3,
\end{aligned}$$

where $0 < \xi_k^j(w) < w$ and we have used the boundedness of β_j^-, $g_{2,k}^n(t)$, $\dot{g}_{2,k}^n(t)$ and $\ddot{g}_{2,k}^n(t)$.

Therefore, combing all the three types of estimates, we have $|Q_{2,l}^n(s)| \lesssim s^3, l = 1, 2, \cdots, d$ and

$$|y_l(t_n + s) - y_l^{n,2}(s)| \le |D_{2,l}^n(s)| + |Q_{2,l}^n(s)| + O(s^3) \lesssim s^3, \quad \forall 1 \le l \le d,$$

which leads to the estimates for local truncation error $\boldsymbol{\xi}^n$ follows:

$$|\xi_l^{n+1}| = |y_l(t_n + \tau) - S_l(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))| = |y_l(t_n + \tau) - y_l^{n,2}(\tau)| \lesssim \tau^3, \quad \forall 1 \le l \le d.$$

For the truncation error $\dot{\boldsymbol{\xi}}^{n+1}$, we have similar estimates. Given first NPI approximation $y^{n,1}(s)$, in view of $|\dot{\kappa}_j(t)| = |i\beta_j^+ e^{\beta_j^+ t} - i\beta_j^- e^{\beta_j^- t}| \le |\beta_j^+| + |\beta_j^-| \lesssim \varepsilon^{-2}$, we get

$$\begin{aligned}|\dot{y}_l(t_n+s)-\dot{y}_l^{n,2}(s)| \leq & \sum_{j,k=1}^{d}|\overline{u_{jl}}u_{jk}\gamma_j|\int_0^s|\dot{\kappa}_j(s-w)|\bigg||y_k^{n,1}(w)|^2y_k^{n,1}(w)\\ & -|y_k(t_n+w)|^2y_k(t_n+w)\bigg|dw+|\dot{R}_{2,l}^n(s)|\\ \leq & C\varepsilon^{-2}\int_0^s L\|\boldsymbol{y}(t_n+w)-\boldsymbol{y}^{n,1}(s)\|_2dw+|\dot{R}_{2,l}^n(s)|\\ \leq & |\dot{R}_{2,l}^n(s)|+C\varepsilon^{-2}s^3, \quad \forall 1\leq l\leq d,\end{aligned}$$

where the remainder function $\dot{\boldsymbol{R}}_2^n(s)=(\dot{R}_{2,1}^n(s),\cdots,\dot{R}_{2,d}^n(s))^T$ can be divided into two terms as $\dot{\boldsymbol{R}}_2^n(s)=\dot{\boldsymbol{D}}_2^n(s)+\dot{\boldsymbol{Q}}_2^n(s)$. $\dot{\boldsymbol{Q}}_2^n(s)$ includes the quadrature error of the integral approximation in (2.2.9) and $\dot{\boldsymbol{D}}_2^n(s)$ includes every discarded terms as

$$\begin{aligned}& D_{2,l}^n(s)\\ =& \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j\int_0^s\dot{\kappa}_j(s-w)\left(e^{3iw/\varepsilon^2}(\sum_{m=1}^{d}f_{+,k,m}^n e^{-i\beta_m^- w})\left(p_{-1}^2(w)|f_k^n|^2\right)\right)dw\\ &+\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j\int_0^s\dot{\kappa}_j(s-w)\left(-e^{3iw/\varepsilon^2}(\sum_{m=1}^{d}f_{+,k,m}^n e^{-i\beta_m^- w})\left(p_{-1}(w)w|f_k^n|^2\right)\right)dw\\ &+\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j\int_0^s\dot{\kappa}_j(s-w)\left(e^{2iw/\varepsilon^2}(\sum_{m=1}^{d}f_{-,k,m}^n e^{i\beta_m^- w})\left(p_{-1}^2(w)|f_k^n|^2\right)\right)dw\\ &+\cdots,\end{aligned}$$

We estimate the first term, and other terms can be done analogously. By direct computation, we have

$$\begin{aligned}&\left|\sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j\int_0^s\dot{\kappa}_j(s-w)\left(e^{3iw/\varepsilon^2}(\sum_{m=1}^{d}f_{+,k,m}^n e^{-i\beta_m^- w})\left(p_{-1}^2(w)|f_k^n|^2\right)\right)dw\right|\\ &\leq C\varepsilon^{-2}\int_0^s\sum_{m=1}^{d}\left(|y_m(t_n)|+\varepsilon^2|\dot{y}_m(t_n)|\right)\left(\sum_{k=1}^{d}w^2|y_k^n|^6\right)dw\\ &\lesssim \varepsilon^{-2}\int_0^s w^2dw\\ &\lesssim \varepsilon^{-2}s^3.\end{aligned}$$

Thus, $\dot{D}^n_{2,l}(s) \lesssim \varepsilon^{-2}s^3,\ l = 1, 2, \cdots, d$. For $\dot{\boldsymbol{Q}}^n_2(s)$, we know

$$
\begin{aligned}
&\dot{Q}^n_{2,l}(s)\\
&= \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(i\beta_j^- \int_0^s e^{i\beta_j^-(s-w)} w g^n_{1,k}(w)dw - i\beta_j^- e^{i\beta_j^- s/2}\frac{s^2}{2}g^n_{1,k}(\frac{s}{2})\right)\\
&\quad + \cdots \text{(error of other type 1 error terms)}\\
&\quad + \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\left(i\beta_j^+ \int_0^s e^{-\frac{i}{\varepsilon^2}w} e^{-i\beta_j^-(s-w)} p_1(w) g^n_{2,k}(w)dw - i\beta_j^+ q_{-1,1}(s) g^n_{2,k}(0)\right)\\
&\quad + \cdots \text{(error of other type 2 error terms)}\\
&\quad + \sum_{j,k=1}^{d} i\overline{u_{jl}}u_{jk}\gamma_j e^{\frac{i}{\varepsilon^2}s}\Bigg(i\beta_j^+ \int_0^s e^{-\frac{i}{\varepsilon^2}w} e^{-i\beta_j^-(s-w)} g^n_{0,k}(w)dw\\
&\quad - i\beta_j^+ e^{-i\beta_j^- s}(p_{-1}(s)g^n_{0,k}(0) + q_{-1,0}(s)(i\beta_l^- g^n_{0,k}(0) + \dot{g}^n_{0,k}(0)))\Bigg)\\
&\quad + \cdots \text{(error of other type 3 error terms)}.
\end{aligned}
$$

As $\beta_j^+ = -\beta_j^- + \varepsilon^{-2} \lesssim \varepsilon^{-2}$ and $\beta_l^- \lesssim 1 \lesssim \varepsilon^{-2}$, it is easy to prove $\dot{Q}^n_{2,l}(s) \lesssim \varepsilon^{-2}s^3,\ l = 1, 2, \cdots, d$ by the same method for estimating $Q^n_{2,l}(s)$.

Now the local truncation error $\dot{\boldsymbol{\xi}}^n$ has the following estimates:

$$
\begin{aligned}
|\dot{\xi}^n_l| &= |\dot{y}_l(t_n+\tau) - \dot{S}_l(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))| = |\dot{y}_l(t_n+\tau) - \dot{y}^{n,2}_l(\tau)|\\
&\le |\dot{D}^n_{2,l}(\tau)| + |\dot{Q}^n_{2,l}(\tau)| + C\tau^3/\varepsilon^2\\
&\lesssim \varepsilon^{-2}\tau^3, \quad \forall 1 \le l \le d.
\end{aligned}
$$

The proof of Lemma 2.1 is complete.

□

Stability. To prove the stability of our scheme, we divide the numerical propagator $\boldsymbol{S}$ into the linear part $\boldsymbol{S}_L$ and the nonlinear part $\boldsymbol{S}_{NL}$:

$$
\begin{aligned}
\boldsymbol{y}^{n+1} &= \boldsymbol{S}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) = \boldsymbol{S}_L(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) + \boldsymbol{S}_{NL}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n),\\
\dot{\boldsymbol{y}}^{n+1} &= \dot{\boldsymbol{S}}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) = \dot{\boldsymbol{S}}_L(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) + \dot{\boldsymbol{S}}_{NL}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n),
\end{aligned}
$$

where for $l = 1, 2, \cdots, d$,

$$
\begin{aligned}
S_{L,l}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) &:= \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} h_{+,j}^{k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) e^{i\beta_j^+ \tau} + \sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} h_{-,j}^{k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) e^{i\beta_j^- \tau}, \\
\dot{S}_{L,l}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) &:= \sum_{j,k=1}^{d} i\overline{u_{jl}} u_{jk} \beta_j^+ h_{+,j}^{k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) e^{i\beta_j^+ \tau} \\
&\quad + \sum_{j,k=1}^{d} i\overline{u_{jl}} u_{jk} \beta_j^- h_{-,j}^{k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) e^{i\beta_j^- \tau}, \\
S_{NL,l}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) &:= \sum_{j,k=1}^{d} i\overline{u_{jl}} u_{jk} \gamma_j (G_{+,0,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) + e^{-i\beta_j^- \tau/2} G_{+,1,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) \\
&\quad + e^{-i\beta_j^- \tau} G_{+,2,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) + i\beta_j^- e^{-i\beta_j^- \tau} G_{+,3,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) \\
&\quad + G_{-,0,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) + e^{i\beta_j^- \tau/2} G_{-,1,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) \\
&\quad + e^{i\beta_j^- \tau} G_{-,2,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) - i\beta_j^- e^{i\beta_j^- \tau} G_{-,3,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau)), \\
\dot{S}_{NL,l}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n) &:= -\sum_{j,k=1}^{d} \overline{u_{jl}} u_{jk} \gamma_j ((\beta_j^+ (G_{+,0,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) \\
&\quad + e^{-i\beta_j^- \tau/2} G_{+,1,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) \\
&\quad + e^{-i\beta_j^- \tau} G_{+,2,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) + i\beta_j^- e^{-i\beta_j^- \tau} G_{+,3,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau)) \\
&\quad + \beta_j^- (G_{-,0,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) + e^{i\beta_j^- \tau/2} G_{-,1,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) \\
&\quad + e^{i\beta_j^- \tau} G_{-,2,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau) - i\beta_j^- e^{i\beta_j^- \tau} G_{-,3,k}(\boldsymbol{y}^n, \dot{\boldsymbol{y}}^n; \tau))).
\end{aligned}
\tag{2.3.4}
$$

The stability of the NPI (2.2.25) is characterized as follows.

Lemma 2.2. *Given* $(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0)$ *and* $(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1)$ *satisfying* $\boldsymbol{y}^j, \dot{\boldsymbol{y}}^j \in \mathbb{C}^d$ $(j = 0, 1)$ *and* $\|\boldsymbol{y}^j\|_\infty + \varepsilon^2 \|\dot{\boldsymbol{y}}^j\|_\infty \leq M + 1$, *introducing diagonal matrix* $\Lambda = \sqrt{-(\beta^+\beta^-)^{-1}}$ *(*$\beta^\pm$ *given in* (2.2.3)*), we have*

$$
\begin{bmatrix} U\boldsymbol{S}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - U\boldsymbol{S}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1) \\ \Lambda U\dot{\boldsymbol{S}}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - \Lambda U\boldsymbol{S}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1) \end{bmatrix} = Q \begin{bmatrix} U(\boldsymbol{y}^0 - \boldsymbol{y}^1) \\ \Lambda U(\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1) \end{bmatrix} + \begin{bmatrix} \boldsymbol{\eta} \\ \dot{\boldsymbol{\eta}} \end{bmatrix},
$$

where $\|\boldsymbol{\eta}\|_2 \leq C\tau(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2)$, $\|\dot{\boldsymbol{\eta}}\|_2 \leq C\frac{\tau}{\varepsilon}(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2)$ *and* Q *is a unitary matrix given by*

$$
Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} = \begin{bmatrix} \beta^{-1}(e^{i\beta^-\tau}\beta^+ - e^{i\beta^+\tau}\beta^-) & i\beta^{-1}(e^{i\beta^-\tau} - e^{i\beta^+\tau})\Lambda^{-1} \\ \beta^{-1}\Lambda^{-1}(-ie^{i\beta^-\tau} + ie^{i\beta^+\tau}) & -\beta^{-1}(e^{i\beta^-\tau}\beta^- - e^{i\beta^+\tau}\beta^+) \end{bmatrix}. \tag{2.3.5}
$$

In the above, C depends on M, d and $\max_{l=1,\cdots d}\{|d_{ll}|\} = \rho(A)$ (spectral radius of A, (2.2.1)). For Q, we have ($k = 1, 2, \cdots ,$)

$$
\begin{aligned}
Q^k &= \begin{bmatrix} Q_{11}^{(k)} & Q_{12}^{(k)} \\ Q_{21}^{(k)} & Q_{22}^{(k)} \end{bmatrix} \\
&= \begin{bmatrix} \beta^{-1}(e^{ik\beta^-\tau}\beta^+ - e^{ik\beta^+\tau}\beta^-) & i\beta^{-1}(e^{ik\beta^-\tau} - e^{ik\beta^+\tau})\Lambda^{-1} \\ \beta^{-1}\Lambda^{-1}(-ie^{ik\beta^-\tau} + ie^{ik\beta^+\tau}) & -\beta^{-1}(e^{ik\beta^-\tau}\beta^- - e^{ik\beta^+\tau}\beta^+) \end{bmatrix},
\end{aligned}
\tag{2.3.6}
$$

and $\|Q_{11}^{(k)}\|_2 \leq 1$, $|Q_{22}^{(k)}\|_2 \leq 1$, $\|Q_{12}^{(k)}\|_2 \lesssim \varepsilon$, $\|Q_{21}^{(k)}\|_2 \lesssim \varepsilon$.

Proof. From (2.2.5) and (2.3.4), it is easy to find that

$$U\boldsymbol{S}_L(\boldsymbol{y}, \dot{\boldsymbol{y}}) = \beta^{-1}(e^{i\beta^-\tau}\beta^+ - e^{i\beta^+\tau}\beta^-)U\boldsymbol{y} + i\beta^{-1}(e^{i\beta^-\tau} - e^{i\beta^+\tau})\Lambda^{-1}\Lambda U\dot{\boldsymbol{y}}, \tag{2.3.7}$$

$$\Lambda U\dot{\boldsymbol{S}}_L(\boldsymbol{y}, \dot{\boldsymbol{y}}) = \beta^{-1}\Lambda^{-1}(-ie^{i\beta^-\tau} + ie^{i\beta^+\tau})U\boldsymbol{y} - \beta^{-1}(e^{i\beta^-\tau}\beta^- - e^{i\beta^+\tau}\beta^+)\Lambda U\dot{\boldsymbol{y}}. \tag{2.3.8}$$

By direct computation, it is easy to verify that Q is unitary. As $\boldsymbol{S}_L$ and $\dot{\boldsymbol{S}}_L$ are linear in $\boldsymbol{y}$ and $\dot{\boldsymbol{y}}$, we conclude that

$$\begin{bmatrix} U\boldsymbol{S}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - U\boldsymbol{S}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1) \\ \Lambda U\dot{\boldsymbol{S}}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - \Lambda U\boldsymbol{S}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1) \end{bmatrix} = Q \begin{bmatrix} U(\boldsymbol{y}^0 - \boldsymbol{y}^1) \\ \Lambda U(\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1) \end{bmatrix}. \tag{2.3.9}$$

The properties of Q and Q^k can be verified by direct computation and the fact that $\beta_l^+ = O(1/\varepsilon^2), \beta_l^- = O(1)$.

For the nonlinear parts, we obtain the component-wise forms of $U\boldsymbol{S}_{NL}$ and $\Lambda U\dot{\boldsymbol{S}}_{NL}$

as $(j = 1, \cdots, d)$,

$$
\begin{aligned}
(US_{NL})_j(\boldsymbol{y}, \dot{\boldsymbol{y}}) :=& \sum_{k=1}^{d} i u_{jk} \gamma_j (G_{+,0,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) + e^{-i\beta_j^- \tau/2} G_{+,1,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) \\
&+ e^{-i\beta_j^- \tau} G_{+,2,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) + i\beta_j^- e^{-i\beta_j^- \tau} G_{+,3,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) \\
&+ G_{-,0,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) + e^{i\beta_j^- \tau/2} G_{-,1,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) \\
&+ e^{i\beta_j^- \tau} G_{-,2,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) - i\beta_j^- e^{i\beta_j^- \tau} G_{-,3,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau)), \\
(\Lambda U \dot{\boldsymbol{S}}_{NL})_j(\boldsymbol{y}, \dot{\boldsymbol{y}}) :=& -\sum_{k=1}^{d} u_{jk} \gamma_j (-\beta_j^- \beta_j^+)^{-1/2} ((\beta_j^+ (G_{+,0,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) \\
&+ e^{-i\beta_j^- \tau/2} G_{+,1,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) \\
&+ e^{-i\beta_j^- \tau} G_{+,2,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) + i\beta_j^- e^{-i\beta_j^- \tau} G_{+,3,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau)) \\
&+ \beta_j^- (G_{-,0,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) + e^{i\beta_j^- \tau/2} G_{-,1,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) \\
&+ e^{i\beta_j^- \tau} G_{-,2,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau) - i\beta_j^- e^{i\beta_j^- \tau} G_{-,3,k}(\boldsymbol{y}, \dot{\boldsymbol{y}}; \tau))).
\end{aligned}
\tag{2.3.10}
$$

Now, we estimate $(U\boldsymbol{S}_{NL})_l(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - (U\boldsymbol{S}_{NL})_l(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1)$ $(l = 1, \cdots, d)$. Since $|u_{jk}| \leq 1$, $|\gamma_l| = \frac{1}{\varepsilon^2 \beta_l^+} \leq 1$, $|\beta_l^-| \leq \rho(A)$ for $\forall j, k, l = 1, 2, \cdots, d$, we only need to consider $G_{+,j,k}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0; \tau) - G_{+,j,k}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1; \tau)$, $j = 0, 1, 2, 3$, and the estimates fall into the following three types in view of the definitions of $G_{\pm,j,k}$ in (2.2.23).

Type 1. Terms containing $g_{k,l}(\cdot; 0)$, for example $e^{is/\varepsilon^2} q_{-1,0}(\tau)(g_{1,l}^0(0) - g_{1,l}^1(0))$, where $g_{1,l}^0(s) = g_{1,l}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0; s)$, $g_{1,l}^1(s) = g_{1,l}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1; s)$. Then we can estimate the difference by:

$$
\begin{aligned}
& e^{is/\varepsilon^2} q_{-1,0}(\tau)(g_{0,l}^0(0) - g_{0,l}^1(0)) \\
&= -e^{is/\varepsilon^2} q_{-1,0}(\tau) \Big((\sum_{j=1}^{d} \overline{f_{+,l,j}^0})(\sum_{j=1}^{d} f_{-,l,j}^0)(\sum_{j=1}^{d} f_{+,l,j}^0) - (\sum_{j=1}^{d} \overline{f_{+,l,j}^1})(\sum_{j=1}^{d} f_{-,l,j}^1)(\sum_{j=1}^{d} f_{+,l,j}^1) \\
&\quad + (\sum_{j=1}^{d} f_{+,l,j}^0)(\sum_{j=1}^{d} \overline{f_{+,l,j}^0})(\sum_{j=1}^{d} f_{-,l,j}^0) - (\sum_{j=1}^{d} f_{+,l,j}^1)(\sum_{j=1}^{d} \overline{f_{+,l,j}^1})(\sum_{j=1}^{d} f_{-,l,j}^1) + \cdots \Big),
\end{aligned}
$$

where $f_{\pm,l,j}^m = f_{\pm,l,j}(\boldsymbol{y}^m, \dot{\boldsymbol{y}}^m)$ $(m = 0, 1)$ are given in (2.2.14), and some terms with similar structure are omitted for brevity. $\forall j, k, l, m = 1, 2, \cdots, d$, there holds

$$
\begin{aligned}
& |\overline{f_{+,l,j}^0} f_{-,l,k}^0 f_{+,l,m}^0 - \overline{f_{+,l,j}^1} f_{-,l,k}^1 f_{+,l,m}^1| \\
& \leq |\overline{f_{+,l,j}^0} - \overline{f_{+,l,j}^1}| |f_{-,l,k}^0 f_{+,l,m}^0| \\
& \quad + |\overline{f_{+,l,j}^1}| \Big(|f_{-,l,k}^0 - f_{-,l,k}^1| |f_{+,l,m}^0| - |f_{-,l,k}^1| |f_{+,l,m}^0 - f_{+,l,m}^1| \Big).
\end{aligned}
$$

Under the hypothesis of the lemma where $\|\boldsymbol{y}^0\|_\infty + \varepsilon^2\|\dot{\boldsymbol{y}}^0\|_\infty \le M+1$ ($m = 0,1$), from (2.2.12), we know for

$$|h^k_{-,j}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0)| \le \frac{\beta_j^+}{\beta_j}|y_k^0| + \frac{1}{\beta_j}|\dot{y}_k^0| \le (|y_k^0| + \varepsilon^2|\dot{y}_k^0|) \le M+1.$$

Analogously $|h^k_{\pm,j}(\boldsymbol{y}^m, \dot{\boldsymbol{y}}^m))| \le M+1$ ($m = 0,1, j,k = 1,\cdots,d$), and by the unitary property of U and (2.2.14), $|f^m_{\pm,l,j}| \lesssim 1$ for $m = 1,2$, and $l,j = 1,2,\cdots,d$. In addition, we have

$$\begin{aligned} |h^k_{-,j}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - h^k_{-,j}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1)| &\le \frac{\beta_j^+}{\beta_j}|y_k^0 - y_k^1| + \frac{1}{\beta_j}|\dot{y}_k^0 - \dot{y}_k^1| \\ &\le \|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2. \end{aligned} \tag{2.3.11}$$

Recalling $|q_{-1,0}(\tau)| \lesssim \tau^2$, we derive from (2.3.11) that

$$\begin{aligned} &|e^{is/\varepsilon^2} q_{-1,0}(\tau)(g^0_{0,l}(0) - g^1_{0,l}(0))| \\ &\le |q_{-1,0}(\tau)| \left(|(\sum_{j=1}^d \overline{f^0_{+,l,j}})(\sum_{j=1}^d f^0_{-,l,j})(\sum_{j=1}^d f^0_{+,l,j}) - (\sum_{j=1}^d \overline{f^1_{+,l,j}})(\sum_{j=1}^d f^1_{-,l,j})(\sum_{j=1}^d f^1_{+,l,j})| + \cdots \right), \\ &\lesssim \tau(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2). \end{aligned}$$

Type 2. Terms containing $g_{k,l}(\tau/2)$, for example $e^{is/\varepsilon^2}\tau(g^n_{7,l}(\tau/2) - g^{[n]}_{7,l}(\tau/2))$. By definition, we have

$$\begin{aligned} &e^{is/\varepsilon^2}\tau(g^0_{7,l}(\tau/2) - g^1_{7,l}(\tau/2)) \\ &= e^{is/\varepsilon^2}\tau\Big((\sum_{j=1}^d f^0_{+,l,j}e^{-i\beta_j^-\tau/2})(\sum_{j=1}^d \overline{f^0_{+,l,j}}e^{i\beta_j^-\tau/2})(\sum_{j=1}^d f^0_{+,l,j}e^{-i\beta_j^-\tau/2}) \\ &\quad - (\sum_{j=1}^d f^1_{+,l,j}e^{-i\beta_j^-\tau/2})(\sum_{j=1}^d \overline{f^1_{+,l,j}}e^{i\beta_j^-\tau/2})(\sum_{j=1}^d f^1_{+,l,j}e^{-i\beta_j^-\tau/2}) \\ &\quad + (\sum_{j=1}^d f^0_{-,l,j}e^{i\beta_j^-\tau/2})(\sum_{j=1}^d \overline{f^0_{-,l,j}}e^{-i\beta_j^-\tau/2})(\sum_{j=1}^d f^0_{+,l,j}e^{-i\beta_j^-\tau/2}) \\ &\quad - (\sum_{j=1}^d f^1_{-,l,j}e^{i\beta_j^-\tau/2})(\sum_{j=1}^d \overline{f^1_{-,l,j}}e^{-i\beta_j^-\tau/2})(\sum_{j=1}^d f^1_{+,l,j}e^{-i\beta_j^-\tau/2}) + \cdots\Big). \end{aligned}$$

Then $\forall j,k,l,m = 1,2,\cdots,d$, there holds

$$\begin{aligned}
&|f^0_{+,l,j}e^{-i\beta_j^-\tau/2}\overline{f^0_{+,l,k}}e^{i\beta_k^-\tau/2}f^0_{+,l,m}e^{-i\beta_m^-\tau/2} - f^1_{+,l,j}e^{-i\beta_j^-\tau/2}\overline{f^1_{+,l,k}}e^{i\beta_k^-\tau/2}f^1_{+,l,m}e^{-i\beta_m^-\tau/2}| \\
&\le |f^0_{+,l,j}\overline{f^0_{+,l,k}}f^0_{+,l,m} - f^1_{+,l,j}\overline{f^1_{+,l,k}}f^1_{+,l,m}| \\
&\lesssim \|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2.
\end{aligned}$$

where the last inequality can be derived by the same arguments for type 1 terms. Thus, we can get

$$|e^{is/\varepsilon^2}\tau(g^n_{7,l}(\tau/2) - g^{[n]}_{7,l}(\tau/2))| \lesssim \tau(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2).$$

Type 3. Terms containing $\dot{g}_{k,l}(0)$, for example $e^{is/\varepsilon^2}q_{-1,0}(\tau)(\dot{g}^0_{0,l}(0) - \dot{g}^1_{0,l}(0))$. For $l = 1,\cdots,d$, we know

$$\begin{aligned}
&e^{is/\varepsilon^2}q_{-1,0}(\tau)(\dot{g}^0_{0,l}(0) - \dot{g}^1_{0,l}(0)) \\
&= e^{is/\varepsilon^2}q_{-1,0}(\tau)\Big((\sum_{j=1}^d -i\beta_j^- f^0_{+,l,j})(\sum_{j=1}^d \overline{f^0_{+,l,j}})(\sum_{j=1}^d f^0_{+,l,j}) \\
&\quad - (\sum_{j=1}^d -i\beta_j^- f^1_{+,l,j})(\sum_{j=1}^d \overline{f^1_{+,l,j}})(\sum_{j=1}^d f^1_{+,l,j}) \\
&\quad + (\sum_{j=1}^d i\beta_j^- f^0_{-,l,j})(\sum_{j=1}^d \overline{f^0_{-,l,j}})(\sum_{j=1}^d f^0_{+,l,j}) - (\sum_{j=1}^d i\beta_j^- f^1_{-,l,j})(\sum_{j=1}^d \overline{f^1_{-,l,j}})(\sum_{j=1}^d f^1_{+,l,j}) + \cdots\Big).
\end{aligned}$$

Noticing the boundedness of β_j^- (independent of ε), by the same arguments for type 1 terms, we have for $j,k,l,m = 1,2,\cdots,d$,

$$|-i\beta_j^- f^0_{+,l,j}\overline{f^0_{+,l,k}}f^0_{+,l,m} + i\beta_j^- f^1_{+,l,j}\overline{f^1_{+,l,k}}f^1_{+,l,m}| \le \|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2.$$

Therefore, in view of the fact $|q_{-1,0}(\tau)| \lesssim \tau^2$, we obtain

$$\begin{aligned}
|e^{is/\varepsilon^2}q_{-1,0}(\tau)(\dot{g}^0_{0,l}(0) - \dot{g}^1_{0,l}(0))| &\lesssim \tau^2(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2) \\
&\lesssim \tau(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2).
\end{aligned}$$

Combining all the three cases above, we can prove the estimates for the nonlinear part $U\boldsymbol{S}_{NL}$ as

$$\|U\boldsymbol{S}_{NL}(\boldsymbol{y}^0, \dot{\boldsymbol{y}}^0) - U\boldsymbol{S}_{NL}(\boldsymbol{y}^1, \dot{\boldsymbol{y}}^1)\|_2 \lesssim \tau(\|\boldsymbol{y}^0 - \boldsymbol{y}^1\|_2 + \varepsilon^2\|\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1\|_2).$$

For the nonlinear part of $\Lambda U\dot{\boldsymbol{S}}$ in (2.3.10), noticing all terms appearing in $\Lambda U\dot{\boldsymbol{S}}$ differ from corresponding terms in $U\boldsymbol{S}$ by a factor $i\frac{\beta_j^+}{\sqrt{-\beta_l^+\beta_l^-}}$ or $i\frac{\beta_j^-}{\sqrt{-\beta_l^+\beta_l^-}}$, $l,j=1,2,\cdots,d$, recalling the coefficients $\beta_j^\pm$ (2.2.3),

$$|\beta_j^+|/\sqrt{-\beta_l^+\beta_l^-}\lesssim\frac{1}{\varepsilon},\quad |\beta_j^-|/\sqrt{-\beta_l^+\beta_l^-}\lesssim 1,\quad j=1,\cdots,d,$$

we have

$$\|U\dot{\boldsymbol{S}}_{NL}(\boldsymbol{y}^0,\dot{\boldsymbol{y}}^0)-U\dot{\boldsymbol{S}}_{NL}(\boldsymbol{y}^1,\dot{\boldsymbol{y}}^1)\|_2\lesssim\frac{\tau}{\varepsilon}\left(\|\boldsymbol{y}^0-\boldsymbol{y}^1\|_2+\varepsilon^2\|\dot{\boldsymbol{y}}^0-\dot{\boldsymbol{y}}^1\|_2\right).$$

Setting $\boldsymbol{\eta}=U\boldsymbol{S}_{NL}(\boldsymbol{y}^0,\dot{\boldsymbol{y}}^0)-U\boldsymbol{S}_{NL}(\boldsymbol{y}^1,\dot{\boldsymbol{y}}^1)$ and $\dot{\boldsymbol{\eta}}=U\dot{\boldsymbol{S}}_{NL}(\boldsymbol{y}^0,\dot{\boldsymbol{y}}^0)-U\dot{\boldsymbol{S}}_{NL}(\boldsymbol{y}^1,\dot{\boldsymbol{y}}^1)$, combining (2.3.9), we draw the conclusions in Lemma 2.2. □

Now, having Lemmas 2.1 and 2.2 at hand, we are ready to prove Theorem 2.1.

Proof of the main result. To control the nonlinearity, we adopt mathematical induction here. Denote the error vector $\boldsymbol{e}^n=y(t_n)-y^n$ and $\dot{\boldsymbol{e}}^n=\dot{\boldsymbol{y}}(t_n)-\dot{\boldsymbol{y}}^n$ and the local truncation error vector as $\xi^n=\boldsymbol{y}(t_{n+1})-\boldsymbol{S}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n))$, $\dot{\xi}^n=\dot{\boldsymbol{y}}(t_{n+1})-\dot{\boldsymbol{S}}(\boldsymbol{y}(t_n),\dot{\boldsymbol{y}}(t_n))$ $(n\geq 0)$. We have $\boldsymbol{e}^0=\dot{\boldsymbol{e}}^0=0$ by the choice of initial value, i.e. (2.3.2) holds for $n=0$.

Assuming (2.3.2) holds for all $0\leq m\leq n\leq\frac{T}{\tau}-1$, we are going to prove the case for $n+1$. From the local truncation error in Lemma 2.1, it holds

$$\boldsymbol{y}(t_{m+1})=\boldsymbol{S}(\boldsymbol{y}(t_m),\dot{\boldsymbol{y}}(t_m))+\boldsymbol{\xi}^m,\quad \dot{\boldsymbol{y}}(t_{m+1})=\dot{\boldsymbol{S}}(\boldsymbol{y}(t_m),\dot{\boldsymbol{y}}(t_m))+\dot{\boldsymbol{\xi}}^m,\quad m\geq 0,$$

which leads to the error equation for $\boldsymbol{e}^m$ and $\dot{\boldsymbol{e}^m}$ in view of Lemma 2.2 and the induction hypothesis,

$$\begin{bmatrix}U\boldsymbol{e}^{m+1}\\ \Lambda U\dot{\boldsymbol{e}}^{m+1}\end{bmatrix}=Q\begin{bmatrix}U\boldsymbol{e}^{m}\\ \Lambda U\dot{\boldsymbol{e}}^{m}\end{bmatrix}+\begin{bmatrix}\boldsymbol{\eta}^{m}\\ \dot{\boldsymbol{\eta}}^{m}\end{bmatrix}+\begin{bmatrix}U\boldsymbol{\xi}^{m}\\ \Lambda U\dot{\boldsymbol{\xi}}^{m}\end{bmatrix},\quad 0\leq m\leq n, \tag{2.3.12}$$

and the following estimates hold

$$\begin{aligned}&\|\boldsymbol{\eta}^m\|_2\leq C\tau(\|\boldsymbol{e}^m\|_2+\varepsilon^2\|\dot{\boldsymbol{e}}^m\|_2),\quad \|\dot{\boldsymbol{\eta}}^m\|_2\leq\frac{C\tau}{\varepsilon}(\|\boldsymbol{e}^m\|_2+\varepsilon^2\|\dot{\boldsymbol{e}}^m\|_2),\\ &\|\boldsymbol{\xi}^m\|_2+\varepsilon^2\|\dot{\boldsymbol{\xi}}^m\|_2\leq C\tau^3.\end{aligned} \tag{2.3.13}$$

(2.3.12) implies that for $0\leq m\leq n$,

$$\begin{bmatrix}U\boldsymbol{e}^{m+1}\\ \Lambda U\dot{\boldsymbol{e}}^{m+1}\end{bmatrix}=Q^{m+1}\begin{bmatrix}U\boldsymbol{e}^{0}\\ \Lambda U\dot{\boldsymbol{e}}^{0}\end{bmatrix}+\sum_{k=0}^{m}Q^{m-k}\begin{bmatrix}\boldsymbol{\eta}^{k}\\ \dot{\boldsymbol{\eta}}^{k}\end{bmatrix}+\sum_{k=0}^{m}Q^{m-k}\begin{bmatrix}U\boldsymbol{\xi}^{k}\\ \Lambda U\dot{\boldsymbol{\xi}}^{k}\end{bmatrix},$$

which can be written in the following form ($\boldsymbol{e}^0 = \dot{\boldsymbol{e}}^0 = 0$)

$$U\boldsymbol{e}^{m+1} = \sum_{k=0}^{m} \left[Q_{11}^{(m-k)}(\boldsymbol{\eta}^k + U\boldsymbol{\xi}^k) + Q_{12}^{(m-k)}(\dot{\eta}^k + \Lambda U \dot{\boldsymbol{\xi}}^k) \right], \tag{2.3.14}$$

$$U\Lambda e^{m+1} = \sum_{k=0}^{m} \left[Q_{21}^{(m-k)}(\boldsymbol{\eta}^k + U\boldsymbol{\xi}^k) + Q_{22}^{(m-k)}(\dot{\boldsymbol{\eta}}^k + \Lambda U \dot{\boldsymbol{\xi}}^k) \right]. \tag{2.3.15}$$

Recalling the properties $\varepsilon \lesssim \|\Lambda\|_2 \lesssim \varepsilon$, $\|Q_{11}^{(m-k)}\|_2 \le 1, \|Q_{12}^{(m-k)}\|_2 \lesssim \varepsilon, \|Q_{21}^{(m-k)}\|_2 \lesssim \varepsilon, \|Q_{22}^{(m-k)}\|_2 \le 1$ in Lemma 2.2, we have

$$\|\boldsymbol{e}^{m+1}\|_2 = \|U\boldsymbol{e}^{m+1}\|_2 \le C \sum_{k=0}^{m} \left(\|\boldsymbol{\eta}^k\|_2 + \varepsilon \|\dot{\boldsymbol{\eta}}^k\|_2 + \|\boldsymbol{\xi}^k\|_2 + \varepsilon^2 \|\dot{\boldsymbol{\xi}}^k\|_2 \right), \tag{2.3.16}$$

and

$$\begin{aligned} \varepsilon \|\dot{\boldsymbol{e}}^{m+1}\|_2 &\le C \|\Lambda U \dot{\boldsymbol{e}}^{m+1}\|_2 \\ &\le C \sum_{k=0}^{m} \left[\varepsilon^{-1} \|\boldsymbol{\eta}^k\|_2 + \|\dot{\boldsymbol{\eta}}^k\|_2 + (\varepsilon^{-1}\|\boldsymbol{\xi}^k\|_2 + \varepsilon \|\dot{\boldsymbol{\xi}}^k\|_2) \right]. \end{aligned} \tag{2.3.17}$$

Combing (2.3.16), (2.3.17) with (2.3.13), we obtain for $m \le \frac{T}{\tau} - 1$,

$$\|\boldsymbol{e}^{m+1}\|_2 \le C\tau \sum_{k=0}^{m} \left(\|\boldsymbol{e}^k\|_2 + \varepsilon^2 \|\dot{\boldsymbol{e}}^k\|_2 \right) + C(m+1)\tau^3, \tag{2.3.18}$$

$$\varepsilon^2 \|\dot{\boldsymbol{e}}^{m+1}\|_2 \le C\tau \sum_{k=0}^{m} \left[\|\boldsymbol{e}^k\|_2 + \varepsilon^2 \|\dot{\boldsymbol{e}}^k\|_2 \right] + C(m+1)\tau^2, \tag{2.3.19}$$

and

$$\|\boldsymbol{e}^{m+1}\|_2 + \varepsilon^2 \|\boldsymbol{e}^{m+1}\|_2 \le C\tau \sum_{k=0}^{m} \left(\|\boldsymbol{e}^k\|_2 + \varepsilon^2 \|\dot{\boldsymbol{e}}^k\|_2 \right) + C(m+1)\tau^3. \tag{2.3.20}$$

Discrete Gronwall inequality would then imply

$$\|\boldsymbol{e}^{m+1}\|_2 + \varepsilon^2 \|\boldsymbol{e}^{m+1}\|_2 \le C_T \tau^2, \quad m = 0, \cdots, n, \tag{2.3.21}$$

where C depends on T, M, d and A. Moreover,

$$\|\boldsymbol{e}^{n+1}\|_\infty + \varepsilon^2 \|\boldsymbol{e}^{n+1}\|_\infty \le \|\boldsymbol{e}^{n+1}\|_2 + \varepsilon^2 \|\boldsymbol{e}^{n+1}\|_2 \le C_T \tau^2, \tag{2.3.22}$$

and for $0 < \tau \le \frac{1}{\sqrt{C_T}}$, $\|\boldsymbol{e}^{n+1}\|_\infty + \varepsilon^2 \|\boldsymbol{e}^{n+1}\|_\infty \le 1$, i.e. conclusion (2.3.2) holds for $n+1$ by using triangle inequality to obtain $\|\boldsymbol{y}^{n+1}\|_\infty + \varepsilon^2 \|\dot{\boldsymbol{y}}^{n+1}\|_\infty \le \|\boldsymbol{y}(t_{n+1})\|_\infty + \varepsilon^2 \|\dot{\boldsymbol{y}}(t_{n+1})\|_\infty + \|\boldsymbol{e}^{n+1}\|_\infty + \varepsilon^2 \|\dot{\boldsymbol{e}}^{n+1}\|_\infty \le M + 1$. Therefore, the proof is complete by mathematical induction. $\square$

Remark Our NPI method (2.2.25) is uniformly second order independent of ε, while later numerical results show for fixed ε, when time step τ decreases the convergence order will increase from 2 to 3. This can be explained by the following observation. For $\kappa_l(t)$ $(1 \leq l \leq d)$ of the integral kernel $\kappa(t)$ (2.2.4), it is easy to check that $|\kappa_l(t)| = |e^{i\beta_l^+ t} - e^{i\beta_l^- t}| \leq |\beta_l^+ - \beta_l^-|\tau \lesssim \frac{\tau}{\varepsilon^2}$. From the local error analysis in Lemma 2.1, we could then derive the local error as

$$\|\boldsymbol{y}(t_{n+1}) - \boldsymbol{S}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))\|_2 \leq \frac{C}{\varepsilon^2}\tau^4, \quad \varepsilon^2\|\dot{\boldsymbol{y}}(t_{n+1}) - \dot{\boldsymbol{S}}(\boldsymbol{y}(t_n), \dot{\boldsymbol{y}}(t_n))\|_2 \leq \frac{C}{\varepsilon^2}\tau^4.$$

It then follows from the error analysis that $\|\boldsymbol{e}^n\|_2 + \varepsilon^2\|\boldsymbol{e}^n\|_2 \lesssim \frac{\tau^3}{\varepsilon^2}$, which confirms that for fixed ε, the order of convergence is 3 for $\tau \ll \varepsilon^2$.

2.4 Numerical results

In this section, we present numerical results to show the performance of the NPI method (2.2.25). Denote $\boldsymbol{y}^n_{\varepsilon,\tau}$ as the numerical solution at t_n obtained by NPI (2.2.25) with time step τ and parameter ε; the reference solution $\boldsymbol{y}_\varepsilon(t)$ is obtained numerically by applying NPI (2.2.25) with a very fine time step, e.g. $\tau_e = 1 \times 10^{-5}$. To quantify the convergence order, we measure the norm of error vector $e_{\varepsilon,\tau}(T) = \|\boldsymbol{y}^n_{\varepsilon,\tau} - \boldsymbol{y}_\varepsilon(T)\|_2$ $(n = T/\tau)$ at a fixed time T.

2.4.1 Single equation examples

Example 1. In this example, $d = 1$, $A = 1$ and the nonlinear function is chosen as $F(|y|^2) = |y|^2$ in (2.1.1). The initial conditions are chosen as: (1) the well-prepared case, Eq. (2.1.4) with $\alpha = 2$, $y_0 = 1, y_1^\varepsilon = i(-y_0 - F(|y_0|^2)y_0) + 0.1\varepsilon^2$; (2) the ill-prepared case, Eq. (2.1.4) with $\alpha = 0$, $y_0 = 1, y_1^\varepsilon = i(-y_0 - F(|y_0|^2)y_0) + 0.1$.

The errors at $T = 1.0$ are shown for (1) and (2) in Tables 2.1 and 2.2, respectively. From the numerical results, we observe that the convergence order is uniform at order 2. For fixed ε, when τ decreases, the convergence order will increase from 2 to 3; for fixed τ, when ε decreases, the convergence order will decrease from 3 to 2.

Table 2.1: Example 1, $d = 1$, well-prepared case, $\alpha = 2$.

$e_{\varepsilon,\tau}(1.0)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$	$\tau_0/2^8$	$\tau_0/2^9$
$\varepsilon_0 = 0.5$	1.69E-03	2.90E-04	4.77E-05	6.65E-06	8.71E-07	1.11E-07	1.41E-08	1.77E-09	2.24E-10	2.98E-11
order	-	2.54	2.60	2.84	2.93	2.97	2.98	2.99	2.98	2.91
$\varepsilon_0/2$	1.10E-02	1.91E-03	3.07E-04	4.20E-05	5.44E-06	6.91E-07	8.70E-08	1.09E-08	1.37E-09	1.72E-10
order	-	2.53	2.63	2.87	2.95	2.98	2.99	3.00	3.00	2.99
$\varepsilon_0/2^2$	2.30E-02	5.62E-03	1.15E-03	2.03E-04	2.88E-05	3.78E-06	4.84E-07	6.11E-08	7.69E-09	9.68E-10
order	-	2.03	2.29	2.50	2.82	2.93	2.97	2.98	2.99	2.99
$\varepsilon_0/2^3$	7.08E-02	1.70E-02	3.23E-03	5.78E-04	1.01E-04	1.59E-05	2.18E-06	2.83E-07	3.61E-08	4.55E-09
order	-	2.06	2.39	2.48	2.52	2.66	2.87	2.94	2.97	2.99
$\varepsilon_0/2^4$	1.07E-01	2.57E-02	5.92E-03	1.33E-03	2.54E-04	4.24E-05	7.30E-06	1.13E-06	1.53E-07	1.98E-08
order	-	2.06	2.12	2.15	2.39	2.58	2.54	2.69	2.88	2.95
$\varepsilon_0/2^5$	2.68E-01	6.74E-02	1.67E-02	3.86E-03	7.94E-04	1.43E-04	2.47E-05	3.95E-06	5.77E-07	7.22E-08
order	-	1.99	2.01	2.11	2.28	2.47	2.53	2.64	2.77	3.00
$\varepsilon_0/2^6$	2.60E-01	6.38E-02	1.58E-02	3.93E-03	9.14E-04	1.84E-04	3.65E-05	6.23E-06	9.45E-07	1.23E-07
order	-	2.03	2.01	2.01	2.11	2.32	2.33	2.55	2.72	2.94
$\varepsilon_0/2^7$	2.31E-01	5.78E-02	1.39E-02	3.35E-03	7.83E-04	1.78E-04	3.80E-05	7.72E-06	1.36E-06	2.01E-07
order	-	2.00	2.06	2.05	2.10	2.13	2.23	2.30	2.50	2.76
$\varepsilon_0/2^8$	1.62E-01	3.79E-02	9.29E-03	2.36E-03	5.85E-04	1.44E-04	3.26E-05	6.81E-06	1.58E-06	2.82E-07
order	-	2.09	2.03	1.98	2.01	2.02	2.15	2.26	2.11	2.49

Table 2.2: Example 1, $d = 1$, ill-prepared case, $\alpha = 0$.

$e_{\varepsilon,\tau}(1.0)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$	$\tau_0/2^8$	$\tau_0/2^9$
$\varepsilon_0 = 0.5$	7.00E-03	1.12E-03	1.57E-04	2.03E-05	2.56E-06	3.22E-07	4.03E-08	5.02E-09	6.04E-10	7.18E-11
order	-	2.64	2.84	2.95	2.98	2.99	3.00	3.01	3.06	3.07
$\varepsilon_0/2$	7.69E-03	1.47E-03	2.40E-04	3.30E-05	4.73E-06	6.29E-07	8.10E-08	1.03E-08	1.29E-09	1.55E-10
order	-	2.39	2.61	2.86	2.80	2.91	2.96	2.98	3.00	3.05
$\varepsilon_0/2^2$	3.33E-02	6.99E-03	1.46E-03	2.38E-04	3.58E-05	4.84E-06	6.28E-07	7.99E-08	1.01E-08	1.27E-09
order	-	2.25	2.26	2.62	2.73	2.89	2.95	2.97	2.99	2.99
$\varepsilon_0/2^3$	8.28E-02	1.82E-02	3.87E-03	8.54E-04	1.50E-04	2.37E-05	3.25E-06	4.23E-07	5.40E-08	6.87E-09
order	-	2.19	2.23	2.18	2.51	2.66	2.87	2.94	2.97	2.97
$\varepsilon_0/2^4$	1.34E-01	3.31E-02	8.13E-03	1.70E-03	3.68E-04	6.51E-05	1.14E-05	1.78E-06	2.41E-07	3.13E-08
order	-	2.01	2.03	2.26	2.20	2.50	2.51	2.68	2.88	2.95
$\varepsilon_0/2^5$	2.35E-01	5.66E-02	1.33E-02	3.03E-03	6.81E-04	1.45E-04	2.81E-05	5.08E-06	8.37E-07	1.15E-07
order	-	2.06	2.09	2.13	2.15	2.23	2.37	2.47	2.60	2.86
$\varepsilon_0/2^6$	2.03E-01	4.93E-02	1.26E-02	3.16E-03	8.05E-04	1.98E-04	4.25E-05	7.18E-06	1.25E-06	1.97E-07
order	-	2.04	1.97	1.99	1.97	2.02	2.22	2.57	2.52	2.67
$\varepsilon_0/2^7$	2.03E-01	4.95E-02	1.26E-02	3.19E-03	7.80E-04	1.86E-04	4.84E-05	1.12E-05	1.84E-06	3.22E-07
order	-	2.03	1.97	1.99	2.03	2.07	1.94	2.11	2.61	2.52
$\varepsilon_0/2^8$	2.04E-01	4.96E-02	1.17E-02	2.90E-03	6.84E-04	1.68E-04	4.13E-05	1.07E-05	2.48E-06	4.50E-07
order	-	2.04	2.09	2.01	2.08	2.03	2.02	1.95	2.11	2.46

2.4.2 Multiple equation case

Example 2. In this example, $d = 3$ $A = \mathrm{diag}(1, 2, 4)$ and nonlinear term is taken as $F(|\boldsymbol{y}|^2) = |\boldsymbol{y}|^2$ in (2.1.1). The initial conditions are given as: (1) the well-prepared data, Eq. (2.1.4) with $\alpha = 2$, $\boldsymbol{y}_0 = [1, 1, 1]^T, \boldsymbol{y}_1^\varepsilon = i(-A\boldsymbol{y}_0 - F(|\boldsymbol{y}|^2)\boldsymbol{y}) + 0.1\varepsilon^2[1, 1, 1]^T$; (2) the ill-prepared data, Eq. (2.1.4) with $\alpha = 0$, $\boldsymbol{y}_0 = [1, 1, 1]^T, \boldsymbol{y}_1^\varepsilon = i(-A\boldsymbol{y}_0 - F(|\boldsymbol{y}|^2)\boldsymbol{y}) + 0.1[1, 1, 1]^T$.

Table 2.3: Example 2, $d = 3$, well-prepared case.

$e_{\varepsilon,\tau}(1.2)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$	$\tau_0/2^8$	$\tau_0/2^9$
$\varepsilon_0 = 0.5$	7.00E-03	1.12E-03	1.57E-04	2.03E-05	2.56E-06	3.22E-07	4.03E-08	5.02E-09	6.04E-10	7.18E-11
order	-	2.64	2.84	2.95	2.98	2.99	3.00	3.01	3.06	3.07
$\varepsilon_0/2$	7.69E-03	1.47E-03	2.40E-04	3.30E-05	4.73E-06	6.29E-07	8.10E-08	1.03E-08	1.29E-09	1.55E-10
order	-	2.39	2.61	2.86	2.80	2.91	2.96	2.98	3.00	3.05
$\varepsilon_0/2^2$	3.33E-02	6.99E-03	1.46E-03	2.38E-04	3.58E-05	4.84E-06	6.28E-07	7.99E-08	1.01E-08	1.27E-09
order	-	2.25	2.26	2.62	2.73	2.89	2.95	2.97	2.99	2.99
$\varepsilon_0/2^3$	8.28E-02	1.82E-02	3.87E-03	8.54E-04	1.50E-04	2.37E-05	3.25E-06	4.23E-07	5.40E-08	6.87E-09
order	-	2.19	2.23	2.18	2.51	2.66	2.87	2.94	2.97	2.97
$\varepsilon_0/2^4$	1.34E-01	3.31E-02	8.13E-03	1.70E-03	3.68E-04	6.51E-05	1.14E-05	1.78E-06	2.41E-07	3.13E-08
order	-	2.01	2.03	2.26	2.20	2.50	2.51	2.68	2.88	2.95
$\varepsilon_0/2^5$	2.35E-01	5.66E-02	1.33E-02	3.03E-03	6.81E-04	1.45E-04	2.81E-05	5.08E-06	8.37E-07	1.15E-07
order	-	2.06	2.09	2.13	2.15	2.23	2.37	2.47	2.60	2.86
$\varepsilon_0/2^6$	2.03E-01	4.93E-02	1.26E-02	3.16E-03	8.05E-04	1.98E-04	4.25E-05	7.18E-06	1.25E-06	1.97E-07
order	-	2.04	1.97	1.99	1.97	2.02	2.22	2.57	2.52	2.67
$\varepsilon_0/2^7$	2.03E-01	4.95E-02	1.26E-02	3.19E-03	7.80E-04	1.86E-04	4.84E-05	1.12E-05	1.84E-06	3.22E-07
order	-	2.03	1.97	1.99	2.03	2.07	1.94	2.11	2.61	2.52
$\varepsilon_0/2^8$	2.04E-01	4.96E-02	1.17E-02	2.90E-03	6.84E-04	1.68E-04	4.13E-05	1.07E-05	2.48E-06	4.50E-07
order	-	2.04	2.09	2.01	2.08	2.03	2.02	1.95	2.11	2.46

Table 2.4: Example 2, $d = 3$, ill-prepared case.

$e_{\varepsilon,\tau}(1.2)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$	$\tau_0/2^8$	$\tau_0/2^9$
$\varepsilon_0 = 0.5$	1.63E-02	2.56E-03	3.55E-04	4.55E-05	5.72E-06	7.24E-07	9.02E-08	1.14E-08	1.40E-09	1.66E-10
order	-	2.67	2.85	2.96	2.99	2.98	3.01	2.99	3.02	3.07
$\varepsilon_0/2$	1.72E-02	3.22E-03	5.34E-04	7.87E-05	1.11E-05	1.49E-06	1.89E-07	2.38E-08	2.92E-09	3.58E-10
order	-	2.42	2.59	2.76	2.82	2.90	2.98	2.99	3.03	3.02
$\varepsilon_0/2^2$	7.10E-02	1.54E-02	3.31E-03	5.50E-04	8.18E-05	1.10E-05	1.44E-06	1.86E-07	2.33E-08	2.94E-09
order	-	2.20	2.22	2.59	2.75	2.90	2.93	2.95	3.00	2.99
$\varepsilon_0/2^3$	2.03E-01	4.48E-02	9.68E-03	2.12E-03	3.74E-04	5.85E-05	7.96E-06	9.87E-07	1.24E-07	1.59E-08
order	-	2.18	2.21	2.19	2.50	2.68	2.88	3.01	2.99	2.96
$\varepsilon_0/2^4$	3.10E-01	7.66E-02	1.88E-02	3.93E-03	8.53E-04	1.51E-04	2.64E-05	4.11E-06	5.59E-07	7.25E-08
order	-	2.01	2.03	2.26	2.20	2.50	2.51	2.68	2.88	2.95
$\varepsilon_0/2^5$	5.53E-01	1.34E-01	3.19E-02	7.27E-03	1.68E-03	3.48E-04	6.94E-05	1.23E-05	1.97E-06	2.66E-07
order	-	2.05	2.07	2.13	2.11	2.27	2.33	2.50	2.64	2.88
$\varepsilon_0/2^6$	5.15E-01	1.25E-01	3.10E-02	7.63E-03	1.93E-03	4.78E-04	9.58E-05	1.66E-05	2.94E-06	4.57E-07
order	-	2.04	2.01	2.02	1.98	2.01	2.32	2.53	2.50	2.69
$\varepsilon_0/2^7$	4.79E-01	1.18E-01	3.17E-02	8.15E-03	2.00E-03	4.76E-04	1.20E-04	2.66E-05	4.29E-06	7.45E-07
order	-	2.02	1.90	1.96	2.02	2.07	1.99	2.17	2.63	2.53
$\varepsilon_0/2^8$	3.97E-01	9.76E-02	2.28E-02	6.08E-03	1.54E-03	4.03E-04	1.07E-04	2.58E-05	5.65E-06	1.04E-06
order	-	2.02	2.10	1.91	1.98	1.93	1.92	2.05	2.19	2.44

The numerical errors at $T = 1.2$ are listed in Tables 2.3 and 2.4 for cases (1) and (2), respectively.

Example 3. In this example, $d = 100$, $\boldsymbol{A} = \mathrm{diag}(1, 2, 3, \cdots, 100)$ and the nonlinear function is $F(|\boldsymbol{y}|^2) = |\boldsymbol{y}|^2$ in (2.1.1). The initial conditions are chosen as: (1) the well-prepared case, Eq. (2.1.4) with $\alpha = 2$, $\boldsymbol{y}_0 = [1, 1, \cdots, 1]^T, \boldsymbol{y}_1^\varepsilon = i(-A\boldsymbol{y}_0 - F(|\boldsymbol{y}_0|^2))\boldsymbol{y}_0 + 0.1\varepsilon^2[1, 1, \cdots, 1]^T$; (2) the ill-prepared case (2.1.4) with $\alpha = 0$, $\boldsymbol{y}_0 = [1, 1, \cdots, 1]^T, \boldsymbol{y}_1^\varepsilon =$

Table 2.5: Example 3, $d = 100$, well-prepared case.

$e_{\varepsilon,\tau}(0.8)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$	$\tau_0/2^8$	$\tau_0/2^9$
$\varepsilon_0 = 0.5$2.41E+00	4.37E-01	7.50E-02	1.11E-02	1.41E-03	1.96E-04	2.41E-05	3.27E-06	3.88E-07	4.88E-08	
order	-	2.46	2.54	2.75	2.98	2.85	3.02	2.88	3.08	2.99
$\varepsilon_0/2$	4.03E+00	7.51E-01	1.33E-01	2.42E-02	3.29E-03	4.25E-04	5.39E-05	6.56E-06	8.27E-07	1.06E-07
order	-	2.42	2.50	2.46	2.88	2.95	2.98	3.04	2.99	2.96
$\varepsilon_0/2^2$	6.76E+00	1.57E+00	3.41E-01	6.13E-02	8.80E-03	1.17E-03	1.50E-04	1.91E-05	2.40E-06	3.01E-07
order	-	2.11	2.20	2.48	2.80	2.91	2.96	2.98	2.99	3.00
$\varepsilon_0/2^3$	1.25E+01	3.13E+00	7.60E-01	1.57E-01	2.69E-02	4.01E-03	5.35E-04	6.87E-05	8.69E-06	1.20E-06
order	-	1.99	2.04	2.27	2.55	2.75	2.91	2.96	2.98	2.86
$\varepsilon_0/2^4$	2.18E+01	5.32E+00	1.41E+00	3.48E-01	8.80E-02	1.50E-02	2.20E-03	3.18E-04	4.20E-05	5.37E-06
order	-	2.04	1.91	2.02	1.98	2.56	2.77	2.79	2.92	2.97
$\varepsilon_0/2^5$	2.26E+01	5.45E+00	1.32E+00	3.15E-01	7.63E-02	1.90E-02	3.58E-03	6.04E-04	8.50E-05	1.08E-05
order	-	2.05	2.05	2.06	2.05	2.01	2.41	2.57	2.83	2.97
$\varepsilon_0/2^6$	2.52E+01	6.22E+00	1.55E+00	3.71E-01	8.90E-02	2.19E-02	4.68E-03	8.63E-04	1.46E-04	1.84E-05
order	-	2.02	2.01	2.06	2.06	2.03	2.22	2.44	2.57	2.98
$\varepsilon_0/2^7$	3.05E+01	7.72E+00	1.90E+00	4.64E-01	1.15E-01	2.85E-02	6.24E-03	1.16E-03	1.85E-04	2.46E-05
order	-	1.98	2.02	2.04	2.01	2.02	2.19	2.43	2.64	2.91
$\varepsilon_0/2^8$	3.39E+01	8.89E+00	2.30E+00	5.56E-01	1.37E-01	3.33E-02	7.75E-03	1.29E-03	2.43E-04	3.22E-05
order	-	1.93	1.95	2.05	2.02	2.04	2.10	2.59	2.41	2.92

Table 2.6: Example 3, $d = 100$, ill-prepared case.

$e_{\varepsilon,\tau}(0.8)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$	$\tau_0/2^8$	$\tau_0/2^9$
$\varepsilon_0 = 0.5$	4.40E+00	8.01E-01	1.38E-01	2.23E-02	3.16E-03	4.51E-04	5.75E-05	7.22E-06	8.34E-07	1.16E-07
order	-	2.46	2.54	2.62	2.82	2.81	2.97	2.99	3.11	2.85
$\varepsilon_0/2$	6.02E+00	1.28E+00	2.24E-01	3.99E-02	6.49E-03	1.05E-03	1.53E-04	1.95E-05	2.49E-06	3.04E-07
order	-	2.23	2.51	2.49	2.62	2.63	2.77	2.97	2.97	3.04
$\varepsilon_0/2^2$	9.73E+00	2.42E+00	5.43E-01	1.00E-01	1.77E-02	2.84E-03	4.68E-04	7.37E-05	9.04E-06	1.11E-06
order	-	2.01	2.16	2.44	2.50	2.64	2.60	2.67	3.03	3.03
$\varepsilon_0/2^3$	1.20E+01	2.99E+00	7.23E-01	1.56E-01	2.94E-02	5.37E-03	9.00E-04	1.46E-04	1.99E-05	2.40E-06
order	-	2.00	2.05	2.21	2.41	2.45	2.58	2.62	2.88	3.05
$\varepsilon_0/2^4$	2.22E+01	5.60E+00	1.32E+00	2.92E-01	5.85E-02	1.08E-02	1.92E-03	3.54E-04	5.11E-05	6.59E-06
order	-	1.99	2.08	2.18	2.32	2.44	2.49	2.44	2.79	2.95
$\varepsilon_0/2^5$	3.39E+01	8.65E+00	2.19E+00	5.60E-01	1.39E-01	2.86E-02	5.40E-03	9.12E-04	1.40E-04	1.77E-05
order	-	1.97	1.98	1.97	2.01	2.28	2.41	2.57	2.70	2.99
$\varepsilon_0/2^6$	4.11E+01	1.02E+01	2.52E+00	6.51E-01	1.59E-01	4.01E-02	7.72E-03	1.38E-03	2.25E-04	2.73E-05
order	-	2.01	2.01	1.96	2.03	1.99	2.38	2.48	2.62	3.04
$\varepsilon_0/2^7$	4.84E+01	1.21E+01	3.03E+00	7.42E-01	1.84E-01	4.87E-02	9.14E-03	1.65E-03	3.11E-04	3.64E-05
order	-	2.00	2.00	2.03	2.01	1.92	2.41	2.47	2.41	3.09
$\varepsilon_0/2^8$	6.35E+01	1.59E+01	4.17E+00	1.02E+00	2.54E-01	6.28E-02	1.51E-02	3.01E-03	5.69E-04	7.44E-05
order	-	2.00	1.93	2.04	2.00	2.01	2.06	2.33	2.40	2.94

$i(-A\boldsymbol{y}_0 - F(|\boldsymbol{y}_0|^2))\boldsymbol{y}_0 + 0.1[1, 1, \cdots, 1]^T$.

The corresponding numerical errors at $T = 0.8$ for cases (1) and (2) are presented in Table 2.5 and 2.6, respectively.

From the numerical results above in Tables 2.3- 2.6, we have the following observations:

1. The NPI method (2.2.25) is uniformly second order accurate in τ w.r.. $\varepsilon \in (0, 1]$, both for well-prepared and ill-prepared cases.

2. For fixed ε, if τ is small enough, the error will converge asymptotically with third order in τ.

Chapter 3

Nested Picard Integrators for NLSW

In this chapter, in order to improve the existing methods and achieve uniformly second order temporal error for the NLSW, a nested Picard integrator sine pseudospectral method (NPI-SP) is developed. The error bound is rigorously proved. For simplicity, the numerical scheme is designed for 1D case. Generalization to higher dimensions can be carried out straightforwardly.

3.1 NLSW on bounded domains

We present the details of our uniform second order nested Picard integrator sine pseudospectral method (NPI-SP) for the following NLSW (1.2.1) in this chapter (denote $\psi = \psi(\boldsymbol{x}, t)$):

$$\begin{cases} i\partial_t\psi - \varepsilon^2\partial_{tt}\psi + \nabla^2\psi + F(|\psi|^2)\psi = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, \quad t > 0 \\ \psi(\boldsymbol{x}, 0) = \psi_0(\boldsymbol{x}), \quad \partial_t\psi(\boldsymbol{x}, 0) = \psi_1^\varepsilon(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d, \end{cases} \tag{3.1.1}$$

For simplicity, we consider the case $F(|\psi|^2) = -|\psi|^2$. The method can be easily generalized to more general $f(\cdot)$, such as polynomial type functions. In practice computation, the NLSW is often truncated on a bounded domain, for example interval $\Omega = (a, b)$ in one dimension ($d = 1$), or a bounded box in two dimensions or three dimensions, with zero Dirichlet boundary condition, and this truncation is accurate if the solution of equation(3.1.1) is localized. Here we discuss the truncated equation in one dimension in the following section, and it can be easily generalized to 2D or 3D cases. In one dimension, the truncated NLSW (3.1.1) is ($\Omega = (a, b)$)

$$\begin{cases} i\partial_t\psi(x,t) - \varepsilon^2\partial_{tt}\psi(x,t) + \Delta\psi(x,t) - |\psi(x,t)|^2\psi(x,t) = 0,\ x \in \Omega,\ t > 0, \\ \psi(x,0) = \psi_0(x), \quad \partial_t\psi(x,0) = \psi_1^\varepsilon(x),\ x \in \Omega,\ t > 0, \\ \psi(a,t) = \psi(b,t) = 0, \quad t > 0. \end{cases} \tag{3.1.2}$$

As the solution of NLSW converge to the solution of NLS as $\varepsilon \to 0^+$, we assume the initial velocity $\psi_1^\varepsilon(x)$ of the truncated problem (3.1.2) satisfy

$$\psi_1^\varepsilon(x) = i(\nabla^2\psi_0(x) + |\psi_0(x)|^2\psi_0(x)) + \varepsilon^\alpha\omega^\varepsilon(x), \quad \alpha \geq 0, \quad x \in (a,b), \tag{3.1.3}$$

where $i(\nabla^2\psi_0(x) - |\psi_0(x)|^2\psi_0(x))$ is the initial velocity for the truncated NLS. $\omega^\varepsilon(x)$ is uniformly bounded in $H_0^1 \cap H^2$ w.r.t. ε, which satisfies $\liminf_{\varepsilon\to 0^+}\|\omega^\varepsilon(x)\|_{H^2} > 0$. $\alpha \geq 0$ is the parameter measuring the compatibility of the initial velocity of NLS and NLSW.

3.2 A NPI sine pseudospectral method

3.2.1 Temporal discretization by NPIs

In this section we present the details of our uniform second order nested Picard integrator (NPI) for equation (3.1.1).

Choose the time step size $\Delta t := \tau > 0$ and denote the time steps as $t_n = n\tau$ $(n = 0, 1, \cdots)$. Choose mesh size $h = \Delta x := (b - a)/M$ with M being a positive integer. The grid points are denoted as:

$$x_j := a + j\Delta x, j = 0, 1, \cdots, M.$$

Define index sets

$$\mathcal{T}_M = \{j | j = 1, 2, \cdots, M - 1\},$$
$$\mathcal{T}_M^0 = \{j | j = 0, 2, \cdots, M\},$$

and denote space

$$X_M = \mathrm{span}\left\{\Phi_l(x) = \sin(\mu_l(x-a)),\ \mu_l = \frac{\pi l}{b-a},\ x \in \Omega,\ l \in \mathcal{T}_M\right\},$$
$$Y_M = \left\{v = (v_0, v_1, \cdots, v_M)^T \in \mathbb{C}^{M+1} |\ v_0 = v_M = 0\right\},$$

Then we define the L^2 projection operator $P_M : L^2(\Omega) \to X_M$ and sine interpolation operator $I_M : Y_M \to X_M$ and $I_M : C_0(\overline{\Omega}) \to X_M$ as:

$$\begin{aligned}(P_M\psi)(x) &= \sum_{l=1}^{M-1} \hat{\psi}_l \sin(\mu_l(x-a)),\\ (I_M\phi)(x) &= \sum_{l=1}^{M-1} \tilde{\phi}_l \sin(\mu_l(x-a)), \quad x \in [a,b],\end{aligned} \tag{3.2.1}$$

where the coefficients are defined as

$$\hat{\psi}_l = \frac{2}{b-a}\int_a^b \psi(x)\sin(\mu_l(x-a))dx, \quad l = 1, 2, \cdots,$$
$$\tilde{\phi}_l = \frac{2}{M}\sum_{j=1}^{M-1} \phi_j \sin(jl\pi/M), \quad l \in \mathcal{T}_M.$$

It can be directly checked that on X_M, P_M and I_M are both identity transforms, and if $\phi(x) \in X_M$, $\hat{\phi}_l = \tilde{\phi}_l$.

On each time interval $t \in [t_n, t_{n+1}]$, using the variation of constants formula, the solution $\psi(t_n+s) := \psi(x, t_n+s)$ can be written as:

$$\begin{aligned}\psi(x, t_n+s) =& e^{i\beta^+ s} h_1(\psi(x,t_n), \partial_t\psi(x,t_n); x) + e^{i\beta^- s} h_2(\psi(x,t_n), \partial_t\psi(x,t_n); x)\\ &+ i\gamma\int_0^s \kappa(s-w)|\psi(x,t_n+w)|^2\psi(x,t_n+w)dw, \quad 0 \le s \le \tau.\end{aligned} \tag{3.2.2}$$

Operators β^+, β^- and γ are defined by:

$$\begin{aligned}\beta^+ &:= \frac{1+\sqrt{1-4\varepsilon^2\Delta}}{2\varepsilon^2} = O\left(\frac{1}{\varepsilon^2}\right),\\ \beta^- &:= \frac{1-\sqrt{1-4\varepsilon^2\Delta}}{2\varepsilon^2} = \frac{2\Delta}{1+\sqrt{1-4\varepsilon^2\Delta}} = O(1),\\ \beta &:= \beta^+ - \beta^- = \frac{\sqrt{1-4\varepsilon^2\Delta}}{\varepsilon^2},\\ \gamma &:= \frac{1}{\varepsilon^2\beta} = \frac{1}{\sqrt{1-4\varepsilon^2\Delta}} = O(1),\end{aligned} \tag{3.2.3}$$

where Δ is the Laplacian. Notice $\beta^+ - \frac{1}{\varepsilon^2} = -\beta^-$.

Function $h_1(\cdot,\cdot;x)$ and $h_2(\cdot,\cdot;x)$ are defined as:

$$\begin{aligned} h_1(\psi(x,t_n),\partial_t\psi(x,t_n);x) &:= -\beta^{-1}(\beta^-\psi(x,t_n)+i\partial_t\psi(x,t_n)), \\ h_2(\psi(x,t_n),\partial_t\psi(x,t_n);x) &:= \beta^{-1}(\beta^+\psi(x,t_n)+i\partial_t\psi(x,t_n)), \end{aligned} \tag{3.2.4}$$

and the integral kernel $\kappa(t)$ is defined by:

$$\kappa(t) := e^{i\beta^+ t} - e^{i\beta^- t}. \tag{3.2.5}$$

Based on the definition of Laplacian, for $\phi(x) \in L^2(\Omega)$, if we define

$$\begin{aligned} &\beta_l^+ := \frac{1+\sqrt{1+4\varepsilon^2|\mu_l|^2}}{2\varepsilon^2}, \quad \beta_l^- := \frac{-2|\mu_l|^2}{1+\sqrt{1+4\varepsilon^2|\mu_l|^2}}, \\ &\beta_l := \beta_l^+ - \beta_l^- = \frac{\sqrt{1+4\varepsilon^2|\mu_l|^2}}{\varepsilon^2}, \quad \gamma_l := \frac{1}{\varepsilon^2\beta_l} = \frac{1}{\sqrt{1+4\varepsilon^2|\mu_l|^2}}, \end{aligned} \tag{3.2.6}$$

$\beta^-\phi$ can be written as

$$(\beta^-\phi)(x) = \sum_{l=1}^{\infty} \widehat{(\beta^-\phi)}_l \sin(\mu_l(x-a)) = \sum_{l=1}^{\infty} \beta_l^- \hat{\phi}_l \sin(\mu_l(x-a)),$$

and other operators β^+, β, γ, $e^{i\beta^+ t}$, $e^{i\beta^- t}$ can be computed accordingly. Specially, if $\phi(x) \in X_M$, then

$$\begin{aligned} (\beta^-\phi)(x) &= \sum_{l=1}^{M-1} \widehat{(\beta^-\phi)}_l \sin(\mu_l(x-a)) \\ &= \sum_{l=1}^{M-1} \beta_l^- \hat{\phi}_l \sin(\mu_l(x-a)) \\ &= \sum_{l=1}^{M-1} \beta_l^- \tilde{\phi}_l \sin(\mu_l(x-a)), \end{aligned}$$

For the above integral form (3.2.2), it can be derived [3] there exists $T > 0$ such that equation (3.1.2) with initial value satisfies (3.1.3) admits solution $\psi(x,t) \in L^\infty[[0,T];L^\infty \cap H^1]$, and $\partial_t\psi(x,t) = O(1)$, $\partial_{tt}\psi(x,t) = O(\varepsilon^{\min\{\alpha-2,0\}})$. The oscillation, which results in the unboundedness of $\partial_t^{(k)}\psi(x,t), k \geq 2$ when $\varepsilon \to 0^+$, makes numerical quadrature for the integral in (3.2.2) difficult.

To overcome this, we propose the following nested Picard integrator, i.e. we construct approximations $\psi^{n,[m]}(x,s)$ to $\psi(x,t_n+s)$ for $s\in[0,\tau]$ based on $\psi(x,t_n)$ and integral equation (3.2.2) via the following nested Picard iteration:

$$\begin{aligned}\psi^{n,[0]}(x,s):=&\psi(x,t_n),\\ \psi^{n,[m+1]}(x,s):=&e^{i\beta^+ s}h_1(\psi(x,t_n),\partial_t\psi(x,t_n);x)\\ &+e^{i\beta^- s}h_2(\psi(x,t_n),\partial_t\psi(x,t_n);x)\\ &+i\gamma\int_0^s\kappa(s-w)|\psi^{n,[m]}(x,w)|^2\psi^{n,[m]}(x,w)dw,\quad 0\le s\le\tau.\end{aligned}\tag{3.2.7}$$

where m stands for the number of Picard integration. Based on the aforementioned properties of $\psi(x,t)$, we have $\psi^{n,[0]}(x,s)-\psi(t_n+s)=O(x,s)$ as $\partial_t\psi(x,t)=O(1)$, and then $\psi^{n,[1]}(x,s)-\psi(x,t_n+s)=O(s^2)$. Recursively, we would obtain the local error as

$$\psi(x,t_n+s)-\psi^{n,[m]}(x,s)=O(s^{m+1}),$$

and the global error would be $O(\tau^m)$.

In order to update NPI approximations from formula (3.2.7), $\partial_t\psi(x,t)$ is also required. By taking the derivative of equation (3.2.2),

$$\begin{aligned}\partial_t\psi(x,t_n+s)=&i\beta^+e^{i\beta^+ s}h_1(\psi(x,t_n),\partial_t\psi(x,t_n);x)+i\beta^-e^{i\beta^- s}h_2(\psi(x,t_n),\partial_t\psi(x,t_n);x)\\ &+i\gamma\int_0^s\dot\kappa(s-w)|\psi(x,t_n+w)|^2\psi(x,t_n+w)dw,\quad 0\le s\le\tau.\end{aligned}$$

where the integral kernel $\dot\kappa(t)$ is defined by $\dot\kappa(t):=i\beta^+e^{i\beta^+t}-i\beta^-e^{i\beta^-t}$.

The corresponding approximations $\dot\psi^{n,[m]}(x,s)$ to $\partial_t\psi(t_n+s)$ are given by,

$$\begin{aligned}\dot\psi^{n,[0]}(x,s):=&\partial_t\psi(x,t_n),\\ \dot\psi^{n,[m+1]}(x,s):=&i\beta^+e^{i\beta^+ s}h_1(\psi(x,t_n),\partial_t\psi(x,t_n);x)\\ &+i\beta^-e^{i\beta^- s}h_2(\psi(x,t_n),\partial_t\psi(x,t_n);x),\\ &+i\gamma\int_0^s\dot\kappa(s-w)|\psi^{n,[m]}(x,w)|^2\psi^{n,[m]}(x,w)dw,\quad 0\le s\le\tau,\end{aligned}\tag{3.2.8}$$

Similarly, we would have:

$$\partial_t\psi(x,t_n+s)-\dot\psi^{n,[m]}(x,s)=\varepsilon^{-2}O(s^{m+1}).$$

Therefore, (3.2.7) and (3.2.8) form a complete numerical scheme for solving the system (3.1.2) from t_n to t_{n+1} by setting $s=\tau$ at $m-th$ iterates with $m-th$ order accuracy.

3.2.2 Detailed formulas for a second order NPI

Here, we construct a second order NPI for solving (3.1.2) with (3.1.3). Our target is a uniformly second order algorithm, so from our previous construction we need to take $m = 2$. Ideally we can directly compute $\psi^{n,[2]}(x,s)$ and $\dot{\psi}^{n,[2]}(x,s)$ from (3.2.7) and (3.2.8), while it would be computationally expensive. In practice, approximations of the integral terms in (3.2.7) and (3.2.8) should be done for evaluating $\psi^{n,[m]}(x,s)$ and $\dot{\psi}^{n,[m]}(x,s)$ to reduce the computational cost. And because of our sine spatial discretization, we need to keep our Picard iterations within X_M. Here we introduce numerical approximations $\psi^{n,m}(x,s)$ and $\dot{\psi}^{n,m}(x,s)$ of Picard iterations with residual functions $R^n_{m+1}(x,s)$ and $\dot{R}^n_{m+1}(x,s)$ $(m = 1, 2, \ldots)$ as following:

$$
\begin{aligned}
\psi^{n,0}(x,s) :=& \psi(x,t_n), \\
\psi^{n,m+1}(x,s) :=& e^{i\beta^+ s} h_1(\psi(x,t_n), \partial_t\psi(x,t_n); x) \\
&+ e^{i\beta^- s} h_2(\psi(x,t_n), \partial_t\psi(x,t_n); x) \\
&+ i\gamma \int_0^s \kappa(s-w) I_M(|\psi^{n,m}(x,w)|^2 \psi^{n,m}(x,w)) dw \\
&- R^n_{m+1}(x,s), \quad 0 \le s \le \tau,
\end{aligned}
\tag{3.2.9}
$$

$$
\begin{aligned}
\dot{\psi}^{n,0}(x,s) :=& \partial_t\psi(x,t_n), \\
\dot{\psi}^{n,m+1}(x,s) :=& i\beta^+ e^{i\beta^+ s} h_1(\psi(x,t_n), \partial_t\psi(x,t_n)) \\
&+ i\beta^- e^{i\beta^- s} h_2(\psi(x,t_n), \partial_t\psi(x,t_n)), \\
&+ i\gamma \int_0^s \dot{\kappa}(s-w) I_M(|\psi^{n,m}(x,w)|^2 \psi^{n,m}(x,w)) dw \\
&- \dot{R}^n_{m+1}(x,s), \quad 0 \le s \le \tau,
\end{aligned}
\tag{3.2.10}
$$

where the residual functions $R^n_{m+1}(x,s)$ and $\dot{R}^n_{m+1}(x,s)$ are introduced when numerically computing the nonlinearity integral after projection. We hope to keep $R^n_{m+1}(x,s) = O(s^{m+1})$, $\varepsilon^2 \dot{R}^n_{m+1}(x,s) = O(s^{m+1})$ and then the accuracy of NPI can be preserved.

In the following part, we only need to specify the approximations of (3.2.7) we choose for residual functions $R^n_{m+1}(s)$, and $\dot{R}^n_{m+1}(s)$ can be obtained by taking the time derivative of (3.2.7).

In order to maintain the ε-dependent accuracy, we find that the highly oscillatory factors in (3.2.9) and (3.2.10) have to be treated properly. Here, we adopt Gautschi-type quadrature, and separate the highly oscillatory part (terms like $e^{i\frac{1}{\varepsilon^2}(s-w)}$) and the slow varying part, then integrate the oscillatory part exactly and approximate the non-oscillatory part by high order quadrature. In the solution the rapid oscillations are caused by $e^{i\beta^+ t}$, which can be decomposed as:

$$e^{i\beta^+ t} = e^{i\frac{1}{\varepsilon^2}t}e^{-i\beta^- t}, \quad \beta^- = O(1).$$

The second term is of $O(1)$ frequency thus slow varying, so the first term $e^{i\frac{1}{\varepsilon^2}t}$ is the leading frequency of the rapid oscillation.

Below, we detail the construction of practical NPIs up to second order. For simplicity, we denote $h_1^n := h_1^n(x) = h_1(\psi(x,t_n), \partial_t\psi(x,t_n); x)$, $h_2^n := h_2^n(x) = h_2(\psi(x,t_n), \partial_t\psi(x,t_n); x)$.

First order NPI Starting with $\psi^{n,0}(s) := \psi(t_n)$, by (3.2.9) we have for $\leq s \leq \tau$:

$$\begin{aligned}\psi^{n,1}(x,s) :=& e^{i\frac{1}{\varepsilon^2}s}e^{-i\beta^- s}h_1^n + e^{i\beta^- s}h_2^n \\ &+ ie^{i\frac{1}{\varepsilon^2}s}\gamma\int_0^s e^{-i\frac{1}{\varepsilon^2}w}e^{-i\beta^-(s-w)}I_M(|\psi(x,t_n)|^2\psi(x,t_n))dw \\ &- i\gamma\int_0^s e^{i\beta^-(s-w)}I_M(|\psi(x,t_n)|^2\psi(x,t_n))dw + O(s^2).\end{aligned} \tag{3.2.11}$$

For the integrals, we apply the approximation $e^{-i\beta^-(s-w)} = e^{-i\beta^-(s-s)} + O(s) = 1 + O(s)$ and $e^{i\beta^-(s-w)} = 1 + O(s)$ $(0 \leq w \leq s)$, we would obtain $\psi^{n,1}(s)$. To show the detailed form of $\psi^{n,1}(s)$, we introduce coefficients function $p_k(s), k = 0, \pm1, \pm2$ defined by:

$$p_k(s) := \int_0^s e^{ik\frac{s_1}{\varepsilon^2}}ds_1 = O(\tau), \quad 0 \leq s \leq \tau, \tag{3.2.12}$$

and for simplicity denote

$$f^n := f(\psi(x,t_n); x) = i\gamma I_M(|\psi(x,t_n)|^2\psi(x,t_n)), \tag{3.2.13}$$

we have the following expression for $\psi^{n,1}(s)$:

$$\psi^{n,1}(x,s) = e^{i\frac{1}{\varepsilon^2}s}(e^{-i\beta^- s}h_1^n + p_{-1}(s)f^n) + (e^{i\beta^- s}h_2^n - sf^n), \quad 0 \leq s \leq \tau. \tag{3.2.14}$$

If we take the time derivative of $\psi^{n,1}(x,s)$, we would get $\dot{\psi}^{n,1}(x,s)$, which could also be derived by taking the same approximation $e^{i\beta^-(s-w)} = 1 + O(s)$ in (3.2.10). However the detailed form of $\dot{\psi}^{n,1}(x,s)$ will not appear in the construction of higher order NPI.

With $\psi^{n,1}(x,s)$ constructed, we need to identify the leading oscillations in the nonlinear integral term in (3.2.9) for $\psi^{n,2}(s)$. By (3.2.14) we have:

$$\begin{aligned} |\psi^{n,1}(x,s)|^2 =& F_0^n(x,s) + sF_1^n(x,s) + p_{-1}(s)F_{-2}^n(x,s) + p_1(s)F_2^n(x,s) \\ &+ e^{-is/\varepsilon^2}(F_{-3}^n(x,s) + sF_{-4}^n(x,s) + p_1(s)F_5^n(x,s)) \\ &+ e^{is/\varepsilon^2}(F_3^n(x,s) + sF_4^n(x,s) + p_{-1}(s)F_{-5}^n(x,s)) + O(s^2), \end{aligned} \tag{3.2.15}$$

where $F_k^n(x,s) := F_k(\psi(t_n), \partial_t\psi(t_n); x, s), k = -5, -4, \cdots, 4, 5$ are given as the following:

$$\begin{aligned} &F_0^n(x,s) = (e^{-i\beta^- s}h_1^n)(e^{i\beta^- s}\overline{h_1^n}) + (e^{i\beta^- s}h_2^n)(e^{-i\beta^- s}\overline{h_2^n}), \\ &F_1^n(x,s) = 2\,\mathrm{Re}(-\overline{f^n}(e^{i\beta^- s}h_2^n)), \quad F_2^n(x,s) = \overline{f^n}(e^{-i\beta^- s}h_1^n), \\ &F_3^n(x,s) = (e^{-i\beta^- s}h_1^n)(e^{-i\beta^- s}\overline{h_2^n}), \quad F_4^n(x,s) = -\overline{f^n}(e^{-i\beta^- s}h_1^n), \\ &F_5^n(x,s) = \overline{f^n}(e^{i\beta^- s}h_2^n), \quad F_{-k}^n(x,s) = \overline{F_k^n(x,s)}. \end{aligned} \tag{3.2.16}$$

Terms in the summation with order no less than $O(s^2)$ are contained in the remainder.

Then the following expression for $|\psi^{n,1}(x,s)|^2\psi^{n,1}(x,s)$ is obtained:

$$\begin{aligned} &|\psi^{n,1}(x,s)|^2\psi^{n,1}(x,s) \\ &= g_0^n(x,s) + sg_1^n(x,s) + p_1(s)g_2^n(x,s) + p_{-1}(s)g_3^n(x,s) \\ &\quad + e^{-is/\varepsilon^2}(g_4^n(x,s) + sg_5^n(x,s) + p_1(s)g_6^n(x,s)) \\ &\quad + e^{is/\varepsilon^2}(g_7^n(x,s) + sg_8^n(x,s) + p_1(s)g_9^n(x,s) + p_{-1}(s)g_{10}^n(x,s)) \\ &\quad + e^{i2s/\varepsilon^2}(g_{11}^n(x,s) + sg_{12}^n(x,s) + p_{-1}(s)g_{13}^n(x,s)) + O(s^2), \end{aligned} \tag{3.2.17}$$

where $g_k^n(x,s) := g_k(\psi(t_n), \partial_t\psi(t_n); x, s), k = 0, 1, \cdots, 13$ are defined by:

$$
\begin{aligned}
g_0^n(x,s) &= F_{-3}^n(x,s)(e^{-i\beta^- s}h_1^n) + F_0^n(x,s)(e^{i\beta^- s}h_2^n),\\
g_1^n(x,s) &= F_{-4}^n(x,s)(e^{-i\beta^- s}h_1^n) + F_1^n(x,s)(e^{i\beta^- s}h_2^n) - F_0^n(x,s)f^n,\\
g_2^n(x,s) &= F_{-5}^n(x,s)(e^{-i\beta^- s}h_1^n) + F_2^n(x,s)(e^{i\beta^- s}h_2^n),\\
g_3^n(x,s) &= F_{-2}^n(x,s)(e^{i\beta^- s}h_2^n) + F_{-3}^n(x,s)f^n,\\
g_4^n(x,s) &= F_{-3}^n(x,s)(e^{i\beta^- s}h_2^n), \quad g_5^n(x,s) = F_{-4}^n(x,s)(e^{i\beta^- s}h_2^n) - F_{-3}^n(x,s)f^n,\\
g_6^n(x,s) &= F_{-5}^n(x,s)(e^{i\beta^- s}h_2^n),\\
g_7^n(x,s) &= F_0^n(x,s)(e^{-i\beta^- s}h_1^n) + F_3^n(x,s)(e^{i\beta^- s}h_2^n),\\
g_8^n(x,s) &= F_1^n(x,s)(e^{-i\beta^- s}h_1^n) + F_4^n(x,s)(e^{i\beta^- s}h_2^n) - F_3^n(x,s)f^n,\\
g_9^n(x,s) &= F_2^n(x,s)(e^{-i\beta^- s}h_1^n),\\
g_{10}^n(x,s) &= F_{-2}^n(x,s)(e^{-i\beta^- s}h_1^n) + F_5^n(x,s)(e^{i\beta^- s}h_2^n) + F_0^n(x,s)f^n,\\
g_{11}^n(x,s) &= F_3^n(x,s)(e^{-i\beta^- s}h_1^n),\\
g_{12}^n(x,s) &= F_4^n(x,s)(e^{-i\beta^- s}h_1^n),\\
g_{13}^n(x,s) &= F_5^n(x,s)(e^{-i\beta^- s}h_1^n) + F_3^n(x,s)f^n.
\end{aligned}
\tag{3.2.18}
$$

Terms in the summation with order no less than $O(s^2)$ are contained in the remainder.

Making use of the expansion (3.2.17), we can now compute $\psi^{n,2}(s)$ for $0 \le s \le \tau$ numerically:

$$
\begin{aligned}
\psi^{n,2}(x,s) :=& e^{i\frac{1}{\varepsilon^2}s}e^{-i\beta^- s}h_1^n + e^{i\beta^- s}h_2^n\\
&+ ie^{i\frac{1}{\varepsilon^2}s}\gamma\int_0^s e^{-i\frac{1}{\varepsilon^2}w}e^{-i\beta^-(s-w)}I_M(|\psi^{n,1}(x,s)|^2\psi^{n,1}(x,s))dw\\
&- i\gamma\int_0^s e^{i\beta^-(s-w)}I_M(|\psi^{n,1}(x,s)|^2\psi^{n,1}(x,s))dw + O(s^3).
\end{aligned}
\tag{3.2.19}
$$

Submitting (3.2.17) into (3.2.19), we can classify those numerical integrals in the nonlinear term into the following three types.

Type 1 Terms without ε-dependent rapid oscillation, for example

$$\int_0^s e^{i\beta^-(s-w)}I_M g_0^n(x,w)dw.$$

We adopt the midpoint rule to approximate the integral as

$$\int_0^s e^{i\beta^-(s-w)}I_M g_0^n(x,w)dw = e^{i\beta^- s/2}sI_M g_0^n(x,s/2) + O(s^3).$$

Type 2 Oscillatory terms (ε dependent) with $O(\tau)$ amplitudes. Take

$$\int_0^s e^{-i\frac{1}{\varepsilon^2}w} e^{-i\beta^-(s-w)} p_{-1}(s) I_M g_3^n(x,w)dw$$

as an example. By Taylor expansion

$$e^{-i\beta^-(s-w)} I_M g_3^n(x,w) = I_M g_3^n(x,0) + O(w),$$

and integrating the leading part accurately, we have

$$\begin{aligned}\int_0^s e^{-i\frac{1}{\varepsilon^2}w} e^{-i\beta^-(s-w)} p_{-1}(s) I_M g_3^n(x,w)dw =& \int_0^s e^{-i\frac{1}{\varepsilon^2}w} p_{-1}(s) I_M g_3^n(x,0)dw + O(s^3)\\ =& q_{-1,-1}(s) I_M g_3^n(x,0) + O(s^3),\end{aligned}$$

where the coefficients $q_{k,l}(s), k = 0, \pm 1, \pm 2, l = 0, \pm 1$ are defined as:

$$q_{k,l}(s) = \int_0^s \int_0^{s_1} e^{iks_1/\varepsilon^2} e^{ils_2/\varepsilon^2} ds_2 ds_1 = O(\tau^2), \quad 0 \le s \le \tau. \tag{3.2.20}$$

Type 3 Oscillatory terms (ε dependent) with $O(1)$ amplitudes, for example

$$\int_0^s e^{-i\frac{1}{\varepsilon^2}w} e^{-i\beta^-(s-w)} I_M g_0^n(x,w)dw.$$

By Taylor expansion $e^{i\beta^- w} I_M g_0^n(x,w) = I_M(g_0^n(x,0) + w(i\beta^- g_0^n(x,0) + \dot{g}_0^n(x,0))) + O(w^2)$. Integrate the leading terms accurately, we have

$$\begin{aligned}&\int_0^s e^{-i\frac{1}{\varepsilon^2}w} e^{-i\beta^-(s-w)} I_M g_0^n(x,w)dw\\ =& e^{-i\beta^- s} \int_0^s e^{-i\frac{1}{\varepsilon^2}w} I_M(g_0^n(x,0) + w(i\beta^- g_0^n(x,0) + \dot{g}_0^n(x,0)))dw + O(s^3)\\ =& e^{-i\beta^- s} \int_0^s e^{-i\frac{1}{\varepsilon^2}w} I_M(g_0^n(x,0)\\ &+ p_0(w)(i\beta^- g_0^n(x,0) + \dot{g}_0^n(x,0)))dw + O(s^3)\\ =& e^{-i\beta^- s}(p_{-1}(s) I_M g_0^n(x,0)\\ &+ q_{-1,0}(s)(i\beta^- I_M g_0^n(x,0) + I_M \dot{g}_0^n(x,0))) + O(s^3),\end{aligned}$$

$\dot{g}_k^n(x,s)$ is obtained by taking the time derivative of $g_k^n(x,s)$ in (3.2.18). For all the type 3 terms we only need $\dot{g}_0^n(x,0)$, $\dot{g}_4^n(x,0)$, $\dot{g}_7^n(x,0)$, $\dot{g}_{11}^n(x,0)$, and the detailed expressions are listed below:

$$\begin{aligned}\dot{g}_0^n(x,0) &= \dot{F}_{-3}^n(x,0)h_1^n - iF_{-3}^n(x,0)(\beta^- h_1^n) + \dot{F}_0^n(x,0)h_2^n + iF_0^n(x,0)(\beta^- h_2^n),\\ \dot{g}_4^n(x,0) &= \dot{F}_{-3}^n(x,0)h_2^n + iF_{-3}^n(x,0)(\beta^- h_2^n),\\ \dot{g}_7^n(x,0) &= \dot{F}_0^n(x,0)h_1^n - iF_0^n(x,0)(\beta^- h_1^n) + \dot{F}_3^n(x,0)h_2^n + iF_3^n(x,0)(\beta^- h_2^n),\\ \dot{g}_{11}^n(x,0) &= \dot{F}_3^n(x,0)h_1^n - iF_3^n(x,0)(\beta^- h_1^n),\end{aligned} \tag{3.2.21}$$

where

$$\begin{aligned}\dot{F}_0^n(x,0) &= -i(\beta^- h_1^n)\overline{h_1^n} + ih_1^n(\beta^- \overline{h_1^n}) + i(\beta^- h_2^n)\overline{h_2^n} - ih_2^n(\beta^- \overline{h_2^n}),\\ \dot{F}_3^n(x,0) &= -i(\beta^- h_1^n)\overline{h_2^n} - ih_1^n(\beta^- \overline{h_2^n}),\\ \dot{F}_{-3}^n(x,0) &= \overline{\dot{F}_3^n(x,0)}.\end{aligned} \tag{3.2.22}$$

However the operator β^- before $g_k^n(x,0)$ and in the expression of $\dot{g}_k^n(x,0)$ will lead to stability issues. Assume $\phi \in X_M$,

$$\begin{aligned}\|\beta^-\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}|\beta_l^-|^2(1+|\mu_l|^2)|\hat{\phi}_l|^2\\ &\lesssim \sum_{l=1}^{M-1}|\mu_l|^4(1+|\mu_l|^2)|\hat{\phi}_l|^2\\ &\leq \sum_{l=1}^{M-1}M^4(1+|\mu_l|^2)|\hat{\phi}_l|^2\\ &\leq M^4\|\phi\|_{H^1}^2,\end{aligned}$$

which means the H^1 norm of β^- restricted on X_M is dependent on M therefore h. It will lead to the possible CFL type condition for stability. To avoid this, we replace operator β^- with the filtered operator $\sin(\beta^-\tau)/\tau$. After the replacement,

$$\begin{aligned}\left\|\frac{\sin(\beta^-\tau)}{\tau}\phi\right\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}|\sin(\beta_l^-\tau)/\tau|^2(1+\mu_l^2)|\hat{\phi}_l|^2\\ &\lesssim \sum_{l=1}^{M-1}\frac{1}{\tau^2}(1+\mu_l^2)|\hat{\phi}_l|^2\\ &\leq \frac{1}{\tau^2}\|\phi\|_{H^1}^2,\end{aligned}$$

the H^1 norm of the filter only depends on τ. The error introduced this way can be bounded when the regularity of ϕ is good enough, and will be discussed in detail in later section.

For type 3 integral, we conclude with the following approximation:

$$\begin{aligned}&\int_0^s e^{-i\frac{1}{\varepsilon^2}w}e^{-i\beta^-(s-w)}I_M g_0^n(x,w)dw\\&=e^{-i\beta^-s}(p_{-1}(s)I_M g_0^n(x,0)+q_{-1,0}(s)(i\frac{\sin(\beta^-\tau)}{\tau}I_M g_0^n(x,0)+I_M\dot{g}_0^{n,f}(x,0)))+O(s^3),\end{aligned}$$

where $\dot{g}_k^{n,f}(x,0) := \dot{g}_k^f(\psi(t_n),\partial_t\psi(t_n);x,0), k=0,4,7,11$ are defined as

$$\begin{aligned}\dot{g}_0^{n,f}(x,0)=&\dot{F}_{-3}^{n,f}(x,0)h_1^n-iF_{-3}^n(x,0)(\frac{\sin(\beta^-\tau)}{\tau}h_1^n)\\&+\dot{F}_0^{n,f}(x,0)h_2^n+iF_0^n(x,0)(\frac{\sin(\beta^-\tau)}{\tau}h_2^n),\\\dot{g}_4^{n,f}(x,0)=&\dot{F}_{-3}^{n,f}(x,0)h_2^n+iF_{-3}^n(x,0)(\frac{\sin(\beta^-\tau)}{\tau}h_2^n),\\\dot{g}_7^{n,f}(x,0)=&\dot{F}_0^{n,f}(x,0)h_1^n-iF_0^n(x,0)(\frac{\sin(\beta^-\tau)}{\tau}h_1^n)\\&+\dot{F}_3^{n,f}(x,0)h_2^n+iF_3^n(x,0)(\frac{\sin(\beta^-\tau)}{\tau}h_2^n),\\\dot{g}_{11}^{n,f}(x,0)=&\dot{F}_3^{n,f}(x,0)h_1^n-iF_3^n(x,0)(\frac{\sin(\beta^-\tau)}{\tau}h_1^n),\end{aligned}\tag{3.2.23}$$

and $\dot{F}_k^{n,f}(x,0) := \dot{F}_k^f(\psi(t_n),\partial_t\psi(t_n);x,0), k=0,4,7,11$ are defined as

$$\begin{aligned}\dot{F}_0^{n,f}(x,0)=&-i(\frac{\sin(\beta^-\tau)}{\tau}h_1^n)\overline{h_1^n}+ih_1^n(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_1^n})\\&+i(\frac{\sin(\beta^-\tau)}{\tau}h_2^n)\overline{h_2^n}-ih_2^n(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_2^n}),\\\dot{F}_3^{n,f}(x,0)=&-i(\frac{\sin(\beta^-\tau)}{\tau}h_1^n)\overline{h_2^n}-ih_1^n(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_2^n}),\\\dot{F}_{-3}^{n,f}(x,0)=&\overline{\dot{F}_3^{n,f}(x,0)}.\end{aligned}\tag{3.2.24}$$

With all the aforementioned approximations and replacements, we have the following expression for $\psi^{n,2}(s)$ for $0\le s\le\tau$:

$$\begin{aligned}\psi^{n,2}(x,s)=&e^{i\beta^+s}h_1^n+e^{i\beta^-s}h_2^n\\&+i\gamma(G_{+,0}^n(x,s)+e^{-i\beta^-s/2}G_{+,1}^n(x,s)+e^{-i\beta^-s}G_{+,2}^n(x,s)\\&+i\frac{\sin(\beta^-\tau)}{\tau}e^{-i\beta^-s}G_{+,3}^n(x,s)\\&+G_{-,0}^n(x,s)+e^{i\beta^-s/2}G_{-,1}^n(x,s)+e^{i\beta^-s}G_{-,2}^n(x,s)\\&+i\frac{\sin(\beta^-\tau)}{\tau}e^{i\beta^-s}G_{-,3}^n(x,s)),\end{aligned}\tag{3.2.25}$$

where the expression $G_{\pm,k}(x,s) := G^n_{\pm,k}(\psi(t_n), \partial_t\psi(t_n); x, s)$, $k = 0, 1, 2, 3$ are defined as the following:

$$
\begin{aligned}
G^n_{+,0}(s) =& e^{is/\varepsilon^2} I_M(q_{-1,0}(s)g^n_1(x,0) + q_{-1,1}(s)g^n_2(x,0) + q_{-1,-1}(s)g^n_3(x,0) \\
&+ q_{-2,0}(s)g^n_5(x,0) + q_{-2,1}(s)g^n_6(x,0) + q_{0,1}(s)g^n_9(x,0) \\
&+ q_{0,-1}(s)g^n_{10}(x,0) + q_{1,0}(s)g^n_{12}(x,0) + q_{1,1}(s)g^n_{13}(x,0)), \\
G^n_{+,1}(s) =& e^{is/\varepsilon^2} I_M(sg^n_7(x,s/2) + s^2/2g^n_8(x,s/2)), \\
G^n_{+,2}(s) =& e^{is/\varepsilon^2} I_M(p_{-1}(s)g^n_0(x,0) + q_{-1,0}(s)\dot{g}^{n,f}_0(x,0) + p_{-2}(s)g^n_4(x,0) \\
&+ q_{-2,0}(s)\dot{g}^{n,f}_4(x,0) + p_1(s)g^n_{11}(x,0) + q_{1,0}(s)\dot{g}^{n,f}_{11}(x,0)), \\
G^n_{+,3}(s) =& e^{is/\varepsilon^2} I_M(q_{-1,0}(s)g^n_0(x,0) + q_{-2,0}(s)g^n_4(x,0) + q_{1,0}(s)g^n_{11}(x,0)), \\
G^n_{-,0}(s) =& I_M(q_{0,1}(s)g^n_2(x,0) + q_{0,-1}(s)g^n_3(x,0) + q_{-1,0}(s)g^n_5(x,0) \\
&+ q_{-1,1}(s)g^n_6(x,0) + q_{-1,-1}(s)g^n_8(x,0) + q_{1,1}(s)g^n_9(x,0) \\
&+ q_{1,-1}(s)g^n_{10}(x,0) + q_{2,0}(s)g^n_{12}(x,0) + q_{2,-1}(s)g^n_{13}(x,0)), \\
G^n_{-,1}(s) =& I_M(sg^n_0(x,s/2) + s^2/2g^n_1(x,s/2)), \\
G^n_{-,2}(s) =& I_M(p_{-1}(s)g^n_4(x,0) + q_{-1,0}(s)\dot{g}^{n,f}_4(x,0) + p_1(s)g^n_7(x,0) \\
&+ q_{1,0}(s)\dot{g}^{n,f}_7(x,0) + p_2(s)g^n_{11}(x,0) + q_{2,0}(s)\dot{g}^{n,f}_{11}(x,0)), \\
G^n_{-,3}(s) =& - I_M(q_{-1,0}(s)g^n_4(x,0) + q_{1,0}(s)g^n_7(x,0) + q_{2,0}(s)g^n_{11}(x,0)).
\end{aligned}
\tag{3.2.26}
$$

Applying the same approximation procedure and filter replacements to (3.2.10), we have the expression for $\dot{\psi}^{n,2}(s)$:

$$
\begin{aligned}
\dot{\psi}^{n,2}(x,s) = & i(\frac{1}{\varepsilon^2} - \beta^-)e^{i\beta^+ s}h^n_1 + i\beta^- e^{i\beta^- s}h^n_2 \\
& - \gamma((\frac{1}{\varepsilon^2} - \beta^-)(G^n_{+,0}(x,s) + e^{-i\beta^- s/2}G^n_{+,1}(x,s) \\
& + e^{-i\beta^- s}G^n_{+,2}(x,s) + i\frac{\sin(\beta^-\tau)}{\tau}e^{-i\beta^- s}G^n_{+,3}(x,s)) \\
& + \beta^-(G^n_{-,0}(x,s) + e^{i\beta^- s/2}G^n_{-,1}(x,s) \\
& + e^{i\beta^- s}G^n_{-,2}(x,s) + i\frac{\sin(\beta^-\tau)}{\tau}e^{i\beta^- s}G^n_{-,3}(x,s))),
\end{aligned}
\tag{3.2.27}
$$

Setting $s = \tau$ in (3.2.25) and (3.2.27) with the filter applied, assuming accurate solution $(\psi(x,t), \partial_t\psi(x,t))$ at time $t = t_n$ is known, we can update numerical approximations

$(\psi^{n+1}(x), \dot{\psi}^{n+1}(x))$ of $(\psi(x,t), \partial_t\psi(x,t))$ at time $t = t_{n+1}$ by:

$$\begin{aligned}
\psi^{n+1}(x) &= e^{i\beta^+\tau}h_1^n + e^{i\beta^-\tau}h_2^n \\
&\quad + i\gamma(G_{+,0}^n(x,\tau) + e^{-i\beta^-\tau/2}G_{+,1}^n(x,\tau) \\
&\quad + e^{-i\beta^-\tau}G_{+,2}^n(x,\tau) + i\frac{\sin(\beta^-\tau)}{\tau}e^{-i\beta^-\tau}G_{+,3}^n(x,\tau) \\
&\quad + G_{-,0}^n(x,\tau) + e^{i\beta^-\tau/2}G_{-,1}^n(x,\tau) + e^{i\beta^-\tau}G_{-,2}^n(x,\tau) \\
&\quad + i\frac{\sin(\beta^-\tau)}{\tau}e^{i\beta^-\tau}G_{-,3}^n(x,\tau)), \\
\dot{\psi}^{n+1}(x) &= i(\frac{1}{\varepsilon^2} - \beta^-)e^{i\beta^+\tau}h_1^n + i\beta^- e^{i\beta^-\tau}h_2^n \\
&\quad - \gamma((\frac{1}{\varepsilon^2} - \beta^-)(G_{+,0}^n(x,\tau) + e^{-i\beta^-\tau/2}G_{+,1}^n(x,\tau) \\
&\quad + e^{-i\beta^-\tau}G_{+,2}^n(x,\tau) + i\frac{\sin(\beta^-\tau)}{\tau}e^{-i\beta^-\tau}G_{+,3}^n(x,\tau)) \\
&\quad + \beta^-(G_{-,0}^n(x,\tau) + e^{i\beta^-\tau/2}G_{-,1}^n(x,\tau) \\
&\quad + e^{i\beta^-\tau}G_{-,2}^n(x,\tau) + i\frac{\sin(\beta^-\tau)}{\tau}e^{i\beta^-\tau}G_{-,3}^n(x,\tau))),
\end{aligned}$$

In the above expression (3.2.28), if $\psi(x,t_n) \in X_M$ and $\partial_t\psi(x,t_n) \in X_M$, then $\psi^{n+1}(x) \in X_M$ and $\dot{\psi}^{n+1}(x) \in X_M$. We denote this scheme by $S : X_M \times X_M \to X_M$

and $\dot{S}: X_M \times X_M \to X_M$, and for any $(\psi^0, \dot{\psi}^0) \in X_M \times X_M$,

$$
\begin{aligned}
S(\psi^0, \dot{\psi}^0; x) = {} & e^{i\beta^+\tau} h_1(\psi^0, \dot{\psi}^0; x) + e^{i\beta^-\tau} h_2(\psi^0, \dot{\psi}^0; x) \\
& + i\gamma(G_{+,0}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + e^{-i\beta^-\tau/2} G_{+,1}(\psi^0, \dot{\psi}^0; x, \tau) + e^{-i\beta^-\tau} G_{+,2}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + i\frac{\sin(\beta^-\tau)}{\tau} e^{-i\beta^-\tau} G_{+,3}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + G_{-,0}(\psi^0, \dot{\psi}^0; x, \tau) + e^{i\beta^-\tau/2} G_{-,1}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + e^{i\beta^-\tau} G_{-,2}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + i\frac{\sin(\beta^-\tau)}{\tau} e^{i\beta^-\tau} G_{-,3}(\psi^0, \dot{\psi}^0; x, \tau)), \\
\dot{S}(\psi^0, \dot{\psi}^0; x) = {} & i(\frac{1}{\varepsilon^2} - \beta^-) e^{i\beta^+\tau} h_1(\psi^0, \dot{\psi}^0; x) + i\beta^- e^{i\beta^-\tau} h_2(\psi^0, \dot{\psi}^0; x) \\
& - \gamma((\frac{1}{\varepsilon^2} - \beta^-)(G_{+,0}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + e^{-i\beta^-\tau/2} G_{+,1}(\psi^0, \dot{\psi}^0; x, \tau) + e^{-i\beta^-\tau} G_{+,2}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + i\frac{\sin(\beta^-\tau)}{\tau} e^{-i\beta^-\tau} G_{+,3}(\psi^0, \dot{\psi}^0; x, \tau)) \\
& + \beta^-(G_{-,0}(\psi^0, \dot{\psi}^0; x, \tau) + e^{i\beta^-\tau/2} G_{-,1}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + e^{i\beta^-\tau} G_{-,2}(\psi^0, \dot{\psi}^0; x, \tau) \\
& + i\frac{\sin(\beta^-\tau)}{\tau} e^{i\beta^-\tau} G_{-,3}(\psi^0, \dot{\psi}^0; x, \tau))).
\end{aligned}
\tag{3.2.28}
$$

3.2.3 Spatial discretization by a sine pseudospectral method

Here we present the sine pseudospectral implementation of the proposed second order NPI scheme. Let $\psi_j^n \in Y_M$ be the approximation of $\psi(x_j, t_n)$, and let $\dot{\psi}_j^n \in Y_M$ be the approximation of $\partial_t \psi(x_j, t_n)$. Choose $\psi_j^0 = \psi_0(x_j)$ and $\dot{\psi}_j^0 = \psi_1^\varepsilon(x_j)$.

Denote the interpolation $\psi_I^n(x) = I_M(\psi^n) \in X_M$ and $\dot{\psi}_I^n(x) = I_M(\dot{\psi}^n) \in X_M$. From t_n to t_{n+1}, given ψ^n and $\dot{\psi}^n$. The proposed second order NPI computes ψ^{n+1} and $\dot{\psi}^{n+1}$ by the following steps:

1. Compute $\psi_I^n(x_j)$ and $\dot{\psi}_I^n(x_j)$ by

$$
\psi_I^n(x_j) = \sum_{l=1}^{M-1} (\widetilde{\psi^n})_l \sin(\mu_l(x_j - a)), \quad \dot{\psi}_I^n(x_j) = \sum_{l=1}^{M-1} (\widetilde{\dot{\psi}^n})_l \sin(\mu_l(x_j - a)),
$$

where

$$(\widetilde{\psi^n})_l = \frac{2}{M}\sum_{j=1}^{M-1} \psi_j^n \sin(\mu_l(x_j - a)), \quad (\widetilde{\dot{\psi}^n})_l = \frac{2}{M}\sum_{j=1}^{M-1} \dot{\psi}_j^n \sin(\mu_l(x_j - a)).$$

2. Compute $\widehat{(h_1^{[n]})}_l$ and $\widehat{(h_2^{[n]})}_l$ by

$$\widehat{(h_1^{[n]})}_l = -\beta_l^{-1}(\beta_l^-(\widehat{\psi_I^n})_l + i(\widehat{\dot{\psi}_I^n})_l), \quad \widehat{(h_2^{[n]})}_l = \beta_l^{-1}(\beta_l^+(\widehat{\psi_I^n})_l + i(\widehat{\dot{\psi}_I^n})_l),$$

where

$$(\widehat{\psi_I^n})_l = (\widetilde{\psi_I^n})_l = \frac{2}{M}\sum_{l=1}^{M-1} \psi_I^n(x_j) \sin(\mu_l(x_j - a)),$$
$$(\widehat{\dot{\psi}_I^n})_l = (\widetilde{\dot{\psi}_I^n})_l = \frac{2}{M}\sum_{l=1}^{M-1} \dot{\psi}_I^n(x_j) \sin(\mu_l(x_j - a)).$$

3. Compute $(h_1^{[n]})_j$, $(h_2^{[n]})_j$, $(e^{-i\beta^-\tau/2}h_1^{[n]})_j$, $(e^{i\beta^-\tau/2}h_2^{[n]})_j$, $(\frac{\sin(\beta^-\tau)}{\tau}h_1^{[n]})_j$ and $(\frac{\sin(\beta^-\tau)}{\tau} h_2^{[n]})_j$ by $\widehat{(h_1^{[n]})}_l$ and $\widehat{(h_2^{[n]})}_l$. For simplicity here we only write formula for $(e^{-i\beta^-\tau/2}h_1^{[n]})_j$, others can be similarly computed.

$$(e^{-i\beta^-\tau/2}h_1^{[n]})_j = \sum_{l=1}^{M-1} e^{-i\beta_l^-\tau/2}\widehat{(h_1^{[n]})}_l \sin(\mu_l(x_j - a)).$$

4. Compute $f_j^{[n]}$ by

$$\widetilde{(f^{[n]})}_l = \frac{2}{M}\sum_{l=1}^{M-1} |\psi_I^n(x_j)|^2\psi_I^n(x_j) \sin(\mu_l(x_j - a)), \quad f_j^{[n]} = \sum_{l=1}^{M-1} \widetilde{(f^{[n]})}_l \sin(\mu_l(x_j - a)).$$

5. Compute $(F_k^{[n]}(0))_j$ for all $k = -5, -4, \cdots, 4, 5$, $(F_k^{[n]}(\tau/2))_j$ for $k = 0, \pm1, \pm3, \pm4$ by formula (3.2.16), for example

$$(F_0^{[n]}(0))_j = (h_1^{[n]})_j\overline{(h_1^{[n]})_j} + (h_2^{[n]})_j\overline{(h_2^{[n]})_j}.$$

And compute $(\dot{F}_k^{[n],f}(0))_j$ for $k = 0, \pm3$ by formula (3.2.24).

6. Compute $(g_k^{[n]}(0))_j$ for $k = 0, 1, \cdots, 13$, $(g_k^{[n]}(\tau/2))_j$ for $k = 0, 1, 2, 3, 7, 8, 9, 10$ by formula (3.2.18), and compute $(\dot{g}_k^{[n],f}(0))_j$ for $k = 0, 4, 7, 11$ by formula (3.2.23).

Then compute $\widetilde{(g_k^{[n]}(0))}_l$ for $k = 0, 1, \cdots, 13$, $\widetilde{(g_k^{[n]}(\tau/2))}_l$ for $k = 0, 1, 2, 3, 7, 8, 9, 10$, $\widetilde{(\dot{g}_k^{[n],f}(0))}_l$ for $k = 0, 4, 7, 11$, for example

$$\widetilde{(g_0^{[n]}(0))}_l = \frac{2}{M}\sum_{l=1}^{M-1} (g_0^{[n]}(0))_j \sin(\mu_l(x_j - a)).$$

7. Compute $(\widetilde{G^{[n]}_{+,k}(\tau)})_l$ and $(\widetilde{G^{[n]}_{-,k}(\tau)})_l$, $k = 0,1,2,3$ by formula (3.2.26). For example,

$$(\widetilde{G^{[n]}_{+,1}(\tau)})_l = e^{i\tau/\varepsilon^2}(s(\widetilde{g^{[n]}_7(\tau/2)})_l + s^2/2(\widetilde{g^{[n]}_8(\tau/2)})_l).$$

8. Compute $(\widetilde{\psi^{n+1}})_l$ and $(\widetilde{\dot\psi^{n+1}})_l$ by

$$\begin{aligned}
(\widetilde{\psi^{n+1}})_l = {} & e^{i\beta_l^+\tau}(\widehat{h^{[n]}_1})_l + e^{i\beta_l^-\tau}(\widehat{h^{[n]}_2})_l \\
& + i\gamma_l((\widetilde{G^{[n]}_{+,0}(\tau)})_l + e^{-i\beta_l^-\tau/2}(\widetilde{G^{[n]}_{+,1}(\tau)})_l + e^{-i\beta_l^-\tau}(\widetilde{G^{[n]}_{+,2}(\tau)})_l \\
& + i\frac{\sin(\beta_l^-\tau)}{\tau}e^{-i\beta_l^-\tau}(\widetilde{G^{[n]}_{+,3}(\tau)})_l \\
& + (\widetilde{G^{[n]}_{-,0}(\tau)})_l + e^{i\beta_l^-\tau/2}(\widetilde{G^{[n]}_{-,1}(\tau)})_l + e^{i\beta_l^-\tau}(\widetilde{G^{[n]}_{-,2}(\tau)})_l \\
& + i\frac{\sin(\beta_l^-\tau)}{\tau}e^{i\beta_l^-\tau}(\widetilde{G^{[n]}_{-,3}(\tau)})_l), \\
(\widetilde{\dot\psi^{n+1}})_l = {} & i(\frac{1}{\varepsilon^2} - \beta_l^-)e^{i\beta_l^+\tau}(\widehat{h^{[n]}_1})_l + i\beta_l^- e^{i\beta_l^-\tau}(\widehat{h^{[n]}_2})_l \\
& - \gamma_l((\frac{1}{\varepsilon^2} - \beta_l^-)((\widetilde{G^{[n]}_{+,0}(\tau)})_l + e^{-i\beta_l^-\tau/2}(\widetilde{G^{[n]}_{+,1}(\tau)})_l + e^{-i\beta_l^-\tau}(\widetilde{G^{[n]}_{+,2}(\tau)})_l \\
& + i\frac{\sin(\beta_l^-\tau)}{\tau}e^{-i\beta_l^-\tau}(\widetilde{G^{[n]}_{+,3}(\tau)})_l) \\
& + \beta_l^-((\widetilde{G^{[n]}_{-,0}(\tau)})_l + e^{i\beta_l^-\tau/2}(\widetilde{G^{[n]}_{-,1}(\tau)})_l + e^{i\beta_l^-\tau}(\widetilde{G^{[n]}_{-,2}(\tau)})_l \\
& + i\frac{\sin(\beta_l^-\tau)}{\tau}e^{i\beta_l^-\tau}(\widetilde{G^{[n]}_{-,3}(\tau)})_l)).
\end{aligned} \tag{3.2.29}$$

Finally compute ψ_j^{n+1} and $\dot\psi_j^{n+1}$ by

$$\psi_j^{n+1} = \sum_{l=1}^{M-1}(\widetilde{\psi^{n+1}})_l\sin(\mu_l(x_j-a)), \quad \dot\psi_j^{n+1} = \sum_{l=1}^{M-1}(\widetilde{\dot\psi^{n+1}})_l\sin(\mu_l(x_j-a)).$$

The NPI-SP scheme (3.2.29) is explicit, and can be solved efficiently by fast sine transform. The memory cost is $O(M)$, and for each step the computational cost is $O(M\log M)$.

Remark By the expression (3.2.28) and (3.2.29) we can directly verify that $\psi_j^{n+1} = S(\psi_I^n, \dot\psi_I^n; x_j)$ and $\psi_j^{n+1} = S(\psi_I^n, \dot\psi_I^n; x_j)$. Because $S(\psi_I^n, \dot\psi_I^n) \in X_M$, $\dot S(\psi_I^n, \dot\psi_I^n) \in X_M$, and I_M is the identity on X_M, we get

$$\psi_I^{n+1}(x) = I_M(\psi^{n+1})(x) = I_M S(\psi_I^n, \dot{\psi}_I^n)(x) = S(\psi_I^n, \dot{\psi}_I^n)(x),$$
$$\dot{\psi}_I^{n+1}(x) = I_M(\dot{\psi}^{n+1})(x) = I_M \dot{S}(\psi_I^n, \dot{\psi}_I^n)(x) = \dot{S}(\psi_I^n, \dot{\psi}_I^n)(x),$$

which means $\psi_j^{n+1} = \psi_I^{n+1}(x_j)$ and $\dot{\psi}_j^{n+1} = \dot{\psi}_I^{n+1}(x_j)$. Therefore for $n \geq 1$, the step 1 in NPI-SP can be skipped.

3.3 Uniform and optimal error estimates

3.3.1 Main Results

Before stating our main results first we introduce some Sobolev space. For $\phi(x) \in H^m(\Omega) \cap H_0^1(\Omega)$, it can be represented as a sine series

$$\phi(x) = \sum_{l=1}^{\infty} \hat{\phi}_l \sin(\mu_l(x-a)), \quad \hat{\phi}_l = \frac{2}{b-a}\int_a^b \psi(x)\sin(\mu_l(x-a))dx.$$

Define the subspace $H_s^m(\Omega) \subset H^m(\Omega) \cap H_0^1(\Omega)$ by $H_s^m(\Omega) = \{\phi \in H^m(\Omega) | \partial_x^{2k}\phi(a) = \partial_x^{2k}\phi(b) = 0, 0 \leq 2k < m\}$. In the following section we will omit Ω when there is no confusion.

Based on the theoretical results [18, 73], we make the following assumptions on the initial data and exact solution to (3.1.2) with (3.1.3). We assume that there exists $T > 0$, such that for $\varepsilon \in (0, 1]$, the solution $\psi(x, t)$ to (3.1.2) exists and

$$\|\psi\|_{L^\infty([0,T];L^\infty \cap H_s^m)} + \|\partial_t \psi\|_{L^\infty([0,T];L^\infty \cap H^{m-1})} \lesssim 1, \quad m \geq 5, \tag{3.3.1}$$

where we denote

$$M_1 = \max\Bigg\{ \sup_{\varepsilon \in (0,1]} \sup_{t \in [0,T]} \|\psi(\cdot, t)\|_{L^\infty} + \varepsilon^2 \sup_{\varepsilon \in (0,1]} \sup_{t \in [0,T]} \|\partial_t \psi(\cdot, t)\|_{L^\infty},$$
$$\sup_{\varepsilon \in (0,1]} \sup_{t \in [0,T]} \|\psi(\cdot, t)\|_{H^1} + \varepsilon^2 \sup_{\varepsilon \in (0,1]} \sup_{t \in [0,T]} \|\partial_t \psi(\cdot, t)\|_{H^1} \Bigg\}.$$

And the initial data satisfies the assumption

$$\begin{aligned} &1 \lesssim \|\omega^\varepsilon(x)\|_{H_s^m} \lesssim 1, \\ &\|\psi_0(x)\|_{H_s^{m+2}} \lesssim 1. \end{aligned} \tag{3.3.2}$$

With assumption (3.3.1) and (3.3.2) it can be shown that $\psi \in L^\infty([0,T]; H_s^m)$.

We can then prove the following error estimates for our NPI:

Theorem 3.1. *Let $\psi^n \in Y_M$ and $\dot{\psi}^n \in Y_M$ be the numerical approximation of $\psi(x,t_n)$ and $\partial_t\psi(x,t_n)$ from NPI-SP (3.2.29). $\psi_I^n := I_M(\psi^n) \in X_M$ and $\dot{\psi}_I^n := I_M(\dot{\psi}^n) \in X_M$ are their interpolation. Under the above assumption (3.3.1) and (3.3.2), $\exists h_0, \tau_0 > 0$, such that $\forall 0 < h < h_0, 0 < \tau < \tau_0$,*

$$\begin{aligned}
&\|\psi(x,t_n) - \psi_I^n(x)\|_{H^1(\Omega)} + \varepsilon^2\|\partial_t\psi(x,t_n) - \dot{\psi}_I^n(x)\|_{H^1(\Omega)} \lesssim h^{m-2} + \tau^2, \\
&\|\psi^n\|_{l^\infty} + \varepsilon^2\|\dot{\psi}^n\|_{l^\infty} \le M_1 + 1, \quad 0 \le n \le \frac{T}{\tau}.
\end{aligned}$$

3.3.2 Proof for the NPI-SP

Before the prof we first introduce some lemmas for the projection operator P_M and interpolation operator I_M.

Lemma 3.1 (L^2 projection)**.** *Let $\phi(x) \in H_s^m(\Omega)$, $m \ge 2$, then*

$$\|\phi(x) - P_M(\phi)(x)\|_{L^2} \lesssim h^m, \quad |\phi(x) - P_M(\phi)(x)|_{H^1} \lesssim h^{m-1}. \tag{3.3.3}$$

For the sine interpolation I_M we have a similar result.

Lemma 3.2 (sine interpolation)**.** *Let $\phi(x) \in H_1^0(\Omega)$, then*

$$\|I_M(\phi)(x)\|_{L^2} \le \|\phi(x)\|_{L^2} + h\|\nabla\phi(x)\|_{L^2}. \tag{3.3.4}$$

The proof can be found in [6, 94]. Combining those two lemmas we find that for any $\phi \in H_0^1$,

$$\begin{aligned}
\|I_M(\phi) - P_M(\phi)\|_{L^2} &= \|I_M(\phi - P_M(\phi))\|_{L^2} \\
&\lesssim \|\phi - P_M(\phi)\|_{L^2} + h\|\nabla(\phi - P_M(\phi))\|_{L^2},
\end{aligned}$$

and if $\phi \in H_s^m (m \ge 2)$, $\|I_M(\phi) - P_M(\phi)\|_{L^2} \lesssim h^m$.

Another lemma will be used when estimate interpolation in X_M.

Lemma 3.3. *Let $\phi(x) \in X_M$, then*

$$\|\nabla \phi\|_{L^2} \le M\|\phi\|_{L^2} \lesssim h^{-1}\|\phi\|_{L^2}. \tag{3.3.5}$$

It can be directly proved as $\phi(x) \in X_M$,

$$\|\nabla \phi\|_{L^2}^2 = \frac{b-a}{2}\sum_{l=1}^{M-1}|\mu_l|^2|\widehat{\phi}_l|^2 \le \frac{b-a}{2}M^2\sum_{l=1}^{M-1}|\widehat{\phi}_l|^2 \le M^2\|\phi\|_{L^2}^2.$$

Local truncation error estimates To prove the Theorem 3.1 we define the error function $e^n(x) := \psi(x,t_n) - \psi_I^n(x)$, $\dot{e}^n(x) := \partial_t\psi(x,t_n) - \dot{\psi}_I^n(x)$, then

$$\begin{aligned}\|e^{n+1}(x)\|_{H^1} &\le \|\psi(x,t_{n+1}) - P_M\psi(x,t_{n+1})\|_{H^1} + \|e_M^{n+1}(x)\|_{H^1},\\ \|\dot{e}^{n+1}(x)\|_{H^1} &\le \|\partial_t\psi(x,t_{n+1}) - P_M\partial_t\psi(x,t_{n+1})\|_{H^1} + \|\dot{e}_M^{n+1}(x)\|_{H^1},\end{aligned} \tag{3.3.6}$$

the error function after projection $e_M^{n+1}(x)$ and $\dot{e}_M^{n+1}(x)$ are

$$\begin{aligned}e_M^{n+1}(x) &:= P_M\psi(x,t_{n+1}) - \psi_I^{n+1}(x) = P_M\psi(x,t_{n+1}) - S(\psi_I^n(x), \dot{\psi}_I^n(x)),\\ \dot{e}_M^{n+1}(x) &:= P_M\partial_t\psi(x,t_{n+1}) - \dot{\psi}_I^{n+1}(x) = P_M\partial_t\psi(x,t_{n+1}) - \dot{S}(\psi_I^n(x), \dot{\psi}_I^n(x)).\end{aligned} \tag{3.3.7}$$

By Lemma 3.1,

$$\|\psi(x,t_{n+1}) - P_M\psi(x,t_{n+1})\|_{H^1} \lesssim h^{m-1}, \quad \|\partial_t\psi(x,t_{n+1}) - P_M\partial_t\psi(x,t_{n+1})\|_{H^1} \lesssim h^{m-1},$$

so we only need to estimate $\|e_M^{n+1}(x)\|_{H^1}$ and $\|\dot{e}_M^{n+1}(x)\|_{H^1}$.

Denote the local truncation error function $\xi^n(x)$ and $\dot{\xi}^n(x)$ by

$$\begin{aligned}\xi^n(x) &:= P_M\psi(x,t_{n+1}) - S(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)),\\ \dot{\xi}^n(x) &:= P_M\partial_t\psi(x,t_{n+1}) - \dot{S}(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)),\end{aligned} \tag{3.3.8}$$

then $e_M^{n+1}(x)$ and $\dot{e}_M^{n+1}(x)$ can be written as

$$\begin{aligned}e_M^{n+1}(x) &= \xi^n(x) + (S(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)) - S(\psi_I^n(x), \dot{\psi}_I^n(x))),\\ \dot{e}_M^{n+1}(x) &= \dot{\xi}^n(x) + (\dot{S}(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)) - \dot{S}(\psi_I^n(x), \dot{\psi}_I^n(x))).\end{aligned}$$

From the construction of the NPI scheme, we can derive the following estimates.

Lemma 3.4. *Under the assumption of Theorem 3.1, for* $\xi^n(x)$ *and* $\dot{\xi}^n(x)$ *defined in* (3.3.8),

$$\|\xi^n(x)\|_{H^1} \le C(\tau^3 + \tau h^{m-1}), \quad \varepsilon^2 \|\dot{\xi}^n(x)\|_{H^1} \le C(\tau^3 + \tau h^{m-2}),$$

where $S(\cdot,\cdot)$ *and* $\dot{S}(\cdot,\cdot)$ *are defined in* (3.2.28), C *is independent of* ε.

Proof. By the construction of the NPI, we define the following functions for $m = 0, 1$:

$$\begin{aligned}
\psi_M^{n,0}(x,s) :=& P_M\psi(x,t_n),\\
\psi_M^{n,m+1}(x,s) :=& e^{i\beta^+ s} h_1(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n); x)\\
&+ e^{i\beta^- s} h_2(P_M\psi(x,t_n), \partial_t P_M\psi(x,t_n); x)\\
&+ i\gamma \int_0^s \kappa(s-w) I_M(|\psi_M^{n,m}(x,w)|^2 \psi_M^{n,m}(x,w)) dw - R_{M,m+1}^n(x,s),\\
\dot{\psi}_M^{n,0}(x,s) :=& P_M\partial_t\psi(x,t_n),\\
\dot{\psi}_M^{n,m+1}(x,s) :=& i\beta^+ e^{i\beta^+ s} h_1(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n))\\
&+ i\beta^- e^{i\beta^- s} h_2(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)),\\
&+ i\gamma \int_0^s \dot{\kappa}(s-w) I_M(|\psi_M^{n,m}(x,w)|^2 \psi_M^{n,m}(x,w)) dw - \dot{R}_{M,m+1}^n(x,s),
\end{aligned}$$

and by the definition of S and $\dot{S}$ in (3.2.28), $S(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)) = \psi_M^{n,2}(x,s)$, $\dot{S}(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n)) = \dot{\psi}_M^{n,2}(x,s)$.

We first estimate $P_M\psi(x,t_n+s) - \psi_M^{n,1}(x,s)$. Notice if $\phi \in H_0^1$,

$$P_M\beta^-\phi(x) = P_M\Big(\sum_{l=1}^{\infty} \beta_l^- \widehat{\phi}_l \sin(\mu_l(x-a))\Big) = \sum_{l=1}^{M-1} \beta_l^- \widehat{\phi}_l \sin(\mu_l(x-a)) = \beta^- P_M\phi(x),$$

which means P_M commutes with β^-. Similaly P_M commutes with β^+, β, γ, $e^{i\beta^+ s}$ and

$e^{i\beta^- s}$. And because P_M is identity on X_M, by the variational form (3.2.2),

$$\begin{aligned}P_M\psi(x,t_n+s)=&P_M e^{i\beta^+ s}h_1(\psi(x,t_n),\partial_t\psi(x,t_n);x)\\&+P_M e^{i\beta^- s}h_2(\psi(x,t_n),\partial_t\psi(x,t_n);x)\\&+P_M i\gamma\int_0^s\kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)))dw,\\=&e^{i\beta^+ s}h_1(P_M\psi(x,t_n),P_M\partial_t\psi(x,t_n);x)\\&+e^{i\beta^- s}h_2(P_M\psi(x,t_n),P_M\partial_t\psi(x,t_n);x)\\&+i\gamma\int_0^s\kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w))dw.\end{aligned}$$

Therefore,

$$\begin{aligned}&P_M\psi(x,t_n+s)-\psi_M^{n,1}(x,s)\\&=i\gamma\int_0^s\kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)\\&\quad-|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw+R_{M,1}^n(x,s),\end{aligned}$$

and for $R_{M,1}^n(x,s)$,

$$\begin{aligned}R_{M,1}^n(x,s)=&\,i\gamma\int_0^s e^{i(s-w)/\varepsilon^2}(1-e^{-i\beta^-(s-w)})I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw\\&+i\gamma\int_0^s(1-e^{-i\beta^-(s-w)})I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw,\end{aligned}$$

where $R_{M,1}^n(x,s)$ is the error when evaluating (3.2.11).

Noticing function $|\psi|^2\psi$ is Lipschitz on bounded interval $[-(M_1+1),(M_1+1)]$ with some Lipschitz constant L, which means:

$$||a|^2a-|b|^2b|\leq L|a-b|,\quad -(M_1+1)\leq a,b\leq M_1+1.$$

For $\phi\in X_M$,

$$\begin{aligned}\|\beta^-\phi\|_{L^2}^2&=\frac{b-a}{2}\sum_{l=1}^{M-1}|\beta^-|^2|\widetilde{\phi}_l|^2\lesssim\frac{b-a}{2}\sum_{l=1}^{M-1}|\mu_l^2|^2|\widetilde{\phi}_l|^2\lesssim\|\phi\|_{H^1}^2,\\\|e^{i\beta^- s}\phi\|_{L^2}^2&=\frac{b-a}{2}\sum_{l=1}^{M-1}|e^{i\beta^- s}|^2|\widetilde{\phi}_l|^2=\frac{b-a}{2}\sum_{l=1}^{M-1}|\widetilde{\phi}_l|^2=\|\phi\|_{L^2}^2,\\\|\gamma\phi\|_{L^2}^2&=\frac{b-a}{2}\sum_{l=1}^{M-1}|\gamma_l|^2|\widetilde{\phi}_l|^2\leq\frac{b-a}{2}\sum_{l=1}^{M-1}|\widetilde{\phi}_l|^2=\|\phi\|_{L^2}^2,\end{aligned}\tag{3.3.9}$$

by (3.2.6), So

$$\begin{aligned}\|R^n_{M,1}(x,s)\|_{H^3} \leq& \|i\gamma\int_0^s e^{i(s-w)/\varepsilon^2}(1-e^{-i\beta^-(s-w)})I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw\|_{H^3}\\ &+\|i\gamma\int_0^s(1-e^{-i\beta^-(s-w)})I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw\|_{H^3}\\ \lesssim&\|\int_0^s(i\beta^-(s-w))I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw\|_{H^3}\\ \lesssim& s^2\|I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))\|_{H^4}.\end{aligned}$$

By Lemma 3.2 and 3.3, because $|P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\in X_{3M}$, by assumption (3.3.1),

$$\begin{aligned}&\|I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))\|_{H^4}\\ &\lesssim \||P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\|_{H^4}+h\|\nabla(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))\|_{H^4}\\ &\lesssim (1+3Mh)\||P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\|_{H^4}\lesssim \||P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\|_{H^4}\\ &\lesssim \|P_M\psi(x,t_n)\|^3_{H^3}\\ &\lesssim \|\psi(x,t_n)\|^3_{H^4}\\ &\lesssim 1.\end{aligned}$$

The last few inequalities hold because when $\varphi,\phi\in H^1$, $\|\varphi\phi\|_{H^1}\lesssim\|\varphi\|_{H^1}\|\phi\|_{H^1}$, and $\|P_M\varphi\|_{H^1}\leq\|\varphi\|_{H^1}$ by Parseval's identity.

For the other part, when $h\leq h_0$ is small enough, by Lemma 3.2,

$$\begin{aligned}&\|i\gamma\int_0^s\kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)-|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw\|_{H^3}\\ &\lesssim\int_0^s\|I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)-|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))\|_{H^3}dw\\ &\lesssim\int_0^s(\||\psi(x,t_n+w)|^2\psi(x,t_n+w)-|P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\|_{H^3}\\ &\quad+h\||\psi(x,t_n+w)|^2\psi(x,t_n+w)-|P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\|_{H^4})dw\\ &\lesssim\int_0^s L\|\psi(x,t_n+w)-P_M\psi(x,t_n)\|_{H^3}dw+h\int_0^s L\|\psi(x,t_n+w)-P_M\psi(x,t_n)\|_{H^4}dw\\ &\lesssim\int_0^s\|\psi(x,t_n+w)-\psi(x,t_n)\|_{H^3}dw+s\|\psi(x,t_n)-P_M\psi(x,t_n)\|_{H^3}\\ &\quad+h\int_0^s\|\psi(x,t_n+w)-\psi(x,t_n)\|_{H^4}dw+hs\|\psi(x,t_n)-P_M\psi(x,t_n)\|_{H^4}.\end{aligned}$$

By Lemma 3.1 and assumption (3.3.1), when $m \geq 5$,

$$\|\psi(x,t_n) - P_M\psi(x,t_n)\|_{H^4} \lesssim h^{m-4}, \quad \|\psi(x,t_n) - P_M\psi(x,t_n)\|_{H^3} \lesssim h^{m-3}.$$

By fundamental theorem of calculus,

$$\psi(x,t_n+w) - \psi(x,t_n) = \int_0^w \partial_t\psi(x,t_n+w_1)dw_1,$$

then by our assumption (3.3.1),

$$\begin{aligned}
&\|i\gamma\int_0^s \kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w) - |P_M\psi(x,t_n)|^2P_M\psi(x,t_n))dw\|_{H^3} \\
&\lesssim \int_0^s\int_0^w \|\partial_t\psi(x,t_n+w_1)\|_{H^3}dw_1dw + sh^{m-3} \\
&\quad + h\int_0^s\int_0^w \|\partial_t\psi(x,t_n+w_1)\|_{H^4}dw_1dw + sh^{m-3} \\
&\lesssim s^2\|\partial_t\psi\|_{L^\infty([0,T];H^3)} + s^2h\|\partial_t\psi\|_{L^\infty([0,T];H^4)} + sh^{m-3} \\
&\lesssim s^2 + sh^{m-3}.
\end{aligned}$$

Combine the above estiamtes, we know for $s \leq \tau \leq \tau_0$ sufficiently small

$$\|P_M\psi(x,t_n+s) - \psi_M^{n,1}(x,s)\|_{H^3} \lesssim s^2 + sh^{m-3},$$

therefore,

$$\begin{aligned}
&\|\psi(x,t_n+s) - \psi_M^{n,1}(x,s)\|_{H^3} \\
&\lesssim \|P_M\psi(x,t_n+s) - \psi_M^{n,1}(x,s)\|_{H^3} + \|\psi(x,t_n+s) - P_M\psi(x,t_n+s)\|_{H^3} \\
&\lesssim s^2 + (1+s)h^{m-4} \\
&\lesssim s^2 + h^{m-3}.
\end{aligned}$$

Similarly we can prove the estimates for H^1 and H^2 norm, i.e.

$$\begin{aligned}
&\|\psi(x,t_n+s) - \psi_M^{n,1}(x,s)\|_{H^1} \lesssim s^2 + h^{m-1}, \\
&\|\psi(x,t_n+s) - \psi_M^{n,1}(x,s)\|_{H^2} \lesssim s^2 + h^{m-2}, \qquad (3.3.10)\\
&\|\psi(x,t_n+s) - \psi_M^{n,1}(x,s)\|_{H^3} \lesssim s^2 + h^{m-3},
\end{aligned}$$

By discrete Sobolev inequality in 1D space,

$$
\begin{aligned}
&\|\psi(x,t_n+s)-\psi_M^{n,1}(x,s)\|_{l^\infty}^2\\
&\lesssim \|\psi(x,t_n+s)-\psi_M^{n,1}(x,s)\|_{L^2}\|\nabla\psi(x,t_n+s)-\nabla\psi_M^{n,1}(x,s)\|_{L^2}\\
&\lesssim \|\psi(x,t_n+s)-\psi_M^{n,1}(x,s)\|_{H^1}^2\\
&\lesssim s^4.
\end{aligned}
$$

if we denote for $\phi(x)\in L^\infty$, $\|\phi\|_{l^\infty}=\max_{i=0,1,\cdots,M}|\phi(x_i)|$. Thus, we know that there exists $\tau_0>0$ sufficiently small such that for $0<s\le\tau\le\tau_0$, $\|\psi_M^{n,1}(x,s)\|_{l^\infty}\le\|\psi(x,t_n+s)\|_{L^\infty}+1\le M+1$.

Continue with the second NPI approximation,

$$
\begin{aligned}
P_M\psi(x,t_n+s)-\psi_M^{n,2}(x,s)=&i\gamma\int_0^s\kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)\\
&-|\psi_M^{n,1}(x,w)|^2\psi_M^{n,1}(x,w))dw+R_{M,2}^n(x,s),
\end{aligned}
\tag{3.3.11}
$$

where $R_{M,2}^n(x,s)$ is the error for approximating the integrals in (3.2.19). By construction, we write $R_{M,2}^n(x,s)=D_{M,2}^n(x,s)+Q_{M,2}^n(x,s)$, where $D_{M,2}^n(x,s)$ is the error introduced by discarded term in formula (3.2.15) and (3.2.17), $Q_{M,2}^n(x,s)$ is the error introduced by numerical quadrature, then $\|R_{M,2}^n(x,s)\|_{H^1}\le\|D_{M,2}^n(x,s)\|_{H^1}+\|Q_{M,2}^n(x,s)\|_{H^1}$.

We estimate $R_{M,2}^n(x,s)$ first. For simplicity, denote

$$
\begin{aligned}
h_{M,1}^n&=h_1(P_M\psi(x,t_n),P_M\partial_t\psi(x,t_n);x),\\
h_{M,2}^n&=h_2(P_M\psi(x,t_n),P_M\partial_t\psi(x,t_n);x),\\
f_M^n&=i\gamma I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n);x).
\end{aligned}
$$

By Parseval's identity,

$$\begin{aligned}
\|\beta^{-1}\beta^{-}P_M\psi(x,t_n)\|_{H^4}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}|\frac{\beta^-}{\beta}|^2(1+|\mu_l|^2+|\mu_l|^4+|\mu_l|^6+|\mu_l|^8)|\widehat{\psi(t_n)}_l|^2\\
&\leq \frac{b-a}{2}\sum_{l=1}^{M-1}(1+|\mu_l|^2+|\mu_l|^4+|\mu_l|^6+|\mu_l|^8)|\widehat{\psi(t_n)}_l|^2\\
&= \|P_M\psi(x,t_n)\|_{H^4}^2\\
&\leq \|\psi(x,t_n)\|_{H^4}^2,\\
\|\beta^{-1}P_M\partial_t\psi(x,t_n)\|_{H^4}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}|\frac{1}{\beta}|^2(1+|\mu_l|^2+|\mu_l|^4+|\mu_l|^6+|\mu_l|^8)|\widehat{\partial_t\psi(t_n)}_l|^2\\
&\leq \frac{b-a}{2}\sum_{l=1}^{M-1}\varepsilon^4(1+|\mu_l|^2+|\mu_l|^4+|\mu_l|^6+|\mu_l|^8)|\widehat{\partial_t\psi(t_n)}_l|^2\\
&= \varepsilon^4\|P_M\partial_t\psi(x,t_n)\|_{H^4}^2\\
&\leq \varepsilon^4\|\partial_t\psi(x,t_n)\|_{H^4}^2,
\end{aligned}$$

so by (3.2.4) and our assumption (3.3.1),

$$\|h_{M,1}^n\|_{H^4} \leq \|\psi(x,t_n)\|_{H^4}+\varepsilon^2\|\partial_t\psi(x,t_n)\|_{H^4} \lesssim 1. \tag{3.3.12}$$

Similarly $\|h_{M,2}^n\|_{H^4} \lesssim 1$.

For f_M^n, with (3.3.9), Lemma 3.2 and Lemma 3.3, we have

$$\begin{aligned}
\|f_M^n\|_{H^4} =& \|i\gamma I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))\|_{H^4}\\
&\leq \|I_M(|P_M\psi(x,t_n)|^2P_M\psi(x,t_n))\|_{H^4}\\
&\leq (1+3Mh)\||P_M\psi(x,t_n)|^2P_M\psi(x,t_n)\|_{H^4}\\
&\leq (1+3Mh)\|P_M\psi(x,t_n)\|_{H^4}^3\\
&\leq (1+3Mh)\|\psi(x,t_n)\|_{H^4}^3\\
&\lesssim 1.
\end{aligned} \tag{3.3.13}$$

To estimate $D^n_{M,2}(x,s)$, we write

$$\begin{aligned} D^n_{M,2}(x,s) =& i\gamma\int_0^s \kappa(s-w)I_M\left(e^{iw/\varepsilon^2}(e^{-i\beta^- s}h^n_{M,1})p^2_{-1}(w)|f^n_M|^2\right)dw \\ &+ i\gamma\int_0^s \kappa(s-w)I_M\left(-e^{iw/\varepsilon^2}(e^{-i\beta^- s}h^n_{M,1})p_{-1}(w)w|f^n_M|^2\right)dw \\ &+ i\gamma\int_0^s \kappa(s-w)I_M\left(e^{iw/\varepsilon^2}p^2_{-1}(w)|f^n_M|^2(e^{i\beta^- s}h^n_{M,2})\right)dw \\ &+\cdots, \end{aligned}$$

where other similar terms are omitted for simplicity. Noticing $p_0(w) = w$, $D^n_2(x,s)$ includes every term containing integrated product of more than one $p_k(w), k = -1, 0, 1$. We estimate one of these terms, and the others can be proved similarly. By the estimates (3.3.9), there holds

$$\begin{aligned} &\|i\gamma\int_0^s \kappa(s-w)I_M\left(e^{iw/\varepsilon^2}(e^{-i\beta^- s}h^n_{M,1})p^2_{-1}(w)|f^n_M|^2\right)dw\|_{H^1} \\ &\lesssim \int_0^s w^2\|h^n_{M,1}|f^n_M|^2\|_{H^1}dw \lesssim \|h^n_{M,1}\|_{H^1}\|f^n_M\|^2_{H^1}\int_0^s w^2 dw \lesssim s^3, \end{aligned}$$

Then we can derive $\|D^n_2(x,s)\|_{L^2} \lesssim s^3$.

For simplicity, denote

$$\begin{aligned} g^n_{M,k}(x,w) &= g^n_k(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n); x, w), \quad m = 1,2,\cdots,13, \\ \dot{g}^{n,f}_{M,k}(x,w) &= \dot{g}^{n,f}_k(P_M\psi(x,t_n), P_M\partial_t\psi(x,t_n); x, w), \quad m = 0,4,7,11. \end{aligned}$$

To estimate $Q^n_{2,M}(x,s)$, we write

$$\begin{aligned}
Q^n_{2,M}(x,s) = &- i\gamma\Bigg(\int_0^s e^{i\beta^-(s-w)} I_M g^n_{M,0}(x,w)dw - e^{i\beta^- s/2} s I_M g^n_{M,0}(x,\frac{s}{2})\Bigg)\\
&+ \cdots (\text{error of other type 1 error terms})\\
&+ i\gamma e^{is/\varepsilon^2}\Bigg(\int_0^s e^{-iw/\varepsilon^2} e^{-i\beta^-(s-w)} p_{-1}(w) I_M g^n_{M,3}(x,w)dw\\
&- q_{-1,1}(s) I_M g^n_{M,3}(x,0)\Bigg)\\
&+ \cdots (\text{error of other type 2 error terms})\\
&+ i\gamma e^{is/\varepsilon^2}\Bigg(\int_0^s e^{-iw/\varepsilon^2} e^{-i\beta^-(s-w)} I_M g^n_{M,0}(x,w)dw\\
&- e^{-i\beta^- s}(p_{-1}(s) I_M g^n_{M,0}(x,0)\\
&+ q_{-1,0}(s)(i\frac{\sin(\beta^-\tau)}{\tau} I_M g^n_{M,0}(x,0) + I_M \dot{g}^{n,f}_{M,0}(x,0)))\Bigg)\\
&+ \cdots (\text{error of other type 3 error terms}),
\end{aligned}$$

where classification of type 1, 2, 3 terms are introduced for numerical quadrature to calculate expression (3.2.19). For simplicity, we prove the estimates for one of each type of terms, and the proof can be easily extended to the other terms.

First we prove the boundedness of $g^n_{M,k}(x,t)$, $\dot{g}^n_{M,k}(x,t) = \partial_t g^n_{M,k}(x,t)$ and $\ddot{g}^n_{M,k}(x,t) = \partial_{tt} g^n_{M,k}(x,t)$, $k = 0, 1, \cdots, 13$ for $\forall 0 \le t \le \tau$. Notice all $g^n_{M,k}(t)$ share a similar structure, here we take $g^n_{M,4}(x,t)$ as an example.

$$\begin{aligned}
g^n_{M,4}(x,t) &= (e^{i\beta^- t}\overline{h^n_{M,1}})(e^{i\beta^- t}h^n_{M,2})^2,\\
\dot{g}^n_{M,4}(x,t) &= (i\beta^- e^{i\beta^- t}\overline{h^n_{M,1}})(e^{i\beta^- t}h^n_{M,2})^2 + 2(e^{i\beta^- t}\overline{h^n_{M,1}})(i\beta^- e^{i\beta^- t}h^n_{M,2})(e^{i\beta^- t}h^n_{M,2}),\\
\ddot{g}^n_{M,4}(x,t) &= (-(\beta^-)^2 e^{i\beta^- t}\overline{h^n_{M,1}})(e^{i\beta^- t}h^n_{M,2})^2 + 4(i\beta^- e^{i\beta^- t}\overline{h^n_{M,1}})(i\beta^- e^{i\beta^- t}h^n_{M,2})(e^{i\beta^- t}h^n_{M,2})\\
&\quad + 2(e^{i\beta^- t}\overline{h^n_{M,1}})(-(\beta^-)^2 e^{i\beta^- t}h^n_{M,2})(e^{i\beta^- t}h^n_{M,2}) + 2(e^{i\beta^- t}\overline{h^n_{M,1}})(i\beta^- e^{i\beta^- t}h^n_{M,2})^2,
\end{aligned}$$

then by (3.3.9),

$$\begin{aligned}
&\|e^{i\beta^- t}\overline{h^n_{M,1}}\|_{H^4} \lesssim \|h^n_{M,1}\|_{H^4} \lesssim 1, \quad \|e^{i\beta^- t}h^n_{M,2}\|_{H^4} \lesssim \|h^n_{M,2}\|_{H^4} \lesssim 1,\\
&\|\beta^- e^{i\beta^- t}\overline{h^n_{M,1}}\|_{H^3} \lesssim \|h^n_{M,1}\|_{H^4} \lesssim 1, \quad \|\beta^- e^{i\beta^- t}h^n_{M,2}\|_{H^3} \lesssim \|h^n_{M,2}\|_{H^3} \lesssim 1,\\
&\|(\beta^-)^2 e^{i\beta^- t}\overline{h^n_{M,1}}\|_{H^2} \lesssim \|h^n_{M,1}\|_{H^4} \lesssim 1, \quad \|(\beta^-)^2 e^{i\beta^- t}h^n_{M,2}\|_{H^2} \lesssim \|h^n_{M,2}\|_{H^4} \lesssim 1,
\end{aligned}$$

thus

$$\|g^n_{M,4}(x,t)\|_{H^4} \lesssim 1,\ \|\dot{g}^n_{M,4}(x,t)\|_{H^3} \lesssim 1,\ \|\ddot{g}^n_{M,4}(x,t)\|_{H^2} \lesssim 1.$$

By this way we can prove that for $\forall 0 \le t \le \tau$,

$$\|g^n_{M,k}(x,t)\|_{H^4} \lesssim 1,\ \|\dot{g}^n_{M,k}(x,t)\|_{H^3} \lesssim 1,\ \|\ddot{g}^n_{M,k}(x,t)\|_{H^2} \lesssim 1, \forall k = 0, 1, \cdots 13,$$

and because $g^n_{M,k}(x,t), \dot{g}^n_{M,k}(x,t), \ddot{g}^n_{M,k}(x,t) \in X_{3M}$, by Lemma 3.2 and 3.3, for $\forall 0 \le t \le \tau$,

$$\|I_M g^n_{M,k}(x,t)\|_{H^4} \lesssim 1,\ \|I_M\dot{g}^n_{M,k}(x,t)\|_{H^3} \lesssim 1,\ \|I_M\ddot{g}^n_{M,k}(x,t)\|_{H^2} \lesssim 1, \forall k = 0, 1, \cdots 13,$$

Then we estimate $Q^n_{M,2}(x,s)$.

Type 1. We have

$$\begin{aligned}
&\|i\gamma\left(\int_0^s e^{i\beta^-(s-w)} I_M g^n_{M,0}(x,w)dw - e^{i\beta^- s/2} s I_M g^n_{M,0}(x,\frac{s}{2})\right)\|_{H^1} \\
&\lesssim \|i\gamma \int_0^s (w - s/2)\dot{\Theta}(x,s/2)dw\|_{H^1} + \|i\gamma \int_0^s \int_{s/2}^w \ddot{\Theta}(x,t)(w-t)dtdw\|_{H^1} \\
&\lesssim \| \int_0^s \int_{s/2}^w \ddot{\Theta}(x,t)(w-t)dtdw\|_{H^1},
\end{aligned}$$

where $\Theta(x,t) = e^{i\beta^-(s-t)} g^n_{M,0}(x,t)$. For derivatives, we get

$$\begin{aligned}
\dot{\Theta}(x,t) =& - i\beta^- e^{i\beta^-(s-t)} I_M g^n_{M,0}(x,t) + e^{i\beta^-(s-t)} I_M \dot{g}^n_{M,0}(x,t), \\
\ddot{\Theta}(x,t) =& - (\beta^-)^2 e^{i\beta^-(s-t)} I_M g^n_{M,0}(x,t) - 2i\beta^- e^{i\beta^-(s-t)} I_M \dot{g}^n_{M,0}(x,t) \\
&+ e^{i\beta^-(s-t)} I_M \ddot{g}^n_{M,0}(x,t),
\end{aligned}$$

therefore by (3.3.9)

$$\begin{aligned}
\|\ddot{\Theta}(x,t)\|_{H^1} &\lesssim \|I_M g^n_{M,0}(x,t)\|_{H^3} + \|I_M \dot{g}^n_{M,0}(x,t)\|_{H^2} + \|I_M \ddot{g}^n_{M,0}(x,t)\|_{H^1} \\
&\lesssim 1.
\end{aligned}$$

Thus,

$$\begin{aligned}
&\|i\gamma\left(\int_0^s e^{i\beta^-(s-w)} I_M g^n_{M,0}(x,w)dw - e^{i\beta^- s/2} s I_M g^n_{M,0}(x,\frac{s}{2})\right)\|_{H^1} \\
&\lesssim \int_0^s \int_{s/2}^w \|\ddot{\Theta}(x,t)\|_{H^1}(w-t)dtdw \\
&\lesssim s^3.
\end{aligned}$$

Type 2. In view of the H^2 boundedness of $I_M g^n_{M,3}(x,t)$ and H^1 boundedness of $I_M\dot{g}^n_{M,3}(x,t)$, we derive that

$$
\begin{aligned}
&\|i\gamma e^{is/\varepsilon^2}\left(\int_0^s e^{-iw/\varepsilon^2}e^{-i\beta^-(s-w)}p_{-1}(w)I_M g^n_{M,3}(x,w)dw - q_{-1,1}(s)I_M g^n_{M,3}(x,0)\right)\|_{H^1}\\
&\lesssim \int_0^s |e^{-\frac{i}{\varepsilon^2}w}p_{-1}(w)|\Bigg(\|(e^{-i\beta^-(s-w)}-1)I_M g^n_{M,3}(x,w)\|_{H^1}\\
&\quad + \|I_M g^n_{M,3}(x,w) - I_M g^n_{M,3}(x,0)\|_{H^1}\Bigg)dw\\
&\lesssim \int_0^s w\left(\int_0^{s-w}\|-i\beta^- e^{-i\beta^- t}I_M g^n_{M,3}(x,w)\|_{H^1}dt + \int_0^w \|I_M\dot{g}^n_{M,3}(x,t)\|_{H^1}dt\right)dw\\
&\lesssim \int_0^s w\left(\int_0^{s-w}\|I_M g^n_{M,3}(x,w)\|_{H^2}dt + \int_0^w \|I_M\dot{g}^n_{M,3}(x,t)\|_{H^1}dt\right)dw\\
&\lesssim \int_0^s ws\,dw\\
&\lesssim s^3.
\end{aligned}
$$

Type 3. We can obtain

$$
\begin{aligned}
&\|i\gamma e^{is/\varepsilon^2}\Bigg(\int_0^s e^{-iw/\varepsilon^2}e^{-i\beta^-(s-w)}I_M g^n_{M,0}(x,w)dw - e^{-i\beta^- s}(p_{-1}(s)I_M g^n_{M,0}(x,0)\\
&\quad + q_{-1,0}(s)(i\frac{\sin(\beta^-\tau)}{\tau}I_M g^n_{M,0}(x,0) + I_M\dot{g}^{n,f}_{M,0}(x,0)))\Bigg)\|_{H^1}\\
&\lesssim \int_0^s \|e^{i\beta^- w}I_M g^n_{M,0}(x,w)\\
&\quad - \left(I_M g^n_{M,0}(x,0) + w(i\beta^- I_M g^n_{M,0}(x,0) + I_M\dot{g}^n_{M,0}(x,0))\right)\|_{H^1}dw\\
&\quad + \int_0^s w\|(\frac{\sin(\beta^-\tau)}{\tau} - \beta)I_M g^n_{M,0}(x,0)\|_{H^1}dw + \int_0^s w\|I_M(\dot{g}^{n,f}_{M,0}(x,0) - \dot{g}^n_{M,0}(x,0))\|_{H^1}.
\end{aligned}
$$

For the first term, by Taylor expansion of $e^{i\beta^- w}I_M g^n_{M,0}(x,w)$ at $w=0$ and (3.3.9),

$$
\begin{aligned}
&\|e^{i\beta^- w}I_M g^n_{M,0}(x,w) - \left(I_M g^n_{M,0}(x,0) + w(i\beta^- I_M g^n_{M,0}(x,0) + I_M\dot{g}^n_{M,0}(x,0))\right)\|_{H^1}\\
&\lesssim \int_0^w (w-t)\|(-\beta^-)^2 e^{i\beta^- t}I_M g^n_{M,0}(x,t) + 2i\beta^- e^{i\beta^- t}I_M\dot{g}^n_{M,0}(x,t)\\
&\quad + e^{i\beta^- t}I_M\ddot{g}^n_{M,0}(x,t)\|_{H^1}dt\\
&\lesssim w\int_0^w \|I_M g^n_{M,0}(x,t)\|_{H^3} + \|I_M\dot{g}^n_{M,0}(x,t)\|_{H^2} + \|I_M\ddot{g}^n_{M,0}(x,t)\|_{H^1}\\
&\lesssim w^2.
\end{aligned}
$$

For the second term, assume $\phi \in X_M$,

$$
\begin{aligned}
\|(\beta^- - \frac{\sin(\beta^-\tau)}{\tau})\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}(\beta_l^- - \sin(\beta_l^-\tau)/\tau)^2(1+\mu_l^2)|\hat{\phi}_l|^2 \\
&\lesssim \sum_{l=1}^{M-1}(\beta_l^-\tau)^2(1+\mu_l^2)|\hat{\phi}_l|^2 \\
&\lesssim \sum_{l=1}^{M-1}\mu_l^4\tau^2(1+\mu_l^2)|\hat{\phi}_l|^2 \\
&\leq \tau\|\phi\|_{H^3}^2,
\end{aligned}
$$

therefore

$$
\|(\frac{\sin(\beta^-\tau)}{\tau} - \beta)I_M g_{M,0}^n(x,0)\|_{H^1} \lesssim \tau\|I_M g_{M,0}^n(x,0)\|_{H^3} \lesssim \tau.
$$

For the last term, by (3.2.21) and (3.2.23)

$$
\begin{aligned}
\dot{g}_{M,0}^{n,f}(x,0) - \dot{g}_{M,0}^n(x,0) =& i(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_{M,1}^n})h_{M,2}^n h_{M,1}^n - i(\beta^-\overline{h_{M,1}^n})h_{M,2}^n h_{M,1}^n \\
&+ i\overline{h_{M,1}^n}(\frac{\sin(\beta^-\tau)}{\tau}h_{M,2}^n)h_{M,1}^n - i\overline{h_{M,1}^n}(\beta^- h_{M,2}^n)h_{M,1}^n \\
&+ \ldots,
\end{aligned}
$$

here we omit other similar terms for simplicity.

$$
\begin{aligned}
&\|i(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_{M,1}^n})h_{M,2}^n h_{M,1}^n - i(\beta^-\overline{h_{M,1}^n})h_{M,2}^n h_{M,1}^n\|_{H^1} \\
&\lesssim \|(\frac{\sin(\beta^-\tau)}{\tau} - \beta^-)\overline{h_{M,1}^n}\|_{H^1}\|h_{M,2}^n\|_{H^1}\|h_{M,1}^n\|_{H^1} \\
&\leq \tau\|h_{M,1}^n\|_{H^3}\|h_{M,2}^n\|_{H^1}\|h_{M,1}^n\|_{H^1} \\
&\lesssim \tau.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\|i\gamma e^{is/\varepsilon^2}\Bigg(\int_0^s e^{-iw/\varepsilon^2}e^{-i\beta^-(s-w)}I_M g^n_{M,0}(x,w)dw \\
&\quad - e^{-i\beta^- s}(p_{-1}(s)I_M g^n_{M,0}(x,0)+q_{-1,0}(s)(i\frac{\sin(\beta^-\tau)}{\tau}I_M g^n_{M,0}(x,0)+I_M\dot{g}^{n,f}_{M,0}(x,0)))\Bigg)\|_{H^1} \\
&\lesssim \int_0^s w^2 dw + \int_0^s w\tau dw \\
&\lesssim s^3 + s^2\tau \\
&\lesssim \tau^3.
\end{aligned}
$$

Therefore, combing all the three types of H^1 estimates, we have $\|Q^n_{M,2}(x,s)\|_{H^1} \lesssim \tau^3, 0 \le s \le \tau$.

For the remaining part in (3.3.11), notice $\|\psi^{n,1}_M\|_{l^\infty} \le M_1 + 1$,

$$
\begin{aligned}
&\|i\gamma\int_0^s \kappa(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi^{n,1}_M(x,w)|^2\psi^{n,1}_M(x,w))dw\|_{H^1} \\
&\lesssim \int_0^s \|I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi^{n,1}_M(x,w)|^2\psi^{n,1}_M(x,w))\|_{H^1}dw \\
&\lesssim \int_0^s (\||\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi^{n,1}_M(x,w)|^2\psi^{n,1}_M(x,w)\|_{H^1} \\
&\quad + h\||\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi^{n,1}_M(x,w)|^2\psi^{n,1}_M(x,w)\|_{H^2})dw \\
&\lesssim \int_0^s L\|\psi(x,t_n+w)-\psi^{n,1}_M(x,w)\|_{H^1}dw + h\int_0^s L\|\psi(x,t_n+w)-\psi^{n,1}_M(x,w)\|_{H^2}dw \\
&\lesssim s^3 + sh^{m-1}.
\end{aligned}
$$

by the H^1 and H^2 estimates of $|\psi(x,t_n+w)-\psi^{n,1}_M(x,w)|$ (3.3.10). Therefore by (3.3.11) and definition of $\xi^n(x)$,

$$
\begin{aligned}
\|\xi^n(x)\|_{H^1} &= \|P_M\psi(x,t_n+\tau)-\psi^{n,2}_M(x,\tau)\| \\
&\lesssim \tau^3 + \tau h^{m-1} + \|R^n_{M,2}(x,\tau)\|_{H^1} \\
&\lesssim \tau^3 + \tau h^{m-1}.
\end{aligned}
$$

For the truncation error $\dot{\xi}^n(x)$, we have similar estimates. Given $\psi_M^{n,1}(x,s)$,

$$\begin{aligned} &P_M\partial_t\psi(x,t_n+s)-\dot{\psi}_M^{n,2}(x,s)\\ &=i\gamma\int_0^s\dot{\kappa}(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w) \\ &\quad-|\psi_M^{n,1}(x,w)|^2\psi_M^{n,1}(x,w))dw+\dot{R}_{M,2}^n(x,s), \end{aligned} \tag{3.3.14}$$

where the remainder function $\dot{R}_{M,2}^n(x,s)$ can be divided into two terms as $\dot{R}_{M,2}^n(x,s)=\dot{D}_{M,2}^n(x,s)+\dot{Q}_{M,2}^n(x,s)$. $\dot{D}_{M,2}^n(x,s)$ includes every discarded terms and $\dot{Q}_{M,2}^n(x,s)$ includes the quadrature error of the integral approximation.

We estimate the integral kernel $\dot{\kappa}(t)$ first. Assume $\phi(x)\in X_M$, then by (3.3.9),

$$\begin{aligned} \|\dot{\kappa}(t)\phi\|_{H^1}&=\|i(\varepsilon^{-2}-\beta^-)e^{i\beta^+t}\phi-i\beta^-e^{i\beta^-t}\phi\|_{H^1}\\ &\lesssim\varepsilon^{-2}\|e^{i\beta^+t}\phi\|_{H^1}+(\|\beta^-e^{i\beta^+t}\phi\|_{H^1}+\|\beta^-e^{i\beta^-t}\phi\|_{H^1})\\ &\lesssim\varepsilon^{-2}\|\phi\|_{H^2}. \end{aligned}$$

Then the first part in (3.3.14) can be estimated by

$$\begin{aligned} &\|i\gamma\int_0^s\dot{\kappa}(s-w)I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi_M^{n,1}(x,w)|^2\psi_M^{n,1}(x,w))dw\|_{H^1}\\ &\lesssim\varepsilon^{-2}\int_0^s\|I_M(|\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi_M^{n,1}(x,w)|^2\psi_M^{n,1}(x,w))\|_{H^2}dw\\ &\lesssim\varepsilon^{-2}\int_0^s(\||\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi_M^{n,1}(x,w)|^2\psi_M^{n,1}(x,w)\|_{H^2}\\ &\quad+h\||\psi(x,t_n+w)|^2\psi(x,t_n+w)-|\psi_M^{n,1}(x,w)|^2\psi_M^{n,1}(x,w)\|_{H^3})dw\\ &\lesssim\varepsilon^{-2}\int_0^sL\|\psi(x,t_n+w)-\psi_M^{n,1}(x,w)\|_{H^2}dw+h\int_0^sL\|\psi(x,t_n+w)-\psi_M^{n,1}(x,w)\|_{H^3}dw\\ &\lesssim\varepsilon^{-2}(s^3+sh^{m-2}). \end{aligned}$$

by the H^2 and H^3 estimates of $|\psi(x,t_n+w)-\psi_M^{n,1}(x,w)|$ (3.3.10).

It only remains to estimate $\dot{D}_{M,2}^n(x,s)$ and $\dot{Q}_{M,2}^n(x,s)$. We write $\dot{D}_{M,2}^n(x,s)$ as

$$\begin{aligned} D_{M,2}^n(x,s)=&i\gamma\int_0^s\dot{\kappa}(s-w)I_M\left(e^{iw/\varepsilon^2}(e^{-i\beta^-s}h_{M,1}^n)p_{-1}^2(w)|f_M^n|^2\right)dw\\ &+i\gamma\int_0^s\dot{\kappa}(s-w)I_M\left(-e^{iw/\varepsilon^2}(e^{-i\beta^-s}h_{M,1}^n)p_{-1}(w)w|f_M^n|^2\right)dw\\ &+i\gamma\int_0^s\dot{\kappa}(s-w)I_M\left(e^{iw/\varepsilon^2}p_{-1}^2(w)|f_M^n|^2(e^{i\beta^-s}h_{M,2}^n)\right)dw\\ &+\cdots, \end{aligned}$$

We estimate the first term, and other terms can be done analogously. By direct computation, we have

$$
\begin{aligned}
&\|i\gamma\int_0^s \dot{\kappa}(s-w)I_M\left(e^{iw/\varepsilon^2}(e^{-i\beta^- s}h^n_{M,1})p^2_{-1}(w)|f^n_M|^2\right)dw\|_{H^1}\\
&\lesssim \varepsilon^{-2}\int_0^s w^2\|h^n_{M,1}|f^n_M|^2\|_{H^2}dw\\
&\lesssim \varepsilon^{-2}\|h^n_{M,1}\|_{H^2}\|f^n_M\|^2_{H^2}\int_0^s w^2dw\\
&\lesssim \varepsilon^{-2}s^3,
\end{aligned}
$$

Thus, $\|\dot{D}^n_{M,2}(x,s)\|_{H^1}\lesssim\varepsilon^{-2}s^3$.

For $\dot{Q}^n_2(s)$, we know

$$
\begin{aligned}
\dot{Q}^n_2(x,s)=&-i\gamma\Bigg(\int_0^s i\beta^- e^{i\beta^-(s-w)}I_M g^n_{M,0}(x,w)dw-i\beta^- e^{i\beta^- s/2}sI_M g^n_{M,0}(x,\frac{s}{2})\Bigg)\\
&+\cdots(\text{error of other type 1 error terms})\\
&+i\gamma e^{is/\varepsilon^2}\Bigg(i\beta^+\int_0^s e^{-iw/\varepsilon^2}e^{-i\beta^-(s-w)}p_{-1}(w)I_M g^n_{M,3}(x,w)dw\\
&-i\beta^+q_{-1,1}(s)I_M g^n_{M,3}(x,0)\Bigg)\\
&+\cdots(\text{error of other type 2 error terms})\\
&+i\gamma e^{is/\varepsilon^2}\Bigg(i\beta^+\int_0^s e^{-iw/\varepsilon^2}e^{-i\beta^-(s-w)}I_M g^n_{M,0}(x,w)dw\\
&-i\beta^+e^{-i\beta^- s}(p_{-1}(s)I_M g^n_{M,0}(x,0)\\
&+q_{-1,0}(s)(i\frac{\sin(\beta^-\tau)}{\tau}I_M g^n_{M,0}(x,0)+I_M\dot{g}^{n,f}_{M,0}(x,0)))\Bigg)\\
&+\cdots(\text{error of other type 3 error terms}).
\end{aligned}
$$

As $\|\beta^+\phi\|_{H^1}\lesssim\varepsilon^{-2}\|\phi\|_{H^2}$ when $\phi\in X_M$, and

$$
\|I_M g^n_{M,k}(x,t)\|_{H^4}\lesssim 1,\ \|I_M\dot{g}^n_{M,k}(x,t)\|_{H^3}\lesssim 1,\ \|I_M\ddot{g}^n_{M,k}(x,t)\|_{H^2}\lesssim 1,\forall k=0,1,\cdots 13,
$$

it is easy to prove $\|\dot{Q}^n_{M,2}(x,s)\|_{H^1}\lesssim\varepsilon^{-2}\tau^3$ when $0\le s\le\tau$ by the same method for estimating $Q^n_{M,2}(x,s)$.

Therefore by (3.3.14) and definition of $\dot{\xi}^n(x)$,

$$\begin{aligned}\varepsilon^2\|\dot{\xi}^n(x)\|_{H^1} &= \varepsilon^2\|P_M\partial_t\psi(x,t_n+\tau)-\dot{\psi}_M^{n,2}(x,\tau)\| \\ &\lesssim \tau^3+\tau h^{m-2}+\varepsilon^2\|R_{M,2}^n(x,\tau)\|_{H^1} \\ &\lesssim \tau^3+\tau h^{m-2}.\end{aligned}$$

The proof of Lemma 3.4 is complete. □

Stability To prove the stability of our scheme, we divide the numerical propagator S into the linear part S_L and the nonlinear part S_{NL}:

$$\begin{aligned}\psi_I^{n+1} &= S(\psi_I^n,\dot{\psi}_I^n) = S_L(\psi_I^n,\dot{\psi}_I^n)+S_{NL}(\psi_I^n,\dot{\psi}_I^n), \\ \dot{\psi}_I^{n+1} &= \dot{S}(\psi_I^n,\dot{\psi}_I^n) = \dot{S}_L(\psi_I^n,\dot{\psi}_I^n)+\dot{S}_{NL}(\psi_I^n,\dot{\psi}_I^n),\end{aligned}$$

where

$$\begin{aligned}S_L(\psi_I^n,\dot{\psi}_I^n;x) :=& e^{i\beta^+\tau}h_1(\psi_I^n,\dot{\psi}_I^n;x)+e^{i\beta^-\tau}h_2(\psi_I^n,\dot{\psi}_I^n;x), \\ \dot{S}_L(\psi^n,\dot{\psi}^n;x) :=& i(\frac{1}{\varepsilon^2}-\beta^-)e^{i\beta^+\tau}h_1(\psi_I^n,\dot{\psi}_I^n;x)+i\beta^-e^{i\beta^-\tau}h_2(\psi_I^n,\dot{\psi}_I^n;x), \\ S_{NL}(\psi_I^n,\dot{\psi}_I^n;x) :=& i\gamma(G_{+,0}(\psi_I^n,\dot{\psi}_I^n;x,\tau)+e^{-i\beta^-\tau/2}G_{+,1}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+e^{-i\beta^-\tau}G_{+,2}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+i\frac{\sin(\beta^-\tau)}{\tau}e^{-i\beta^-\tau}G_{+,3}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+G_{-,0}(\psi_I^n,\dot{\psi}_I^n;x,\tau)+e^{i\beta^-\tau/2}G_{-,1}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+e^{i\beta^-\tau}G_{-,2}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+i\frac{\sin(\beta^-\tau)}{\tau}e^{i\beta^-\tau}G_{-,3}(\psi_I^n,\dot{\psi}_I^n;x,\tau)), \\ \dot{S}_{NL}(\psi_I^n,\dot{\psi}_I^n;x) :=& -\gamma((\frac{1}{\varepsilon^2}-\beta^-)(G_{+,0}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+e^{-i\beta^-\tau/2}G_{+,1}(\psi_I^n,\dot{\psi}_I^n;x,\tau)+e^{-i\beta^-\tau}G_{+,2}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+i\frac{\sin(\beta^-\tau)}{\tau}e^{-i\beta^-\tau}G_{+,3}(\psi_I^n,\dot{\psi}_I^n;x,\tau)) \\ &+\beta^-(G_{-,0}(\psi_I^n,\dot{\psi}_I^n;x,\tau)+e^{i\beta^-\tau/2}G_{-,1}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+e^{i\beta^-\tau}G_{-,2}(\psi_I^n,\dot{\psi}_I^n;x,\tau) \\ &+i\frac{\sin(\beta^-\tau)}{\tau}e^{i\beta^-\tau}G_{-,3}(\psi_I^n,\dot{\psi}_I^n;x,\tau))).\end{aligned} \tag{3.3.15}$$

The stability of the NPI (3.2.28) is characterized as follows.

Lemma 3.5. *Given* $(\psi^0, \dot{\psi}^0)$ *and* $(\psi^1, \dot{\psi}^1)$ *satisfying* $\psi^j, \dot{\psi}^j \in X_M$ $(j = 0, 1)$ *and* $\|\psi^j\|_{H^1} + \varepsilon^2\|\dot{\psi}^j\|_{H^1} \leq M_1 + 1$, *introducing operator* $\lambda = \sqrt{-(\beta^+\beta^-)^{-1}}$ *(*$\beta^\pm$ *given in* (3.2.3)*), we have*

$$\begin{bmatrix} S(\psi^0, \dot{\psi}^0) - S(\psi^1, \dot{\psi}^1) \\ \lambda\dot{S}(\psi^0, \dot{\psi}^0) - \lambda\dot{S}(\psi^1, \dot{\psi}^1) \end{bmatrix} = Q \begin{bmatrix} (\psi^0 - \psi^1) \\ \lambda(\dot{\psi}^0 - \dot{\psi}^1) \end{bmatrix} + \begin{bmatrix} \eta \\ \dot{\eta} \end{bmatrix},$$

where $\|\eta\|_{H^1} \leq C\tau(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot{\psi}^0 - \dot{\psi}^1\|_{H^1})$, $\|\dot{\eta}\|_{H^1} \leq C\frac{\tau}{\varepsilon}(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot{\psi}^0 - \dot{\psi}^1\|_{H^1})$ *and* Q *is a unitary matrix given by*

$$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} = \begin{bmatrix} \beta^{-1}(e^{i\beta^-\tau}\beta^+ - e^{i\beta^+\tau}\beta^-) & i\beta^{-1}(e^{i\beta^-\tau} - e^{i\beta^+\tau})\lambda^{-1} \\ \beta^{-1}\lambda^{-1}(-ie^{i\beta^-\tau} + ie^{i\beta^+\tau}) & -\beta^{-1}(e^{i\beta^-\tau}\beta^- - e^{i\beta^+\tau}\beta^+) \end{bmatrix}. \tag{3.3.16}$$

For Q $(k = 1, 2, \cdots,)$ *we have*

$$\begin{aligned} Q^k &= \begin{bmatrix} Q_{11}^{(k)} & Q_{12}^{(k)} \\ Q_{21}^{(k)} & Q_{22}^{(k)} \end{bmatrix} \\ &= \begin{bmatrix} \beta^{-1}(e^{ik\beta^-\tau}\beta^+ - e^{ik\beta^+\tau}\beta^-) & i\beta^{-1}(e^{ik\beta^-\tau} - e^{ik\beta^+\tau})\lambda^{-1} \\ \beta^{-1}\lambda^{-1}(-ie^{ik\beta^-\tau} + ie^{ik\beta^+\tau}) & -\beta^{-1}(e^{ik\beta^-\tau}\beta^- - e^{ik\beta^+\tau}\beta^+) \end{bmatrix} \end{aligned} \tag{3.3.17}$$

and $\|Q_{11}^{(k)}\|_{H^1} \leq 1$, $|Q_{22}^{(k)}\|_{H^1} \leq 1$, $\|Q_{12}^{(k)}\|_{H^1} \lesssim \varepsilon$, $\|Q_{21}^{(k)}\|_{H^1} \lesssim \varepsilon$.

Proof. From (3.2.4) and (3.3.15), it is easy to find that

$$\begin{aligned} S_L(\psi^0, \dot{\psi}^0) =& \beta^{-1}(e^{i\beta^-\tau}\beta^+ - e^{i\beta^+\tau}\beta^-)\psi^0 + i\beta^{-1}(e^{i\beta^-\tau} - e^{i\beta^+\tau})\lambda^{-1}\lambda\dot{\psi}^0, \\ \lambda\dot{S}_L(\psi^0, \dot{\psi}^0) =& \beta^{-1}\lambda^{-1}(-ie^{i\beta^-\tau} + ie^{i\beta^+\tau})\psi^0 - \beta^{-1}(e^{i\beta^-\tau}\beta^- - e^{i\beta^+\tau}\beta^+)\lambda\dot{\psi}^0. \end{aligned}$$

It is easy to verify that Q is unitary and Q^k has the form (3.3.17) by direct computation. As S_L and $\dot{S}_L$ are linear in ψ^0 and $\dot{\psi}^0$, we conclude that

$$\begin{bmatrix} S_L(\psi^0, \dot{\psi}^0) - S_L(\psi^1, \dot{\psi}^1) \\ \lambda\dot{S}_L(\psi^0, \dot{\psi}^0) - \lambda\dot{S}_L(\psi^1, \dot{\psi}^1) \end{bmatrix} = Q \begin{bmatrix} U(\boldsymbol{y}^0 - \boldsymbol{y}^1) \\ \Lambda U(\dot{\boldsymbol{y}}^0 - \dot{\boldsymbol{y}}^1) \end{bmatrix}. \tag{3.3.18}$$

To verify the properties of $Q_{11}^{(k)}$, assume $\phi \in H_0^1$,

$$\begin{aligned}
\|Q_{11}^{(k)}\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{\infty}|\beta_l^{-1}(e^{ik\beta_l^-\tau}\beta_l^+ - e^{ik\beta_l^+\tau}\beta_l^-)|^2(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&\le \frac{b-a}{2}\sum_{l=1}^{\infty}|\beta_l^{-1}(|\beta_l^+| + |\beta_l^-|)|^2(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&= \frac{b-a}{2}\sum_{l=1}^{\infty}(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&\le \frac{b-a}{2}\sum_{l=1}^{\infty}(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&= \|\phi\|_{H^1}^2,
\end{aligned}$$

thus $\|Q_{11}^{(k)}\|_{H^1} \le 1$.

For $Q_{12}^{(k)}$, denote $\lambda_l = \sqrt{-(\beta_l^+\beta_l^-)^{-1}}$,

$$\begin{aligned}
\|Q_{12}^{(k)}\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{\infty}|i\beta_l^{-1}(e^{ik\beta_l^-\tau} - e^{ik\beta_l^+\tau})\lambda_l^{-1}|^2(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&\le \frac{b-a}{2}\sum_{l=1}^{\infty}\frac{|\varepsilon\mu_l|^2}{1+4\varepsilon^2|\mu_l|^2}(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&\lesssim \frac{b-a}{2}\sum_{l=1}^{\infty}\varepsilon^2(1+|\mu_l|^2)|\widehat{\phi}_l|^2 \\
&= \varepsilon^2\|\phi\|_{H^1}^2,
\end{aligned}$$

thus $\|Q_{12}^{(k)}\|_{H^1} \lesssim \varepsilon$.

$\|Q_{21}^{(k)}\|_{H^1} \lesssim \varepsilon$ and $\|Q_{22}^{(k)}\|_{H^1} \le 1$ can be proved analogously.

For the nonlinear parts, first we estimate $g_k(\psi^0, \dot{\psi}^0; x, s) - g_k(\psi^1, \dot{\psi}^1; x, s), k = 0, 1, \cdots, 13$. For simplicity we denote $g_k^j(x,s) := g_k(\psi^j, \dot{\psi}^j; x, s), j = 0, 1$, then in view of the definition of g_k (3.2.18) the estimates fall into the following two types:

Type 1. Terms containing $g_k(\cdot, \cdot; x, 0)$, for example $g_0^0(x,0) - g_0^1(x,0)$. Then we can estimate the difference by

$$g_0^0(x,0) - g_0^1(x,0) = (\overline{h_1^0}h_2^0h_1^0 - \overline{h_1^1}h_2^1h_1^1 + h_1^0\overline{h_1^0}h_2^0 - h_1^1\overline{h_1^1}h_2^1 + \cdots),$$

where $h_1^j = h_1(\psi^j, \dot{\psi}^j; x)$, $h_2^j = h_2(\psi^j, \dot{\psi}^j; x)$, $j = 0, 1$, and some terms with similar structure are omitted for brevity. Then there holds

$$\begin{aligned}\|\overline{h_1^0}h_2^0h_1^0-\overline{h_1^1}h_2^1h_1^1\|_{H^1}\le\|\overline{h_1^0}-\overline{h_1^1}\|_{H^1}\|h_2^0h_1^0\|_{H^1}\\+\|\overline{h_1^1}\|_{H^1}\Big(\|h_2^0-h_2^1\|_{H^1}\|h_1^0\|_{H_1}-\|h_2^1\|_{H^1}\|h_1^0-h_1^1\|_{H^1}\Big).\end{aligned}$$

We can prove analogously to (3.3.12) that for $j=0,1$

$$\begin{aligned}\|h_1^j\|_{H^1}=\|h_1(\psi^j,\dot\psi^j;x)\|_{H^1}\le\|\psi^j\|_{H^1}+\varepsilon^2\|\dot\psi^j\|_{H^1}\le M_1+1,\\\|h_2^j\|_{H^1}=\|h_2(\psi^j,\dot\psi^j;x)\|_{H^1}\le\|\psi^j\|_{H^1}+\varepsilon^2\|\dot\psi^j\|_{H^1}\le M_1+1,\end{aligned}\tag{3.3.19}$$

by the hypothesis of the lemma. In addition, because $h_1(\cdot,\cdot;x)$ and $h_2(\cdot,\cdot;x)$ are linear, we have

$$\begin{aligned}\|h_1^0-h_1^1\|_{H^1}\le\|\psi^0-\psi^1\|_{H^1}+\varepsilon^2\|\dot\psi^0-\dot\psi^1\|_{H^1},\\\|h_2^0-h_2^1\|_{H^1}\le\|\psi^0-\psi^1\|_{H^1}+\varepsilon^2\|\dot\psi^0-\dot\psi^1\|_{H^1}.\end{aligned}\tag{3.3.20}$$

Thus we can derive

$$\|g_0^0(x,0)-g_0^1(x,0)\|_{H^1}\lesssim\|\psi^0-\psi^1\|_{H^1}+\varepsilon^2\|\dot\psi^0-\dot\psi^1\|_{H^1}.$$

Type 2. Terms containing $g_k(\cdot,\cdot;x,\tau/2)$, for example $g_7^0(x,\tau/2)-g_7^1(x,\tau/2)$. Then by definition,

$$\begin{aligned}g_1^0(x,0)-g_1^1(x,0)=&(e^{-i\beta^-\tau/2}h_1^0)(e^{i\beta^-\tau/2}\overline{h_1^0})(e^{-i\beta^-\tau/2}h_1^0)\\&-(e^{-i\beta^-\tau/2}h_1^1)(e^{i\beta^-\tau/2}\overline{h_1^1})(e^{-i\beta^-\tau/2}h_1^1)\\&+(e^{i\beta^-\tau/2}h_2^0)(e^{-i\beta^-\tau/2}\overline{h_2^0})(e^{-i\beta^-\tau/2}h_1^0)\\&-(e^{i\beta^-\tau/2}h_2^1)(e^{-i\beta^-\tau/2}\overline{h_2^1})(e^{-i\beta^-\tau/2}h_1^1)+\cdots,\end{aligned}$$

Then there holds

$$\begin{aligned}&\|(e^{-i\beta^-\tau/2}h_1^0)(e^{i\beta^-\tau/2}\overline{h_1^0})(e^{-i\beta^-\tau/2}h_1^0)-(e^{-i\beta^-\tau/2}h_1^1)(e^{i\beta^-\tau/2}\overline{h_1^1})(e^{-i\beta^-\tau/2}h_1^1)\|_{H^1}\\&\le\|e^{-i\beta^-\tau/2}(h_1^0-h_1^1)\|_{H^1}\|(e^{i\beta^-\tau/2}\overline{h_1^0})(e^{-i\beta^-\tau/2}h_1^0)\|_{H^1}\\&\quad+\|e^{-i\beta^-\tau/2}h_1^1\|_{H^1}\Big(\|e^{i\beta^-\tau/2}(\overline{h_1^0}-\overline{h_1^1})\|_{H^1}\|e^{-i\beta^-\tau/2}h_1^0\|_{H_1}\\&\quad-\|e^{i\beta^-\tau/2}\overline{h_1^1}\|_{H^1}\|e^{-i\beta^-\tau/2}(h_1^0-h_1^1)\|_{H^1}\Big).\end{aligned}$$

It is obvious that $\|e^{-i\beta^-\tau/2}\|_{H^1} = \|e^{i\beta^-\tau/2}\|_{H^1} = 1$, then by (3.3.19) and (3.3.20),

$$\begin{aligned}&\|(e^{-i\beta^-\tau/2}h_1^0)(e^{i\beta^-\tau/2}\overline{h_1^0})(e^{-i\beta^-\tau/2}h_1^0) - (e^{-i\beta^-\tau/2}h_1^1)(e^{i\beta^-\tau/2}\overline{h_1^1})(e^{-i\beta^-\tau/2}h_1^1)\|_{H^1}\\ &\lesssim \|\psi^0-\psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1},\end{aligned}$$

thus

$$\|g_7^0(x,\tau/2) - g_7^1(x,\tau/2)\|_{H^1} \lesssim \|\psi^0-\psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0-\dot\psi^1\|_{H^1}.$$

It remains to estimate $\dot g_k^f(\psi^0,\dot\psi^0;x,0) - \dot g_k^f(\psi^1,\dot\psi^1;x,0), k = 0,4,7,11$. Similarly, we denote $\dot g_k^{j,f}(x,0) := \dot g_k^f(\psi^j,\dot\psi^j;x,0), j = 0,1$. Then we estimate $\dot g_0^{0,f}(x,0) - \dot g_0^{1,f}(x,0)$ as an example. By its definition (3.2.23),

$$\begin{aligned}\dot g_0^{0,f}(x,0) - \dot g_0^{1,f}(x,0) = (i(&\frac{\sin(\beta^-\tau)}{\tau}\overline{h_1^0})h_2^0h_1^0 - i(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_1^1})h_2^1h_1^1\\ &+ i\overline{h_1^0}(\frac{\sin(\beta^-\tau)}{\tau}h_2^0)h_1^0 - i\overline{h_1^1}(\frac{\sin(\beta^-\tau)}{\tau}h_2^1)h_1^1 + \cdots).\end{aligned}$$

Then there holds

$$\begin{aligned}&\|i(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_1^0})h_2^0h_1^0 - i(\frac{\sin(\beta^-\tau)}{\tau}\overline{h_1^1})h_2^1h_1^1\|_{H^1}\\ &\le \|\frac{\sin(\beta^-\tau)}{\tau}(\overline{h_1^0} - \overline{h_1^1})\|_{H^1}\|h_2^0h_1^0\|_{H^1}\\ &\quad + \|\frac{\sin(\beta^-\tau)}{\tau}\overline{h_1^0}\|_{H^1}\Big(\|h_2^0 - h_2^1\|_{H^1}\|h_1^0\|_{H_1} - \|h_2^1\|_{H^1}\|h_1^0 - h_1^1\|_{H^1}\Big),\end{aligned}$$

and because $\|\frac{\sin(\beta^-\tau)}{\tau}\|_{H^1} \le \frac{1}{\tau}$, by estimates (3.3.19) and (3.3.20),

$$\|\dot g_0^{0,f}(x,0) - \dot g_0^{1,f}(x,0)\|_{H^1} \lesssim \tau^{-1}(\|\psi^0-\psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0-\dot\psi^1\|_{H^1}).$$

Next we estimate $G_{p,k}(\psi^0,\dot\psi^0;x,\tau) - G_{p,k}(\psi^1,\dot\psi^1;x,\tau), p = +,-, k = 0,1,2,3$. Denote $G_{p,k}^j(x,\tau) = G_{p,k}(\psi^j,\dot\psi^j;x,\tau)$. We have $|e^{i\tau/\varepsilon^2}| = 1$, $|p_i(\tau)| \lesssim \tau, i = -1,0,1$, $|q_{i_1,i_2}(\tau)| \lesssim \tau^2, i_1,i_2 = 0,\pm1,\pm2$. Because $g_k(\cdot,\cdot;x,s) \in X_{3M}$, $\dot g_k^f(\cdot,\cdot;x,s) \in X_{3M}$, by

Lemma 3.2 and Lemma 3.3, there holds

$$
\begin{aligned}
&\|G^j_{+,0}(x,\tau) - G^j_{+,0}(x,\tau)\|_{H^1} \\
&\le \|q_{-1,0}(\tau)I_M(g_1^0(x,0) - g_1^1(x,0))\|_{H^1} + \|q_{-1,1}(\tau)I_M(g_2^0(x,0) - g_2^1(x,0))\|_{H^1} + \cdots \\
&\lesssim \tau^2(\|g_1^0(x,0) - g_1^1(x,0)\|_{H^1} + \|g_2^0(x,0) - g_2^1(x,0)\|_{H^1} + \cdots) \\
&\lesssim \tau(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1}), \\
&\|G^j_{+,1}(x,\tau) - G^j_{+,1}(x,\tau)\|_{H^1} \\
&\le \|\tau I_M(g_7^0(x,\tau/2) - g_7^1(x,\tau/2))\|_{H^1} + \|\tau^2/2 I_M(g_8^0(x,\tau/2) - g_8^1(x,\tau/2))\|_{H^1} \\
&\lesssim \tau(\|g_7^0(x,\tau/2) - g_7^1(x,\tau/2)\|_{H^1} + \|g_8^0(x,\tau/2) - g_8^1(x,\tau/2)\|_{H^1}) \\
&\lesssim \tau(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1}), \\
&\|G^j_{+,2}(x,\tau) - G^j_{+,2}(x,\tau)\|_{H^1} \\
&\le \|p_{-1}(\tau)I_M(g_1^0(x,0) - g_1^1(x,0))\|_{H^1} + \|q_{-1,0}(\tau)I_M(\dot g_0^{0,f}(x,0) - \dot g_0^{1,f}(x,0))\|_{H^1} + \cdots \\
&\lesssim \tau\|g_1^0(x,0) - g_1^1(x,0)\|_{H^1} + \tau^2\|\dot g_0^{0,f}(x,0) - \dot g_0^{1,f}(x,0)\|_{H^1} + \cdots \\
&\lesssim \tau(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1}), \\
&\|G^j_{+,3}(x,\tau) - G^j_{+,2}(x,\tau)\|_{H^1} \\
&\le \|q_{-1,0}(\tau)I_M(g_0^0(x,0) - g_0^1(x,0))\|_{H^1} + \|q_{-2,0}(\tau)I_M(g_4^0(x,0) - g_4^1(x,0))\|_{H^1} + \cdots \\
&\lesssim \tau^2(\|g_0^0(x,0) - g_0^1(x,0)\|_{H^1} + \tau^2\|g_4^0(x,0) - g_4^1(x,0)\|_{H^1} + \cdots) \\
&\lesssim \tau^2(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1}).
\end{aligned}
$$

We can prove analogously that

$$
\begin{aligned}
&\|G^j_{-,k}(x,\tau) - G^j_{-,k}(x,\tau)\|_{H^1} \lesssim \tau(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1}), \quad k = 0,1,2, \\
&\|G^j_{-,3}(x,\tau) - G^j_{-,3}(x,\tau)\|_{H^1} \lesssim \tau^2(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot\psi^0 - \dot\psi^1\|_{H^1}).
\end{aligned}
$$

Then we estimate $\eta = S_{NL}(\psi^0, \dot\psi^0) - S_{NL}(\psi^1, \dot\psi^1)$. Assume $\phi \in X_M$, by Parseval's identity,

$$\begin{aligned}
\|\gamma\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}\Big|\frac{1}{\sqrt{1+4\varepsilon^2|\mu_l|^2}}\Big|^2(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&\le \frac{b-a}{2}\sum_{l=1}^{M-1}(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&= \|\phi\|_{H^1}^2.
\end{aligned}$$

Then by (3.3.15), there holds

$$\begin{aligned}
\|\eta\|_{H^1} \le& \sum_{k=0}^{2}\|G^j_{+,k}(x,\tau)-G^j_{+,k}(x,\tau)\|_{H^1}+\tau^{-1}\|G^j_{+,3}(x,\tau)-G^j_{+,3}(x,\tau)\|_{H^1} \\
&+\sum_{k=0}^{2}\|G^j_{-,k}(x,\tau)-G^j_{-,k}(x,\tau)\|_{H^1}+\tau^{-1}\|G^j_{-,3}(x,\tau)-G^j_{-,3}(x,\tau)\|_{H^1} \\
\lesssim& \ \tau(\|\psi^0-\psi^1\|_{H^1}+\varepsilon^2\|\dot{\psi}^0-\dot{\psi}^1\|_{H^1}).
\end{aligned}$$

Lastly we estimate $\dot{\eta}=\lambda S_{NL}(\psi^0,\dot{\psi}^0)-\lambda S_{NL}(\psi^1,\dot{\psi}^1)$. If $\phi\in H_0^1$, because $\lambda=\sqrt{-(\beta^+\beta^-)^{-1}}$, by the definition (3.2.6) we know

$$\begin{aligned}
\|\lambda\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}\Big|\frac{\varepsilon}{\mu_l}\Big|^2(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&\lesssim \frac{b-a}{2}\sum_{l=1}^{M-1}\varepsilon^2(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&= \varepsilon^2\|\phi\|_{H^1}^2, \\
\|\lambda\phi\|_{H^1}^2 &\gtrsim \frac{b-a}{2}\sum_{l=1}^{M-1}\varepsilon^2(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&= \varepsilon^2\|\phi\|_{H^1}^2, \\
\|\lambda\beta^-\phi\|_{H^1}^2 &= \frac{b-a}{2}\sum_{l=1}^{M-1}\Big|\frac{\varepsilon\mu_l}{\sqrt{1+4\varepsilon^2|\mu_l|^2}}\Big|^2(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&\lesssim \frac{b-a}{2}\sum_{l=1}^{M-1}(1+|\mu_l|^2)|\widetilde{\phi}_l|^2 \\
&= \|\phi\|_{H^1}^2,
\end{aligned}$$

which means $\varepsilon\lesssim\|\lambda\|_{H^1}\lesssim\varepsilon$, $\|\lambda\beta^-\|_{H^1}\lesssim 1$.

By (3.2.3), λ commutes with $\gamma = 1/\varepsilon^2\beta$, Then by (3.3.15), there holds

$$\begin{aligned}\|\dot{\eta}\|_{H^1} \leq & (\frac{1}{\varepsilon^2}\|\lambda\|_{H^1} + \|\lambda\beta^-\|_{H^1})(\sum_{k=0}^{2}\|G^j_{+,k}(x,\tau) - G^j_{+,k}(x,\tau)\|_{H^1} \\ & + \tau^{-1}\|G^j_{+,3}(x,\tau) - G^j_{+,3}(x,\tau)\|_{H^1}) \\ & + \|\lambda\beta^-\|_{H^1}(\sum_{k=0}^{2}\|G^j_{-,k}(x,\tau) - G^j_{-,k}(x,\tau)\|_{H^1} \\ & + \tau^{-1}\|G^j_{-,3}(x,\tau) - G^j_{-,3}(x,\tau)\|_{H^1}) \\ \lesssim & \frac{\tau}{\varepsilon}(\|\psi^0 - \psi^1\|_{H^1} + \varepsilon^2\|\dot{\psi}^0 - \dot{\psi}^1\|_{H^1}).\end{aligned}$$

The proof of Lemma 3.5 is completed. □

Now, having Lemmas 3.4 and 3.5 at hand, we are ready to prove Theorem 3.1.

Proof of the main result. To control the nonlinearity, we adopt mathematical induction here. We have

$$\begin{aligned}\|e^0(x)\|_{H^1} &= \|\psi_0(x) - I_M\psi_0(x)\|_{H^1} \lesssim h^{m-1}, \\ \|\dot{e}^0(x)\|_{H^1} &= \|\psi_1(x) - I_M\psi_1(x)\|_{H^1} \lesssim h^{m-1},\end{aligned}$$

by the choice of initial value, i.e. (3.3.2) holds for $n = 0$. For the error function after projection $e^0_M(x)$ and $\dot{e}^0_M(x)$ defined in (3.3.7),

$$\begin{aligned}\|e^0(x) - e^0_M(x)\|_{H^1} &= \|\psi_0(x) - P_M\psi_0(x)\|_{H^1} \lesssim h^{m-1}, \\ \|\dot{e}^0(x) - \dot{e}^0_M(x)\|_{H^1} &= \|\psi_1(x) - P_M\psi_1(x)\|_{H^1} \lesssim h^{m-1},\end{aligned}$$

so

$$\|e^0_M(x)\|_{H^1} + \|\dot{e}^0_M(x)\|_{H^1} \lesssim h^{m-1} \lesssim h^{m-2}. \tag{3.3.21}$$

Assuming (3.3.1) holds for all $0 \leq m \leq n \leq \frac{T}{\tau} - 1$, we are going to prove the case for $n+1$. From the local truncation error in Lemma 3.4, it holds

$$\begin{aligned}P_M\psi(x,t_{m+1}) &= S(P_M\psi(x,t_m), P_M\partial_t\psi(x,t_m)) + \xi^m, \\ P_M\partial_t\psi(x,t_{m+1}) &= \dot{S}(P_M\psi(x,t_m), P_M\partial_t\psi(x,t_m)) + \dot{\xi}^m, \quad m \geq 0,\end{aligned}$$

which leads to the error equation for e_M^m and $\dot{e}_M^m$ in view of (3.3.7), Lemma 3.5 and the induction hypothesis,

$$\begin{bmatrix} e_M^{m+1} \\ \lambda \dot{e}_M^{m+1} \end{bmatrix} = Q \begin{bmatrix} e_M^{m} \\ \lambda \dot{e}_M^{m} \end{bmatrix} + \begin{bmatrix} \eta^m \\ \dot{\eta}^m \end{bmatrix} + \begin{bmatrix} \xi^m \\ \lambda \dot{\xi}^m \end{bmatrix}, \quad 0 \le m \le n, \tag{3.3.22}$$

and the following estimates hold

$$\begin{aligned} &\|\eta^m\|_{H^1} \le C\tau(\|e_M^m\|_{H^1} + \varepsilon^2 \|\dot{e}_M^m\|_{H^1}), \\ &\|\dot{\eta}^m\|_{H^1} \le \frac{C\tau}{\varepsilon}(\|e_M^m\|_{H^1} + \varepsilon^2 \|\dot{e}_M^m\|_{H^1}), \\ &\|\xi^m\|_{H^1} + \varepsilon^2 \|\dot{\xi}^m\|_{H^1} \le C(\tau^3 + \tau h^{m-2}). \end{aligned} \tag{3.3.23}$$

(3.3.22) implies that for $0 \le m \le n$,

$$\begin{bmatrix} e_M^{m+1} \\ \lambda \dot{e}_M^{m+1} \end{bmatrix} = Q^{m+1} \begin{bmatrix} e_M^{0} \\ \lambda \dot{e}_M^{0} \end{bmatrix} + \sum_{k=0}^{m} Q^{m-k} \begin{bmatrix} \eta^k \\ \dot{\eta}^k \end{bmatrix} + \sum_{k=0}^{m} Q^{m-k} \begin{bmatrix} \xi^k \\ \lambda \dot{\xi}^k \end{bmatrix},$$

which can be written in the following form

$$e_M^{m+1} = Q_{11}^{(m+1)} e_M^0 + Q_{12}^{(m+1)} \dot{e}_M^0 + \sum_{k=0}^{m} \left[Q_{11}^{(m-k)}(\eta^k + \xi^k) + Q_{12}^{(m-k)}(\dot{\eta}^k + \lambda \dot{\xi}^k) \right], \tag{3.3.24}$$

$$\lambda e^{m+1} = Q_{21}^{(m+1)} e_M^0 + Q_{22}^{(m+1)} \dot{e}_M^0 + \sum_{k=0}^{m} \left[Q_{21}^{(m-k)}(\eta^k + \xi^k) + Q_{22}^{(m-k)}(\dot{\eta}^k + \lambda \dot{\xi}^k) \right]. \tag{3.3.25}$$

Recalling the properties $\varepsilon \lesssim \|\Lambda\|_{H^1} \lesssim \varepsilon$, $\|Q_{11}^{(k)}\|_{H^1} \le 1, \|Q_{12}^{(k)}\|_{H^1} \lesssim \varepsilon, \|Q_{21}^{(k)}\|_{H^1} \lesssim \varepsilon, \|Q_{22}^{(k)}\|_{H^1} \le 1$, $k = 1, 2, \cdots, m+1$ in Lemma 3.5, we have

$$\begin{aligned} \|e_M^{m+1}\|_{H^1} \le &\|e_M^0(x)\|_{H^1} + \|\dot{e}_M^0(x)\|_{H^1} \\ &+ C \sum_{k=0}^{m} \left(\|\eta^k\|_{H^1} + \varepsilon \|\dot{\eta}^k\|_{H^1} + \|\xi^k\|_{H^1} + \varepsilon^2 \|\dot{\xi}^k\|_{H^1} \right), \end{aligned} \tag{3.3.26}$$

$$\begin{aligned} \varepsilon \|\dot{e}_M^{m+1}\|_2 \le &C \|\lambda \dot{e}_M^{m+1}\|_{H^1} \\ \le &\|e_M^0(x)\|_{H^1} + \|\dot{e}_M^0(x)\|_{H^1} \\ &+ C \sum_{k=0}^{m} \left[\varepsilon^{-1} \|\eta^k\|_{H^1} + \|\dot{\eta}^k\|_{H^1} + (\varepsilon^{-1} \|\xi^k\|_{H^1} + \varepsilon \|\dot{\xi}^k\|_{H^1}) \right]. \end{aligned} \tag{3.3.27}$$

Combing (3.3.26), (3.3.27) with (3.3.21), (3.3.23), we obtain for $m \le \frac{T}{\tau} - 1$,

$$\begin{aligned} \|e_M^{m+1}\|_{H^1} \le &C\tau \sum_{k=0}^{m} \left(\|e_M^k\|_{H^1} + \varepsilon^2 \|\dot{e}_M^k\|_{H^1} \right) \\ &+ C(m+1)(\tau^3 + \tau h^{m-2}) + Ch^{m-2}, \end{aligned} \tag{3.3.28}$$

$$\begin{aligned}\varepsilon^2\|\dot{e}_M^{m+1}\|_{H^1} \leq & C\tau\sum_{k=0}^{m}\left(\|e_M^k\|_{H^1}+\varepsilon^2\|\dot{e}_M^k\|_{H^1}\right) \\ & + C(m+1)(\tau^3+\tau h^{m-2})+Ch^{m-2},\end{aligned} \tag{3.3.29}$$

and

$$\begin{aligned}\|e_M^{m+1}\|_{H^1}+\varepsilon^2\|e_M^{m+1}\|_{H^1} \leq & C\tau\sum_{k=0}^{m}\left(\|e_M^k\|_{H^1}+\varepsilon^2\|\dot{e}_M^k\|_{H^1}\right) \\ & + C(m+1)(\tau^3+\tau h^{m-2})+Ch^{m-2}.\end{aligned} \tag{3.3.30}$$

Discrete Gronwall inequality would then imply

$$\|e_M^{m+1}\|_{H^1}+\varepsilon^2\|e_M^{m+1}\|_{H^1} \leq C_T(\tau^2+h^{m-2}), \quad m=0,\cdots,n. \tag{3.3.31}$$

The error function e^{m+1} and $\dot{e}^{m+1}$ can be then estimated by (3.3.31) and (3.3.6),

$$\|e^{m+1}\|_{H^1}+\varepsilon^2\|e^{m+1}\|_{H^1} \leq C(\tau^2+h^{m-2}), \quad m=0,\cdots,n. \tag{3.3.32}$$

Moreover, by Sobolev embedding theorem, there exists an independent constant C_1,

$$\|e^{n+1}\|_{L^\infty}+\varepsilon^2\|e^{n+1}\|_{L^\infty} \leq C_1\|e^{n+1}\|_{H^1}+\varepsilon^2\|e^{n+1}\|_{H^1} \leq C_1C(\tau^2+h^{m-2}), \tag{3.3.33}$$

and for τ, h sufficiently small, $\|e^{n+1}\|_{L^\infty}+\varepsilon^2\|e^{n+1}\|_{L^\infty} \leq 1$, $\|e^{n+1}\|_{H^1}+\varepsilon^2\|e^{n+1}\|_{H^1} \leq 1$, i.e. conclusion (3.3.1) holds for $n+1$ by using triangle inequality to obtain

$$\begin{aligned}&\|\psi_I^{n+1}(x)\|_{L^\infty}+\varepsilon^2\|\dot{\psi}_I^{n+1}(x)\|_{L^\infty} \\ &\leq \|\psi(x,t_{n+1})\|_{L^\infty}+\varepsilon^2\|\dot{\psi}(x,t_{n+1})\|_{L^\infty} \\ &\quad + \|e^{n+1}\|_{L^\infty}+\varepsilon^2\|\dot{e}^{n+1}\|_{L^\infty} \\ &\leq M+1,\end{aligned}$$

and the condition in Lemma 3.5 is satisfied because $\|\psi_I^{n+1}(x)\|_{H^1}+\varepsilon^2\|\dot{\psi}_I^{n+1}(x)\|_{H^1} \leq M+1$. Therefore, the proof is complete by mathematical induction. □

Remark 1 In 2D/3D case, by the corresponding discrete Sobolev inequalities, Theorem 3.1 still holds under the condition $\tau^2 \lesssim C_d(h)$, where $C_d(h) = |\ln h|^{-1}$ in 2D and $C_d(h) = h^{1/2}$ in 3D.

Remark 2 Our NPI method (3.2.28) is uniformly second order independent of ε, while later numerical results show for fixed ε, when time step τ decreases the convergence order will increase from 2 to 3. This can be explained by the following observation. For the integral kernel $\kappa(t)$ (3.2.5), it is easy to check that $\|\kappa(t)\|_{H^1} = \|e^{i\beta^+ t} - e^{i\beta^- t}\|_{H^1} \leq \|\beta^+ - \beta^-\|_{H^1}\tau \leq \frac{\tau}{\varepsilon^2}$. From the local error analysis in Lemma 3.4, we could then derive the local error as

$$\|\psi(t_n) - S(\psi(t_n), \partial_t\psi(t_n))\|_{H_1} \leq C(\frac{\tau^4}{\varepsilon^2} + \tau h^{m-2}),$$
$$\varepsilon^2\|\partial_t\psi(t_n) - \dot{S}(\psi(t_n), \partial_t\psi(t_n))\|_{H_1} \leq C(\frac{\tau^4}{\varepsilon^2} + \tau h^{m-2}).$$

It then follows from the error analysis that $\|e^n\|_{H_1} + \varepsilon^2\|e^n\|_{H_1} \lesssim \frac{\tau^3}{\varepsilon^2} + h^{m-2}$, which confirms that for fixed ε, the order of temporal convergence is 3 for $\tau \ll \varepsilon^2$.

3.4 Numerical results

In this section, we present the numerical results of our scheme NPI-SP (3.2.28) to confirm our error estimates in Theorem 3.1.

We choose the initial value $\psi_0(x) = \pi^{-1/4}e^{-x^2/2}$ and $\omega^\varepsilon(x) = e^{-x^2/2}$ in (3.1.2). The computational domain is chosen to be $[a, b] = [-16, 16]$. The 'exact' solution is computed by our proposed scheme (3.2.28) with a very fine mesh $h = 1/128$ and time step $\tau = 10^{-6}$. We computed under the following two cases: $\alpha = 2$ for the well-prepared initial data, and $\alpha = 0$ for the ill-prepared data.

The errors are defined as $e^n(x) = \psi(x, t_n) - \psi_I^n(x)$, and we measure the H^1 norm of $e^n(x)$. The errors are displayed at $T = 1$. For spatial error analysis, we choose time step $\tau = 10^{-6}$ such that the temporal error can be neglected. The result is shown in Table 3.1, and the results confirms the spectral spatial convergence.

For temporal error analysis, we choose $h = 1/32$ such that the spatial error can be ignored. The results is shown in Table 3.2 and Table 3.3.

To better show how the temporal convergence rates change with τ, Figure 3.1 and 3.2 presents the temporal convergence rate curves of different ε, for both well-prepared case and ill-prepared case. The order 2 and order 3 temporal convergence rate curves are also presented in those figures for reference.

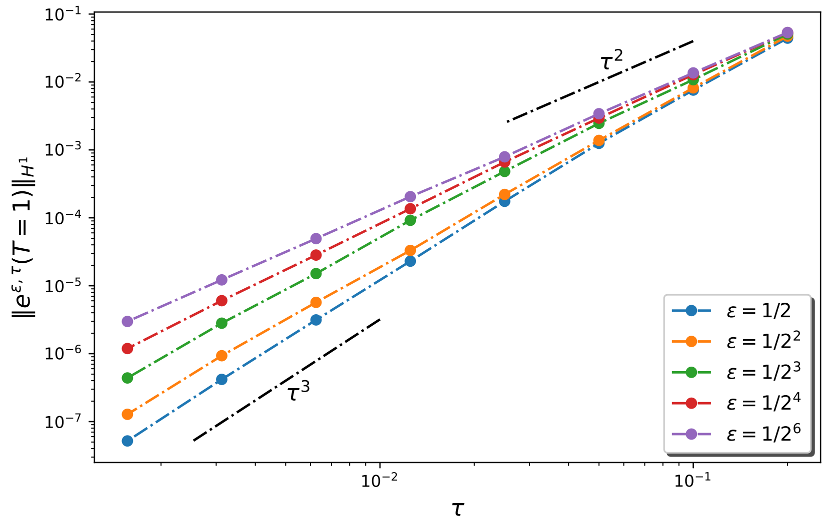

Figure 3.1: The convergence rate of $\|e^n(\cdot,\tau)\|_{H^1}$ with different ε for $\alpha = 2$.

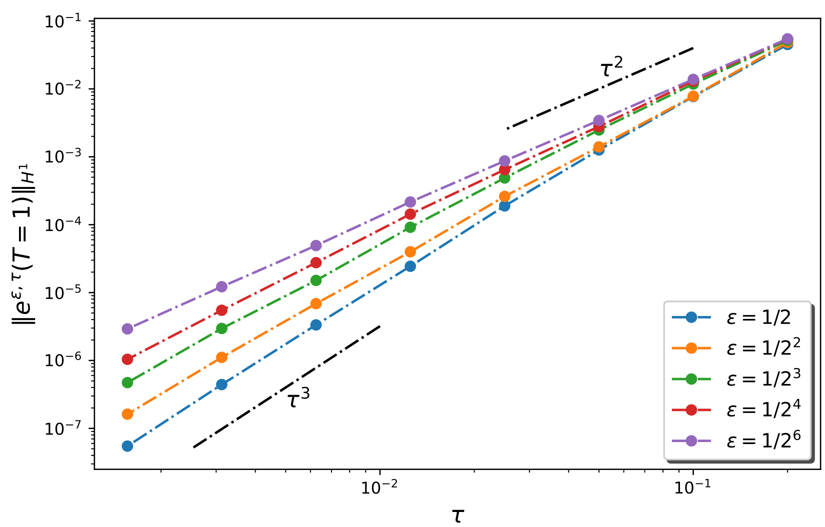

Figure 3.2: The convergence rate of $\|e^n(\cdot,\tau)\|_{H^1}$ with different ε for $\alpha = 0$.

	$\alpha=2$			$\alpha=0$		
	$h=1$	$h=1/2$	$h=1/4$	$h=1$	$h=1/2$	$h=1/4$
$\varepsilon=1/2$	9.97E-1	6.81E-4	3.89E-8	1.02E-1	6.97E-4	4.20E-8
$\varepsilon=1/2^2$	6.43E-2	3.42E-4	1.67E-9	8.48E-2	3.53E-4	2.11E-9
$\varepsilon=1/2^3$	7.38E-2	1.36E-4	1.15E-10	7.51E-2	1.45E-4	1.17E-10
$\varepsilon=1/2^4$	7.38E-2	1.36E-4	1.02E-10	7.52E-2	1.40E-4	1.10E-10
$\varepsilon=1/2^6$	7.38E-2	1.36E-4	1.02E-10	7.52E-2	1.40E-4	1.10E-10
$\varepsilon=1/2^8$	7.38E-2	1.36E-4	1.02E-10	7.52E-2	1.40E-4	1.10E-10

Table 3.1: Spatial error analysis for NPI-SP (3.2.28), with different ε for $\alpha=2$ and $\alpha=0$, for $\|e^n(\cdot)\|_{H^1}$.

$\alpha=2$	$\tau=0.2$	$\tau=0.2/2$	$\tau=0.2/2^2$	$\tau=0.2/2^3$	$\tau=0.2/2^4$	$\tau=0.2/2^5$	$\tau=0.2/2^6$	$\tau=0.2/2^7$
$\varepsilon=1/2$	4.42E-2	7.60E-3	1.25E-3	1.75E-4	2.30E-5	3.14E-6	4.18E-7	5.19E-8
rate	-	2.54	2.60	2.84	2.93	2.87	2.91	3.01
$\varepsilon=1/2^2$	4.73E-2	8.19E-3	1.38E-3	2.21E-4	3.31E-5	5.69E-6	9.33E-7	1.28E-7
rate	-	2.53	2.57	2.64	2.74	2.54	2.61	2.87
$\varepsilon=1/2^3$	5.08E-2	1.08E-2	2.46E-3	4.82E-4	9.19E-5	1.51E-5	2.81E-6	4.39E-7
rate	-	2.23	2.14	2.35	2.39	2.61	2.42	2.68
$\varepsilon=1/2^4$	5.33E-2	1.28E-2	2.94E-3	6.63E-4	1.36E-4	2.83E-5	6.03E-6	1.19E-6
rate	-	2.06	2.12	2.15	2.28	2.27	2.23	2.34
$\varepsilon=1/2^6$	5.35E-2	1.36E-2	3.41E-3	7.91E-4	2.05E-4	4.94E-5	1.22E-5	2.98E-6
rate	-	1.98	1.99	2.11	1.95	2.05	2.02	2.03
$\varepsilon=1/2^8$	5.35E-2	1.36E-2	3.41E-3	7.91E-4	2.05E-4	4.94E-5	1.22E-5	2.98E-6
rate	-	1.98	1.99	2.11	1.95	2.05	2.02	2.03

Table 3.2: Temporal error analysis for NPI-SP when $\alpha=2$, with different ε, for $\|e^n(\cdot)\|_{H^1}$. The convergence rate is computed as $\log_2(\|e^n(\cdot,2\tau)\|_{H^1}/\|e^n(\cdot,\tau)\|_{H^1})$.

From the above numerical results we can conclude: the NPI-SP method is uniformly second order accurate in τ w.r.t. $\varepsilon\in(0,1]$, for both well-prepare and ill-prepared initial data; for fixed ε, if τ is small enough, the error will converge asymptotically with third order in τ.

$\alpha=0$	$\tau=0.2$	$\tau=0.2/2$	$\tau=0.2/2^2$	$\tau=0.2/2^3$	$\tau=0.2/2^4$	$\tau=0.2/2^5$	$\tau=0.2/2^6$	$\tau=0.2/2^7$
$\varepsilon=1/2$	4.51E-2	7.70E-3	1.26E-3	1.89E-4	2.44E-5	3.34E-6	4.42E-7	5.48E-8
rate	-	2.55	2.61	2.74	2.95	2.87	2.92	3.01
$\varepsilon=1/2^2$	4.83E-2	7.80E-3	1.40E-3	2.61E-4	3.99E-5	6.87E-6	1.11E-6	1.62E-7
rate	-	2.63	2.48	2.42	2.71	2.54	2.63	2.78
$\varepsilon=1/2^3$	5.17E-2	1.18E-2	2.48E-3	4.87E-4	9.16E-5	1.51E-5	2.96E-6	4.72E-7
rate	-	2.13	2.25	2.35	2.41	2.60	2.35	2.65
$\varepsilon=1/2^4$	5.42E-2	1.30E-2	2.79E-3	6.46E-4	1.43E-4	2.76E-5	5.49E-6	1.04E-6
rate	-	2.06	2.22	2.11	2.18	2.37	2.33	2.40
$\varepsilon=1/2^6$	5.45E-2	1.38E-2	3.43E-3	8.69E-4	2.16E-4	4.93E-5	1.22E-5	2.92E-6
rate	-	1.98	2.01	1.98	2.01	2.13	2.02	2.06
$\varepsilon=1/2^8$	5.45E-2	1.38E-2	3.43E-3	8.69E-4	2.16E-4	4.93E-5	1.22E-5	2.92E-6
rate	-	1.98	2.01	1.98	2.01	2.13	2.02	2.06

Table 3.3: Temporal error analysis for NPI-SP when $\alpha=0$, with different ε, for $\|e^n(\cdot)\|_{H^1}$. The convergence rate is computed as $\log_2(\|e^n(\cdot,2\tau)\|_{H^1}/\|e^n(\cdot,\tau)\|_{H^1})$.

Chapter 4

An EWI-FP Method for Long-time Dynamics of NLSW

This chapter is devoted to study the long-time dynamics of the NLSW with weak nonlinearities. An exponential wave integrator Fourier spectral pseudospectral (EWI-FP) method is applied to the NLSW to numerically solve the equation in the long-time regime. The error bound of the EWI-FP method up to the long-time is carried out. Numerical results are reported to support the theoretical error estimates, and 2D dynamics presented as examples.

4.1 The NLSW with weak nonlinearity on torus

In this chapter we propose and analyze a exponential wave integrator Fourier pseudospectral method for the following NLSW with weak nonlinearity ($\psi := \psi(\boldsymbol{x}, t)$ is the complex wave function on the torus),

$$\begin{cases} i\partial_t\psi - \alpha\partial_{tt}\psi + \nabla^2\psi - \varepsilon^{2p}|\psi|^{2p}\psi = 0, \quad \boldsymbol{x} \in \mathbb{T}^d, \quad t > 0 \\ \psi(\boldsymbol{x}, 0) = \psi_0(\boldsymbol{x}), \quad \partial_t\psi(\boldsymbol{x}, 0) = \psi_1(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{T}^d, \end{cases} \tag{4.1.1}$$

where $\alpha = O(1)$ is a constant and $0 < \varepsilon \leq 1$ is a parameter controlling the nonlinearity. $\psi_0(\boldsymbol{x}) = O(1)$ and $\psi_1(\boldsymbol{x}) = O(1)$ are the initial wave and velocity. The solution of the

NLSW with weak nonlinearity (4.1.1) propagates waves in both space and time with wavelength at $O(1)$. The wave speed in space is also at $O(1)$.

The long-time dynamics of the Klein-Gordon equations and Dirac equations with weak nonlinearity or small potential are thoroughly studied in the literature [12, 13, 38–41]. However, there still lacks understanding of the long-time dynamics of the NLSW with weak nonlinearity (4.1.1). This motivates us to design numerical methods for solving the equation (4.1.1) on the time interval $[0, T_0/\varepsilon^\beta]$ with $0 \leq \beta \leq 2p$ in this chapter.

Rescaling the amplitude of the wave function $\psi(\boldsymbol{x}, t)$ by introduction $\phi := \phi(\boldsymbol{x}, t) = \varepsilon\psi(\boldsymbol{x}, t)$, the NLSW with weak nonlinearity can be reformulated as the following NLSW with $O(1)$ nonlinearity and small initial data:

$$\begin{cases} i\partial_t\phi - \alpha\partial_{tt}\phi + \nabla^2\phi - |\phi|^{2p}\phi = 0, \quad \boldsymbol{x} \in \mathbb{T}^d, \quad t > 0, \\ \phi(\boldsymbol{x}, 0) = \varepsilon\psi_0(\boldsymbol{x}), \quad \partial_t\phi(\boldsymbol{x}, 0) = \varepsilon\psi_1(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{T}^d, \end{cases} \tag{4.1.2}$$

thus equation (4.1.1) and (4.1.2) are equivalent.

For simplicity of notations, we only present the numerical methods in one dimension (1D) when $p = 1$. It is easy to generalize this method to higher dimensions or larger p. For 1D and $p = 1$, the NLSW (4.1.1) collapse to ($\Omega = (a, b)$):

$$\begin{cases} i\partial_t\psi(x,t) - \alpha\partial_{tt}\psi(x,t) + \partial_{xx}\psi(x,t) - \varepsilon^2|\psi(x,t)|^2\psi(x,t) = 0, x \in \Omega, t > 0, \\ \psi(x, 0) = \psi_0(x), \quad \partial_t\psi(x, 0) = \psi_1(x), \quad x \in \overline{\Omega} = [a, b], \\ \psi(a, t) = \psi(b, t), \quad \partial_x\psi(a, t) = \partial_x\psi(b, t), \quad t \geq 0. \end{cases} \tag{4.1.3}$$

4.2 An exponential wave integrator Fourier pseudospectral (EWI-FP) method

4.2.1 Temporal discretization by EWI

In this section we present the details of our uniform second order exponential wave integrator (EWI) method for equation (4.1.3).

Choose the time step size $\Delta t := \tau > 0$ and denote the time steps as $t_n = n\tau$ $(n = 0, 1, \cdots)$. Choose mesh size $h = \Delta x := (b-a)/M$ with M being a positive integer. The grid points are denoted as:

$$x_j := a + j\Delta x, j = 0, 1, \cdots, M.$$

Define index sets

$$\mathcal{T}_M = \{j | j = -\frac{M}{2}, -\frac{M}{2}+1, \cdots, \frac{M}{2}-1\},$$

and denote space

$$X_M = \text{span}\left\{\Phi_l(x) = e^{i\mu_l(x-a)},\ \mu_l = \frac{2\pi l}{b-a},\ x \in \overline{\Omega},\ l \in \mathcal{T}_M\right\},$$
$$Y_M = \left\{v = (v_0, v_1, \cdots, v_M)^T \in \mathbb{C}^{M+1} |\ v_0 = v_M\right\},$$

Define $C_p(\Omega) = \{u \in C(\Omega) | u(a) = u(b)\}$. Then we denote the L^2 projection operator $P_M : L^2(\Omega) \to X_M$ and trigonometric interpolation operator $I_M : Y_M \to X_M$ and $I_M : C_p(\Omega) \to X_M$ as:

$$\begin{aligned}(P_M\psi)(x) &= \sum_{l\in\mathcal{T}_M} \hat{\psi}_l e^{i\mu_l(x-a)},\\ (I_M\phi)(x) &= \sum_{l\in\mathcal{T}_M} \tilde{\phi}_l e^{i\mu_l(x-a)}, \quad x \in [a, b],\end{aligned} \tag{4.2.1}$$

where the coefficients are defined as

$$\begin{aligned}\hat{\psi}_l &= \frac{1}{b-a}\int_a^b \psi(x) e^{-i\mu_l(x-a)} dx, \quad l \in \mathbb{Z},\\ \tilde{\phi}_l &= \frac{2}{M}\sum_{j=0}^{M-1} \phi_j \sin(jl\pi/M), \quad l \in \mathcal{T}_M,\end{aligned}$$

where ϕ_j interpreted as $\phi(x_j)$ when involved. It can be directly checked that on X_M, P_M and I_M are both identity transforms, and if $\phi(x) \in X_M$, $\hat{\phi}_l = \tilde{\phi}_l$.

We begin with the Fourier pseudospectral method for discretizing the NLSW (4.1.3) in space. That is to find

$$\psi_M(x,t) = \sum_{l\in\mathcal{T}_M} \widehat{\psi}_l(t) e^{i\mu_l(x-a)} \in X_M, \quad x \in \Omega, t \geq 0, \tag{4.2.2}$$

such that

$$i\partial_t\psi_M(x,t) - \alpha\partial_{tt}\psi_M(x,t) + \partial_{xx}\psi_M(x,t) - \varepsilon^2 f(\psi_M(x,t)) = 0 \quad x\in\Omega, t\geq 0, \tag{4.2.3}$$

where $f(v) = |v|^2 v$. Plug (4.2.2) into (4.2.3), by the orthogonality of $\Phi_l(x)$ we get

$$i\frac{d}{dt}\widehat{\psi}_l(t) - \alpha\frac{d^2}{dt^2}\widehat{\psi}_l(t) - |\mu_l|^2\widehat{\psi}_l(t) - \varepsilon^2(\widehat{f(\psi_M)})_l(t) = 0, l\in\mathcal{T}_M, t>0. \tag{4.2.4}$$

Around time $t_n = n\tau$ the above equation can be reformulated as

$$i\frac{d}{dt}\widehat{\psi}_l(t_n+s) - \alpha\frac{d^2}{dt^2}\widehat{\psi}_l(t_n+s) - |\mu_l|^2\widehat{\psi}_l(t_n+s) - \varepsilon^2 f_l^n(s) = 0, l\in\mathcal{T}_M, t>0, \tag{4.2.5}$$

where

$$f_l^n(s) = (f(\widehat{\psi_M(t_n+s)}))_l. \tag{4.2.6}$$

Now, we proceed to apply an exponential wave integrator for solving the ODE (4.2.5). By the variation of constants formula, the solution can be written as:

$$\begin{aligned}\widehat{\psi}_l(t_n+s) =& e^{i\beta_l^+ s}\Big(-\frac{\beta_l^-\widehat{\psi}_l(t_n) + i\partial_t\widehat{\psi}_l(t_n)}{\beta_l}\Big) + e^{i\beta_l^- s}\Big(\frac{\beta_l^+\widehat{\psi}_l(t_n) + i\partial_t\widehat{\psi}_l(t_n)}{\beta_l}\Big) \\ &+ \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^s \kappa_l(s-w) f_l^n(w)dw, \quad 0\leq s\leq\tau.\end{aligned} \tag{4.2.7}$$

Here

$$\begin{aligned}\beta_l^+ &:= \frac{1+\sqrt{1+4\alpha|\mu_l|^2}}{2\alpha}, \\ \beta_l^- &:= \frac{1-\sqrt{1+4\alpha|\mu_l|^2}}{2\alpha} = \frac{-2|\mu_l|^2}{1+\sqrt{1+4\alpha|\mu_l|^2}}, \\ \beta_l &:= \beta_l^+ - \beta_l^- = \frac{\sqrt{1+4\alpha|\mu_l|^2}}{\alpha},\end{aligned} \tag{4.2.8}$$

and the integral kernel is defined by

$$\kappa_l(t) = e^{i\beta_l^+ t} - e^{i\beta_l^- t}. \tag{4.2.9}$$

Using the formula (4.2.7), we are to determine the numerical approximations of $\widehat{\psi}_l$ at different time steps t_n. For $n=0$, let $s=\tau$ in (4.2.7), by the initial condition of equation (4.1.3),

$$\begin{aligned}\widehat{\psi}_l(t_1) =& e^{i\beta_l^+\tau}(-\frac{\beta_l^-\widehat{\psi}_l(0)+i\partial_t\widehat{\psi}_l(0)}{\beta_l}) + e^{i\beta_l^-\tau}(\frac{\beta_l^+\widehat{\psi}_l(0)+i\partial_t\widehat{\psi}_l(0)}{\beta_l}) \\ &+ \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau \kappa_l(\tau-w)f_l^0(w)dw, \\ =& \frac{\beta_l^+e^{i\beta_l^-\tau}-\beta_l^-e^{i\beta_l^+\tau}}{\beta_l}(\widehat{\psi_0})_l - i\tau e^{\frac{i\tau}{2\alpha}}\mathrm{sinc}(\tau\beta_l/2)(\widehat{\psi_1})_l \\ &+ \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau \kappa_l(\tau-w)f_l^0(w)dw,\end{aligned} \tag{4.2.10}$$

if we define the sinc function as

$$\mathrm{sinc}(s) = \frac{\sin(s)}{s} \quad \text{for} \quad s \neq 0, \quad \mathrm{sinc}(0) = 1. \tag{4.2.11}$$

For $n \geq 1$, let $s = \pm\tau$ in (4.2.7), and eliminate the $\partial_t\widehat{\psi}_l(t_n)$, we know

$$\begin{aligned}\widehat{\psi}_l(t_{n+1}) =& -e^{\frac{i\tau}{\alpha}}\widehat{\psi}_l(t_{n-1}) + 2e^{\frac{i\tau}{2\alpha}}\cos(\frac{\beta_l\tau}{2})\widehat{\psi}_l(t_n) + \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau \kappa_l(\tau-w)f_l^n(w)dw \\ &- \frac{i\varepsilon^2}{\alpha\beta_l}e^{\frac{i\tau}{\alpha}}\int_0^\tau \kappa_l(-w)f_l^{n-1}(w)dw.\end{aligned} \tag{4.2.12}$$

For convenience we introduce the following notation for $l \in \mathcal{T}_M$:

$$\sigma_l^+(s) = e^{\frac{i\beta_l^+s}{2}}\mathrm{sinc}(\frac{\beta_l^+s}{2}), \quad \sigma_l^-(s) = e^{\frac{i\beta_l^-s}{2}}\mathrm{sinc}(\frac{\beta_l^-s}{2}), \quad s > 0. \tag{4.2.13}$$

We then approximate the integrals in (4.2.10) and (4.2.12). For $n = 0$, by Taylor expansion, when $l \neq 0$,

$$\begin{aligned}&\int_0^\tau \kappa_l(\tau-w)f_l^0(w)dw \\ &= \int_0^\tau \kappa_l(\tau-w)(f_l^0(0)+w\partial_t f_l^0(0)+O(w^2))dw \\ &= \tau f_l^0(0)(\sigma_l^+(\tau)-\sigma_l^-(\tau)) + i\tau\partial_t f_l^0(0)(\frac{1-\sigma_l^+(\tau)}{\beta_l^+} - \frac{1-\sigma_l^-(\tau)}{\beta_l^-}) + O(\tau^3), \\ &\int_0^\tau \kappa_l(-w)f_l^0(w)dw \\ &= \tau f_l^0(0)(\overline{\sigma_l^+(\tau)}-\overline{\sigma_l^-(\tau)}) + i\tau\partial_t f_l^0(0)(\frac{1-\sigma_l^+(\tau)}{\beta_l^+e^{i\beta_l^+\tau}} - \frac{1-\sigma_l^-(\tau)}{\beta_l^-e^{i\beta_l^-\tau}}) + O(\tau^3),\end{aligned} \tag{4.2.14}$$

and when $l = 0$, as $\beta_0^- = 0$,

$$\begin{aligned}
&\int_0^\tau \kappa_0(\tau - w) f_0^0(w) dw \\
&= \int_0^\tau \kappa_0(\tau - w)(f_l^0(0) + w\partial_t f_0^0(0) + O(w^2))dw \\
&= \tau f_0^0(0)(\sigma_0^+(\tau) - 1) + i\tau\partial_t f_0^0(0)(\frac{1 - \sigma_0^+(\tau)}{\beta_0^+} + \frac{i\tau}{2}) + O(\tau^3), \qquad (4.2.15) \\
&\int_0^\tau \kappa_0(-w) f_0^0(w) dw \\
&= \tau f_0^0(0)(\overline{\sigma_0^+(\tau)} - 1) + i\tau\partial_t f_0^0(0)(\frac{1 - \sigma_0^+(\tau)}{\beta_0^+ e^{i\beta_0^+\tau}} + \frac{i\tau}{2}) + O(\tau^3).
\end{aligned}$$

$\overline{c}$ is the complex conjugate of c, and $\partial_t f_0^0(0)$ can be computed accurately since $\partial_t\psi(x, 0) = \psi_1(x)$ is known in the initial condition.

For $n \geq 1$, when $l \neq 0$,

$$\begin{aligned}
&\int_0^\tau \kappa_l(\tau - w) f_l^n(w) dw \\
&= \int_0^\tau \kappa_l(\tau - w)(f_l^n(0) + w\partial_t f_l^n(0) + O(w^2))dw \\
&= \tau f_l^n(0)(\sigma_l^+(\tau) - \sigma_l^-(\tau)) + i\tau\delta_t^- f_l^n(0)(\frac{1 - \sigma_l^+(\tau)}{\beta_l^+} - \frac{1 - \sigma_l^-(\tau)}{\beta_l^-}) + O(\tau^3), \quad (4.2.16) \\
&\int_0^\tau \kappa_l(-w) f_l^n(w) dw \\
&= \tau f_l^n(0)(\overline{\sigma_l^+(\tau)} - \overline{\sigma_l^-(\tau)}) + i\tau\delta_t^- f_l^n(0)(\frac{1 - \sigma_l^+(\tau)}{\beta_l^+ e^{i\beta_l^+\tau}} - \frac{1 - \sigma_l^-(\tau)}{\beta_l^- e^{i\beta_l^-\tau}}) + O(\tau^3),
\end{aligned}$$

and when $l = 0$,

$$\begin{aligned}
&\int_0^\tau \kappa_0(\tau - w) f_0^n(w) dw \\
&= \int_0^\tau \kappa_0(\tau - w)(f_l^n(0) + w\partial_t f_0^n(0) + O(w^2))dw \\
&= \tau f_0^n(0)(\sigma_0^+(\tau) - 1) + i\tau\delta_t^- f_0^n(0)(\frac{1 - \sigma_0^+(\tau)}{\beta_0^+} + \frac{i\tau}{2}) + O(\tau^3), \qquad (4.2.17) \\
&\int_0^\tau \kappa_0(-w) f_0^n(w) dw \\
&= \tau f_0^n(0)(\overline{\sigma_0^+(\tau)} - 1) + i\tau\delta_t^- f_0^n(0)(\frac{1 - \sigma_0^+(\tau)}{\beta_0^+ e^{i\beta_0^+\tau}} + \frac{i\tau}{2}) + O(\tau^3),
\end{aligned}$$

where the finite difference $\delta_t^- f_0^n(0) := (f_0^n(0) - f_0^{n-1}(0))/\tau$ is the approximation of $\partial_t f_0^n(0)$.

Then the Fourier pseudospectral method can be formulated as follows. For convenience, we denote $g(\phi(x,t_n))$ for $\phi(x,t)$ as

$$g(\phi(0)) = \frac{d}{dt}f(\phi(t))|_{t=0}, \quad g(\phi(t_n)) = \delta_t^- f(\phi(t_n)), n \geq 1, \tag{4.2.18}$$

Denote $\psi_M^n(x)$ be the approximation of $\psi_M(x,t_n)$. Choose $\psi_M^0 = P_M(\psi_0)$, then we can update the approximation $\psi_M^{n+1} \in X_M (n \geq 0)$ as

$$\psi_M^{n+1}(x) = \sum_{l\in\mathcal{T}_M} \widehat{(\psi_M^{n+1})}_l e^{i\mu_l(x-a)}, x \in \overline{\Omega}, \tag{4.2.19}$$

where

$$\begin{aligned}
\widehat{(\psi_M^1)}_l =& c_l^0 \widehat{(\psi_0)}_l + d_l^0 \widehat{(\psi_1)}_l + p_l \widehat{(f(\psi_0))}_l + q_l \widehat{(g(\psi_0))}_l,\\
\widehat{(\psi_M^{n+1})}_l =& c_l \widehat{(\psi_M^{n-1})}_l + d_l \widehat{(\psi_M^n)}_l + p_l \widehat{(f(\psi_M^n))}_l\\
&+ q_l \widehat{(g(\psi_M^n))}_l - p_l^* \widehat{(f(\psi_M^{n-1}))}_l - q_l^* \widehat{(g(\psi_M^{n-1}))}_l, \quad n \geq 1.
\end{aligned} \tag{4.2.20}$$

Functions in (4.2.20) are defined as

$$\begin{aligned}
&c_l^0 = \frac{\beta_l^+ e^{i\beta_l^-\tau} - \beta_l^- e^{i\beta_l^+\tau}}{\beta_l}, \quad d_l^0 = -i\tau e^{\frac{i\tau}{2\alpha}} \mathrm{sinc}(\tau\beta_l/2),\\
&c_l = -e^{\frac{i\tau}{\alpha}}, \quad d_l = 2e^{\frac{i\tau}{2\alpha}} \cos(\tau\beta_l/2),\\
&p_l = \frac{i\varepsilon^2\tau}{\alpha\beta_l}(\sigma_l^+(\tau) - \sigma_l^-(\tau)) \quad (l \neq 0), \quad p_0 = \frac{i\varepsilon^2\tau}{\alpha\beta_0}(\sigma_0^+(\tau) - 1),\\
&p_l^* = \frac{i\varepsilon^2\tau e^{\frac{i\tau}{\alpha}}}{\alpha\beta_l}(\overline{\sigma_l^+(\tau)} - \overline{\sigma_l^-(\tau)}) \quad (l \neq 0), \quad p_0^* = \frac{i\varepsilon^2\tau e^{\frac{i\tau}{\alpha}}}{\alpha\beta_0}(\overline{\sigma_0^+(\tau)} - 1),\\
&q_l = \frac{-\varepsilon^2\tau}{\alpha\beta_l}(\frac{1-\sigma_l^+(\tau)}{\beta_l^+} - \frac{1-\sigma_l^-(\tau)}{\beta_l^-}) \quad (l \neq 0),\\
&q_0 = \frac{-\varepsilon^2\tau}{\alpha\beta_0}(\frac{1-\sigma_0^+(\tau)}{\beta_0^+} + \frac{i\tau}{2}),\\
&q_l^* = \frac{-\varepsilon^2\tau e^{\frac{i\tau}{\alpha}}}{\alpha\beta_l}(\frac{1-\sigma_l^+(\tau)}{\beta_l^+ e^{i\beta_l^+\tau}} - \frac{1-\sigma_l^-(\tau)}{\beta_l^- e^{i\beta_l^-\tau}}) \quad (l \neq 0),\\
&q_0^* = \frac{-\varepsilon^2\tau e^{\frac{i\tau}{\alpha}}}{\alpha\beta_0}(\frac{1-\sigma_0^+(\tau)}{\beta_0^+ e^{i\beta_0^+\tau}} + \frac{i\tau}{2}),
\end{aligned} \tag{4.2.21}$$

and $g(\psi_M^n)$ defined in (4.2.18) can be computed by

$$\begin{aligned}
&g(\psi_M^0) = 2|\psi_M^0|^2 P_M(\psi_1) + (\psi_M^0)^2 \overline{P_M(\psi_1)},\\
&g(\psi_M^n) = \delta_t^- f(\psi_M^n) = \frac{f(\psi_M^n) - f(\psi_M^{n-1})}{\tau}, \quad n \geq 1.
\end{aligned} \tag{4.2.22}$$

It can be shown by direct computation and (4.2.8) that $|c_l|, |d_l|, |c_l^0| \lesssim 1$, $|d_l^0| \lesssim \tau^2$, $|p_l|, |p_l^*| \lesssim \varepsilon^2\tau$ and $|q_l|, |q_l^*| \lesssim \varepsilon^2\tau^2$.

4.2.2 Spatial discretization by Fourier pseudospectral method

In practice the above scheme is impractical to compute, due to the difficulties in computing the Fourier coefficients in (4.2.20). If we replace the projections by interpolations, we will get the full discretized EWI-FP scheme. Let ψ_j^n be the approximation of $\psi(x_j, t_n)$, $\psi_0^n = \psi_M^n$. Choose $\psi_j^0 = \psi_0(x_j)$. Then the numerical approximation $\psi^{n+1} \in Y_M$ at $t = t_{n+1}$ can be computed by

$$\psi_j^{n+1} = \sum_{l \in \mathcal{T}_M} \widetilde{(\psi^{n+1})}_l e^{i\mu_l(x_j - a)}, \quad j = 0, 1, \cdots, M, \tag{4.2.23}$$

where

$$\begin{aligned}\widetilde{(\psi^1)}_l =& c_l^0 \widetilde{(\psi_0)}_l + d_l^0 \widetilde{(\psi_1)}_l + p_l \widetilde{(f(\psi_0))}_l + q_l \widetilde{(g(\psi_0))}_l, \quad l \in \mathcal{T}_M, \\ \widetilde{(\psi^{n+1})}_l =& c_l \widetilde{(\psi^{n-1})}_l + d_l \widetilde{(\psi^n)}_l + p_l \widetilde{(f(\psi^n))}_l + q_l \widetilde{(g(\psi^n))}_l \\ & - p_l^* \widetilde{(f(\psi^{n-1}))}_l - q_l^* \widetilde{(g(\psi^{n-1}))}_l, \quad l \in \mathcal{T}_M, \quad n \geq 1,\end{aligned} \tag{4.2.24}$$

with the coefficients c_l^0, d_l^0, c_l, d_l, p_l, p_l^*, q_l and q_l^* are given in (4.2.21). $g(\psi^n)$ defined by (4.2.18) can be computed by

$$g(\psi_0) = 2|\psi_0|^2\psi_1 + (\psi_0)^2\overline{\psi_1}, \quad g(\psi^n) = \delta_t^- f(\psi^n), \quad n \geq 1. \tag{4.2.25}$$

The EWI-FP is explicit and can be solved by fast Fourier transform. For each time step, the computational cost is $O(M \log M)$ and the memory cost is $O(M)$. We will prove the error estimates for this pseudospectral method EWI-FP in the next section.

4.3 Uniform error estimates for the long-time dynamics

4.3.1 Main Results

In this section we rigorously prove the uniform error estimates of the EWI-FP for NLSW (4.1.3) up to the time $t \in [0, T_0/\varepsilon^\beta]$, $0 \leq \beta \leq 2$. Denote the subspace

$H_p^m(\Omega) \subset H^m(\Omega) \cap H_0^1(\Omega)$ by $H_p^m(\Omega) = \{\phi \in H^m(\Omega) | \partial_x^k \phi(a) = \partial_x^k \phi(b), 0 \leq k < m\}$. In the following parts we will omit Ω when there is no confusion.

Denote $T_\varepsilon = \varepsilon^{-\beta} T_0$ for $0 \leq \beta \leq 2$ and $T_0 > 0$. We assume the solution $\psi(x,t)$ satisfies

$$\|\psi\|_{L^\infty([0,T_\varepsilon];W^{1,\infty}\cap H_p^m)} + \|\partial_t \psi\|_{L^\infty([0,T_\varepsilon];H^1)} + \|\partial_{tt}\psi\|_{L^\infty([0,T_\varepsilon];H^1)} \lesssim 1, \quad m \geq 2, \quad (4.3.1)$$

And the initial data satisfies the assumption

$$\|\psi_0(x)\|_{H_p^{m+2}} \lesssim 1, \quad \|\psi_1(x)\|_{H_p^{m+1}} \lesssim 1. \quad (4.3.2)$$

We denote

$$M_1 = \sup_{\varepsilon \in (0,1]} \sup_{t \in [0,T]} \|\psi(\cdot,t)\|_{L^\infty}.$$

We can then prove the following error estimates for our NPI:

Theorem 4.1. *Let $\psi^n \in Y_M$ be the numerical approximation of $\psi(x,t_n)$ from EWI-FP* (4.2.24) *with fixed $0 < \alpha \leq 1$. $\psi_I^n := I_M(\psi^n) \in X_M$ are their interpolation. Under the above assumption* (4.3.1) *and* (4.3.2)*, $\exists h_0, \tau_0 > 0$ independent of ε, such that $\forall 0 < h < h_0, 0 < \tau < \tau_0$,*

$$\begin{aligned} &\|\psi(x,t_n) - \psi_I^n(x)\|_{H^1(\Omega)} \lesssim h^{m-1} + \varepsilon^{2-\beta}\tau^2, \\ &\|\psi^n\|_{l^\infty(\Omega)} \leq M_1 + 1, \quad 0 \leq n \leq \frac{T_\varepsilon}{\tau}, \end{aligned} \quad (4.3.3)$$

for any $0 < \varepsilon \leq 1$ and $0 \leq \beta \leq 2$.

Remark In 2D/3D case, by the corresponding discrete Sobolev inequalities, Theorem 4.1 still holds under the condition $\tau^2 \lesssim C_d(h)$, where $C_d(h) = |\ln h|^{-1}$ in 2D and $C_d(h) = h^{1/2}$ in 3D.

4.3.2 Proof for the EWI-FP

Before the proof we first introduce some lemmas for the projection operator P_M and interpolation operator I_M.

Lemma 4.1 (L^2 projection). *Let $\phi(x) \in H_p^m(\Omega)$, $m \geq 2$, then*

$$\|\phi(x) - P_M(\phi)(x)\|_{L^2} \lesssim h^m, \quad |\phi(x) - P_M(\phi)(x)|_{H^1} \lesssim h^{m-1}. \tag{4.3.4}$$

For the sine interpolation I_M we have a similar result.

Lemma 4.2 (Fourier interpolation). *Let $\phi(x) \in H_p^1(\Omega)$, then*

$$\|I_M(\phi)(x)\|_{L^2} \leq \|\phi(x)\|_{L^2} + h\|\nabla\phi(x)\|_{L^2}, \tag{4.3.5}$$

and if $\phi(x) \in X_M$, then

$$\|\nabla\phi\|_{L^2} \lesssim h^{-1}\|\phi\|_{L^2}. \tag{4.3.6}$$

Combining those two lemmas we find that for any $\phi \in H_0^1$,

$$\|I_M(\phi) - P_M(\phi)\|_{L^2} = \|I_M(\phi - P_M(\phi))\|_{L^2} \lesssim \|\phi - P_M(\phi)\|_{L^2} + h\|\nabla(\phi - P_M(\phi))\|_{L^2},$$

and if $\phi \in H_p^m(m \geq 2)$, $\|I_M(\phi) - P_M(\phi)\|_{L^2} \lesssim h^m$.

Another lemma will be used when proving the stability. For $\phi = (\phi_0, \phi_1, \cdots, \phi_M) \in Y_M$, we define the l^2 and l^∞ norm on Y_M to be

$$\|\phi\|_{l^2}^2 = h\sum_{j=0}^{M-1}|\phi_j|^2, \quad \|\phi\|_{l^\infty} = \max_{0\leq j\leq M-1}|\phi_j|. \tag{4.3.7}$$

Lemma 4.3. *Let $\phi(x) \in H_p^1(\Omega)$, $\phi = (\phi_0, \phi_1, \cdots, \phi_M) := (\phi(x_0), \phi(x_1), \cdots, \phi(x_M)) \in Y_M$, then*

$$\|\delta_x^+\phi\|_{l^2} \lesssim \|\nabla I_M(\phi)(x)\|_{L^2} \lesssim \|\delta_x^+\phi\|_{l^2}. \tag{4.3.8}$$

where $\delta_x^+\phi_M = h^{-1}(\phi_1 - \phi_M)$.

It can be directly proved as by Bessel's equality,

$$\|\nabla I_M(\phi)(x)\|_{L^2} = (b-a)\sum_{l\in\mathcal{T}_M}|\mu_l|^2|\widetilde{\phi}_l|^2,$$

$$\delta_x^+\phi_j = h^{-1}\sum_{l\in\mathcal{T}_M} e^{i\mu_l h/2}(2i\sin(\mu_l h/2))\widetilde{\phi}_l e^{i\mu_l(x_j-a)},$$

$$\|\delta_x^+\phi\|_{l^2} = (b-a)\sum_{l\in\mathcal{T}_M}|\text{sinc}(\mu_l h/2)|^2|\mu_l|^2|\widetilde{\phi}_l|^2,$$

and because $0 \leq \frac{\mu_l h}{2} \leq \frac{\pi}{2}$, $\frac{2}{\pi} \leq |\text{sinc}(\mu_l h/2)| \leq 1$.

To prove the Theorem 4.1 we define the error function $e^n(x) := \psi(x,t_n) - \psi_I^n(x)$, then

$$\|e^{n+1}(x)\|_{H^1} \le \|\psi(x,t_{n+1}) - P_M\psi(x,t_{n+1})\|_{H^1} + \|e_M^{n+1}(x)\|_{H^1}, \tag{4.3.9}$$

the error function after projection $e_M^{n+1}(x)$ are defined as

$$e_M^{n+1}(x) := P_M\psi(x,t_{n+1}) - \psi_I^{n+1}(x). \tag{4.3.10}$$

By Lemma 4.1,

$$\|\psi(x,t_{n+1}) - P_M\psi(x,t_{n+1})\|_{H^1} \lesssim h^{m-1},$$

so we only need to estimate $\|e_M^{n+1}(x)\|_{H^1}$.

Local truncation error estimates Denote the local truncation error function $\xi^n(x) \in X_M$ by

$$\xi^n(x) = \sum_{l\in\mathcal{T}_M} \widetilde{(\xi^n)}_l e^{i\mu_l(x-a)}, \tag{4.3.11}$$

where

$$\begin{aligned}
\widetilde{(\xi^0)}_l =& \widehat{(\psi(t_1))}_l - c_l^0\widehat{(\psi_0)}_l - d_l^0\widehat{(\psi_1)}_l - p_l\widetilde{(f(\psi_0))}_l - q_l\widetilde{(g(\psi_0))}_l,\\
\widetilde{(\xi^n)}_l =& \widehat{(\psi(t_{n+1}))}_l - c_l\widehat{(\psi(t_{n-1}))}_l - d_l\widehat{(\psi(t_n))}_l - p_l\widetilde{(f(\psi(t_n)))}_l\\
&- q_l\widetilde{(g(\psi(t_n)))}_l + p_l^*\widetilde{(f(\psi(t_{n-1})))}_l + q_l^*\widetilde{(g(\psi(t_{n-1})))}_l, \quad n \ge 1.
\end{aligned} \tag{4.3.12}$$

We need the following decomposition of coefficients defined in (4.2.21): define

$$\begin{aligned}
p_l^+ &= \frac{i\varepsilon^2\tau}{\alpha\beta_l}\overline{\sigma_l^+(\tau)}, \quad p_l^- = \frac{i\varepsilon^2\tau}{\alpha\beta_l}\overline{\sigma_l^-(\tau)} \quad (l\ne 0), \quad p_0^- = \frac{i\varepsilon^2\tau^2}{\alpha\beta_0},\\
q_l^+ &= \frac{-\varepsilon^2\tau}{\alpha\beta_l}\Big(\frac{1-\sigma_l^+(\tau)}{\beta_l^+e^{i\beta_l^+\tau}}\Big), \quad q_l^- = \frac{-\varepsilon^2\tau}{\alpha\beta_l}\Big(\frac{1-\sigma_l^-(\tau)}{\beta_l^-e^{i\beta_l^-\tau}}\Big) \quad (l\ne 0), \quad q_0^- = \frac{-i\varepsilon^2\tau^2}{2\alpha\beta_0},
\end{aligned} \tag{4.3.13}$$

then

$$\begin{aligned}
p_l &= e^{i\beta_l^+\tau}p_l^+ - e^{i\beta_l^-\tau}p_l^-, \quad p_l^* = e^{\frac{i\tau}{\alpha}}(p_l^+ - p_l^-),\\
q_l &= e^{i\beta_l^+\tau}q_l^+ - e^{i\beta_l^-\tau}q_l^-, \quad q_l^* = e^{\frac{i\tau}{\alpha}}(q_l^+ - q_l^-),
\end{aligned} \tag{4.3.14}$$

direct computation shows $|p_l^\pm| \lesssim \varepsilon^2\tau$, $|q_l^\pm| \lesssim \varepsilon^2\tau^2$. Then we have the following estimates.

Lemma 4.4. *Under the assumption of Theorem 4.1, for $\xi^n(x)$ defined in (4.3.12), we have the decomposition for $l \in \mathcal{T}_M$,*

$$\begin{aligned} \widetilde{(\xi^0)}_l =& e^{i\beta_l^+\tau}\widetilde{(\xi^{0,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\xi^{0,-})}_l, \\ \widetilde{(\xi^n)}_l =& e^{i\beta_l^+\tau}\widetilde{(\xi^{n,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\xi^{n,-})}_l - e^{\frac{i\tau}{\alpha}}(\widetilde{(\xi^{n-1,+})}_l - \widetilde{(\xi^{n-1,-})}_l), \quad n \geq 1, \end{aligned} \tag{4.3.15}$$

where $\xi^{n,\pm}(x) = \sum_{l\in\mathcal{T}_M} \widetilde{(\xi^{n,\pm})}_l e^{i\mu_l(x-a)} \in X_M$. And we have the estimates

$$\|\xi^{n,\pm}(x)\|_{H^1} \lesssim \varepsilon^2\tau(\tau^2 + h^{m-1}). \tag{4.3.16}$$

Proof. In (4.2.20), we replace $\psi_M(x,t)$ by $\psi(x,t)$, the equation (4.2.20) still holds for $l \in \mathcal{T}_\mathcal{M}$. We use the same notation $f_l^n(s) = (f(\widetilde{\psi(t_n+s)}))_l$ without confusion. Submit (4.2.20) into (4.3.12), we know for $l \in \mathcal{T}_m$,

$$\begin{aligned} \widetilde{(\xi^0)}_l =& \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau \kappa_l(\tau-w)f_l^0(w)dw - p_l(\widetilde{f(\psi_0)})_l - q_l(\widetilde{g(\psi_0)})_l, \\ \widetilde{(\xi^n)}_l =& \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau \kappa_l(\tau-w)f_l^n(w)dw - \frac{i\varepsilon^2}{\alpha\beta_l}e^{\frac{i\tau}{\alpha}}\int_0^\tau \kappa_l(-w)f_l^{n-1}(w)dw \\ & - p_l(f(\widetilde{\psi(t_n)}))_l - q_l(g(\widetilde{\psi(t_n)}))_l \\ & + p_l^*(f(\widetilde{\psi(t_{n-1})}))_l + q_l^*(g(\widetilde{\psi(t_{n-1})}))_l, \quad n \geq 1. \end{aligned} \tag{4.3.17}$$

We denote the integral approximation errors $Q^{n,\pm}(x) = \sum_{l\in\mathcal{T}_M} \widetilde{(Q^{n,\pm})}_l e^{i\mu_l(x-a)} \in X_M$ as follows

$$\widetilde{(Q^{n,\pm})}_l = \frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau e^{-i\beta_l^\pm w} f_l^n(w)dw \mp (p_l^\pm(f(\widehat{\psi(t_n)}))_l + q_l^\pm(g(\widehat{\psi(t_n)}))_l), \tag{4.3.18}$$

and the interpolation errors $P^{n,\pm}(x) = \sum_{l\in\mathcal{T}_M} \widetilde{(P^{n,\pm})}_l e^{i\mu_l(x-a)} \in X_M$ given by

$$\begin{aligned} \widetilde{(P^{0,\pm})}_l =& p_l^\pm((\widehat{f(\psi_0)})_l - (\widetilde{f(\psi_0)})_l) + q_l^\pm((2\widehat{|\psi_0|^2\psi_1})_l \\ & + (\widehat{(\psi_0)^2\overline{\psi_1}})_l - (2\widetilde{|\psi_0|^2\psi_1})_l - (\widetilde{(\psi_0)^2\overline{\psi_1}})_l), \\ \widetilde{(P^{n,\pm})}_l =& p_l^\pm((f(\widehat{\psi(t_n)}))_l - (f(\widetilde{\psi(t_n)}))_l) + q_l^\pm((\delta_t^- \widehat{f(\psi(t_n))})_l - (\delta_t^- \widetilde{f(\psi(t_n))})_l). \end{aligned} \tag{4.3.19}$$

Combining (4.3.14) and (4.3.17), if we define

$$\xi^{n,\pm}(x) = Q^{n,\pm}(x) + P^{n,\pm}(x), \tag{4.3.20}$$

then decomposition (4.3.15) holds. Now, to estimate $\xi^{n,\pm}(x)$, we only need to estimate $Q^{n,\pm}(x)$ and $P^{n,\pm}(x)$.

First we estimate $Q^{n,\pm}(x)$. By its definition,

$$\begin{aligned}
\widetilde{(Q^{0,\pm})}_l =&\frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau e^{-i\beta_l^\pm w}(f_l^0(w)-f_l^0(0)-w\partial_t f_l^0(0))dw\\
=&\frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau\int_0^w\int_0^{w_1} e^{-i\beta_l^\pm w}(\partial_{tt}f_l^0(w_2))dw_2dw_1dw,\\
\widetilde{(Q^{n,\pm})}_l =&\frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau e^{-i\beta_l^\pm w}(f_l^n(w)-f_l^n(0)-w\delta_t^- f_l^n(0))dw\\
=&\frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau\int_0^w\int_0^{w_1} e^{-i\beta_l^\pm w}(\partial_{tt}f_l^n(w_2))dw_2dw_1dw\\
&-\frac{i\varepsilon^2}{\alpha\beta_l}\int_0^\tau e^{-i\beta_l^\pm w}w(\int_0^\tau\int_0^{w_1}\partial_{tt}f_l^n(-w_2)dw_2dw_1)dw,
\end{aligned} \tag{4.3.21}$$

thus

$$\begin{aligned}
|\widetilde{(Q^{0,\pm})}_l| \lesssim&\varepsilon^2\int_0^\tau\int_0^w\int_0^{w_1}|(\partial_{tt}\widehat{f(\psi(w_2))})_l|dw_2dw_1dw,\\
|\widetilde{(Q^{n,\pm})}_l| \lesssim&\varepsilon^2\int_0^\tau\int_0^w\int_0^{w_1}|(\partial_{tt}f(\widehat{\psi(t_n+w_2)}))_l|dw_2dw_1dw\\
&+\varepsilon^2\int_0^\tau\int_0^\tau\int_0^{w_1}|(\partial_{tt}f(\widehat{\psi(t_n-w_2)}))_l|dw_2dw_1dw
\end{aligned} \tag{4.3.22}$$

By assumption (4.3.1) and (4.3.2), $\|\psi(x,t)\|_{H^1}, \|\partial_t\psi(x,t)\|_{H^1}, \|\partial_{tt}\psi(x,t)\|_{H^1}\lesssim 1$ for $t\in[0,T_\varepsilon]$. Noticing $f(\phi)=|\phi|^2\phi$ is smooth, then direct computation shows that

$$\|\partial_{tt}f(\psi(t))\|_{H^1}\lesssim 1,\quad t\in[0,T_\varepsilon]. \tag{4.3.23}$$

By Cauchy's inequalities and Bessel's inequalities, we know when $n=0$,

$$\begin{aligned}
\|Q^{0,\pm}(x)\|_{H^1}^2 =&(b-a)\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)|\widetilde{(Q^{0,\pm})}_l|^2\\
\lesssim&\varepsilon^4\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)(\int_0^\tau\int_0^w\int_0^{w_1}|(\partial_{tt}\widehat{f(\psi(w_2))})_l|dw_2dw_1dw)^2\\
\lesssim&\varepsilon^4\tau^3\int_0^\tau\int_0^w\int_0^{w_1}\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)|(\partial_{tt}\widehat{f(\psi(w_2))})_l|^2dw_2dw_1dw\\
\lesssim&\varepsilon^4\tau^3\int_0^\tau\int_0^w\int_0^{w_1}\|\partial_{tt}f(\psi(w_2))\|_{H^1}^2dw_2dw_1dw\\
\lesssim&\varepsilon^4\tau^6.
\end{aligned}$$

Similarly for $n \geq 1$,

$$\begin{aligned}\|Q^{n,\pm}(x)\|_{H^1}^2 =&(b-a)\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)|\widetilde{(Q^{n,\pm})}_l|^2\\ \lesssim&\varepsilon^4\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)\Big(\int_0^\tau\int_0^w\int_0^{w_1}|(\partial_{tt}f(\widehat{\psi(t_n+w_2)}))_l|dw_2dw_1dw\\ &+\int_0^\tau\int_0^\tau\int_0^{w_1}|(\partial_{tt}f(\widehat{\psi(t_n-w_2)}))_l|dw_2dw_1dw\Big)^2\\ \lesssim&\varepsilon^4\tau^3\Big(\int_0^\tau\int_0^w\int_0^{w_1}\|\partial_{tt}f(\psi(t_n+w_2))\|_{H^1}^2dw_2dw_1dw\\ &+\int_0^\tau\int_0^\tau\int_0^{w_1}\|\partial_{tt}f(\psi(t_n-w_2))\|_{H^1}^2dw_2dw_1dw\Big)\\ \lesssim&\varepsilon^4\tau^6.\end{aligned}$$

Thus we have proved $\|Q^{n,\pm}(x)\|_{H^1}\lesssim\varepsilon^2\tau^3, n\geq 0$. Then we estimate $P^{n,\pm}(x)$. By the definition,

$$\begin{aligned}\|P^{0,\pm}(x)\|_{H^1}\leq&p_l^\pm\|P_M(f(\psi_0))-I_M(f(\psi_0))\|_{H^1}\\ &+q_l^\pm(\|P_M(2|\psi_0|^2\psi_1)-I_M(2|\psi_0|^2\psi_1)\|_{H^1}\\ &+\|P_M((\psi_0)^2\overline{\psi_1}))-I_M((\psi_0)^2\overline{\psi_1})\|_{H^1}),\end{aligned}$$

and for $n\geq 1$,

$$\begin{aligned}\|P^{n,\pm}(x)\|_{H^1}\leq&p_l^\pm\|P_M(f(\psi(t_n)))-I_M(f(\psi(t_n)))\|_{H^1}\\ &+q_l^\pm\|P_M(\delta_t^-f(\psi(t_n)))-I_M(\delta_t^-f(\psi(t_n)))\|_{H^1}.\end{aligned}$$

Because $\psi(x,t),\psi_0(x),\psi_1(x)\in H_p^m$, it is obvious that $|\psi_0|^2\psi_1$, $(\psi_0)^2\overline{\psi_1}$, $f(\psi(t_n))$, $\delta_t^-f(\psi(t_n))\in H_p^m$. So by Lemma 4.1, noticing $p_l^\pm\lesssim\varepsilon^2\tau$, $q_l^\pm\lesssim\varepsilon^2\tau^2$,

$$\|P^{n,\pm}(x)\|_{H^1}\lesssim\varepsilon^2(\tau h^{m-1}+\tau^2h^{m-1})\lesssim\varepsilon^2\tau h^{m-1}. \tag{4.3.24}$$

Combining the above estimates for $Q^{n,\pm}(x)$ and $P^{n,\pm}(x)$, we finally prove

$$\|\xi^{n,\pm}(x)\|_{H^1}\lesssim\varepsilon^2\tau(\tau^2+h^{m-1}). \tag{4.3.25}$$

□

Stability With $\xi^n(x)$ already estimated, we will continue to estimate $e_M^{n+1}(x)$. By (4.3.10) and (4.3.12),

$$
\begin{aligned}
\widetilde{(e_M^1)}_l =&\widetilde{(\xi^0)}_l + c_l^0(\widehat{(\psi_0)}_l - \widetilde{(\psi_0)}_l) + d_l^0(\widehat{(\psi_1)}_l - \widetilde{(\psi_1)}_l),\\
\widetilde{(e_M^{n+1})}_l =&\widetilde{(\xi^n)}_l + c_l(\widehat{(\psi(t_{n-1}))}_l - \widetilde{(\psi^{n-1})}_l) + d_l(\widehat{(\psi(t_n))}_l - \widetilde{(\psi^n)}_l)\\
&+ p_l(\widetilde{(f(\psi(t_n)))}_l - \widetilde{(f(\psi^n))}_l) + q_l(\widetilde{(g(\psi(t_n)))}_l - \widetilde{(g(\psi^n))}_l)\\
&- p_l^*(\widetilde{(f(\psi(t_{n-1})))}_l - \widetilde{(f(\psi^{n-1}))}_l) - q_l^*(\widetilde{(g(\psi(t_{n-1})))}_l - \widetilde{(g(\psi^{n-1}))}_l),\\
=&\widetilde{(\xi^n)}_l + \widetilde{(\eta^n)}_l + c_l\widetilde{(e_M^n)}_l + d_l\widetilde{(e_M^{n-1})}_l, \quad n \ge 1,
\end{aligned}
\tag{4.3.26}
$$

where we define $\eta^n(x) = \sum_{l\in\mathcal{T}_m}\widetilde{(\eta^n)}_l e^{i\mu_l(x-a)} \in X_M$ for $n \ge 1$ by

$$
\begin{aligned}
\widetilde{(\eta^n)}_l =&p_l(\widetilde{(f(\psi(t_n)))}_l - \widetilde{(f(\psi^n))}_l) + q_l(\widetilde{(g(\psi(t_n)))}_l - \widetilde{(g(\psi^n))}_l)\\
&- p_l^*(\widetilde{(f(\psi(t_{n-1})))}_l - \widetilde{(f(\psi^{n-1}))}_l) - q_l^*(\widetilde{(g(\psi(t_{n-1})))}_l - \widetilde{(g(\psi^{n-1}))}_l).
\end{aligned}
\tag{4.3.27}
$$

We then have the following decomposition and estimates for $\eta^n(x)$.

Lemma 4.5. *Under the assumption of Theorem 4.1, for $\eta^n(x)$ defined in* (4.3.27)*, we have the decomposition for $l \in \mathcal{T}_M$,*

$$
\widetilde{(\eta^n)}_l =e^{i\beta_l^+\tau}\widetilde{(\eta^{n,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\eta^{n,-})}_l - e^{\frac{i\tau}{\alpha}}(\widetilde{(\eta^{n-1,+})}_l - \widetilde{(\eta^{n-1,-})}_l), \quad n \ge 1, \tag{4.3.28}
$$

where $\eta^{n,\pm}(x) = \sum_{l\in\mathcal{T}_M}\widetilde{(\eta^{n,\pm})}_l e^{i\mu_l(x-a)} \in X_M$. And assume $\|\psi^n\|_{l^\infty} \le M_1 + 1$, we have the estimates

$$
\|\eta^{n,\pm}(x)\|_{H^1} \lesssim \varepsilon^2\tau(\|e_M^{n-1}\|_{H^1} + \|e_M^n\|_{H^1} + h^{m-1}), \quad n \ge 1. \tag{4.3.29}
$$

Proof. Define $\eta^{n,\pm}(x)$ as

$$
\widetilde{(\eta^{n,\pm})}_l = p_l^\pm(\widetilde{(f(\psi(t_n)))}_l - \widetilde{(f(\psi^n))}_l) + q_l^\pm(\widetilde{(g(\psi(t_n)))}_l - \widetilde{(g(\psi^n))}_l), \tag{4.3.30}
$$

then by it is easy to verify decomposition (4.3.28) holds. Notice $\widetilde{(f(\psi(t_0)))}_l = \widetilde{(f(\psi^0))}_l$, $\widetilde{(g(\psi(t_0)))}_l = \widetilde{(g(\psi^0))}_l$, and definition of g for $n \ge 1$ (4.2.18),

$$
\widetilde{(\eta^{n,\pm})}_l = \begin{cases} 0, \quad n = 0,\\ p_l^\pm(\widetilde{(f(\psi(t_n)))}_l - \widetilde{(f(\psi^n))}_l)\\ \quad +q_l^\pm(\widetilde{(\delta_t^- f(\psi(t_n)))}_l - \widetilde{(\delta_t^- f(\psi^n))}_l), \quad n \ge 1. \end{cases} \tag{4.3.31}
$$

We then estimate $\eta^{n,\pm}(x)$. By Parseval's equality and Cauchy inequality, noticing $|p_l^\pm| \lesssim \varepsilon^2\tau$, $|q_l^\pm| \lesssim \varepsilon^2\tau^2$,

$$\begin{aligned}\|\eta^{n,\pm}(x)\|_{H_1}^2 =&(b-a)\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)|\widetilde{(\eta^{n,\pm})}_l|^2\\ \lesssim&\varepsilon^4\tau^2(b-a)\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)|(\widetilde{f(\psi(t_n))})_l-(\widetilde{f(\psi^n)})_l|^2\\ &+\varepsilon^4\tau^4(b-a)\sum_{l\in\mathcal{T}_M}(1+|\mu_l|^2)|(\widetilde{\delta_t^- f(\psi(t_n))})_l-(\widetilde{\delta_t^- f(\psi^n)})_l|^2\\ \lesssim&\varepsilon^4\tau^2\|I_M(f(\psi(t_n)))-I_M(f(\psi^n))\|_{H^1}^2\\ &+\varepsilon^4\tau^4\|I_M(\delta_t^- f(\psi(t_n)))-I_M(\delta_t^- f(\psi^n))\|_{H^1}^2.\end{aligned} \tag{4.3.32}$$

To estimate $\|I_M(f(\psi(t_n)))-I_M(f(\psi^n))\|_{H^1}$, first

$$\begin{aligned}&\|I_M(f(\psi(t_n)))-I_M(f(\psi^n))\|_{L^2}^2 = h\sum_{j=0}^{M-1}|f(\psi(x_j,t_n))-f(\psi_j^n)|^2\\ &\le C_{M_1}h\sum_{j=0}^{M-1}|\psi(x_j,t_n)-\psi_j^n|^2 = C_{M_1}\|I_M(\psi(t_n))-I_M(\psi^n)\|_{L^2}^2\\ &\le 2C_{M_1}(\|I_M(\psi(t_n))-P_M(\psi(t_n))\|_{L^2}^2+\|P_M(\psi(t_n))-I_M(\psi^n)\|_{L^2}^2)\\ &\lesssim \|e_M^n(x)\|_{L^2}^2+h^{2m},\end{aligned} \tag{4.3.33}$$

as f is locally Lipschitz on interval $[-(M_1+1), M_1+1]$ with C_{M_1} being the Lipschitz coefficients, and by our assumption of lemma $\|\psi^n\|_{l^\infty} \le M_1+1$. The last inequality holds because of our Lemma 4.2.

To estimate $\|\nabla(I_M(f(\psi(t_n)))-I_M(f(\psi^n)))\|_{L^2}$, by our Lemma 4.3 we only need to estimate $\|\delta_x^+(f(\psi(x_j,t_n))-f(\psi_j^n))\|_{l^2}$. We have

$$\begin{aligned}\delta_x^+(f(\psi(x_j,t_n))-f(\psi_j^n)) = &\int_0^1 |\phi_{1,j}(\theta)|^2\delta_x^+\psi(x_j,t_n)-|\phi_{2,j}(\theta)|^2\delta_x^+\psi_j^n d\theta\\ &+\int_0^1(\phi_{1,j}(\theta))^2\delta_x^+\overline{\psi(x_j,t_n)}-(\phi_{2,j}(\theta))^2\delta_x^+\overline{\psi_j^n}d\theta,\end{aligned} \tag{4.3.34}$$

where

$$\begin{aligned}\phi_{1,j}(\theta) =&\theta\psi(x_{j+1},t_n)+(1-\theta)\psi(x_j,t_n),\\ \phi_{2,j}(\theta) =&\theta\psi_{j+1}^n+(1-\theta)\psi_j^n, \quad 0\le\theta\le 1.\end{aligned} \tag{4.3.35}$$

By our assumption of lemma $\|\psi^n\|_{l^\infty} \le M_1+1$, it is obvious that $|\phi_{1,j}(\theta)|, |\phi_{2,j}(\theta)| \le M_1+1$. By our assumption (4.3.1), $\|\delta_x^+\psi(x_j,t_n)\|_{l^\infty} \lesssim \|\partial_x\psi(x,t_n)\|_{L^\infty} \lesssim 1$.

Then by the locally Lipschitz property of $|\cdot|^2$, for $j \in \mathcal{T}_M$,

$$
\begin{aligned}
&|\int_0^1 |\phi_{1,j}(\theta)|^2\delta_x^+\psi(x_j,t_n) - |\phi_{2,j}(\theta)|^2\delta_x^+\psi_j^n d\theta| \\
&\le |\int_0^1 (|\phi_{1,j}(\theta)|^2 - |\phi_{2,j}(\theta)|^2)\delta_x^+\psi(x_j,t_n)d\theta| \\
&\quad + |\int_0^1 |\phi_{2,j}(\theta)|^2(\delta_x^+\psi(x_j,t_n) - \delta_x^+\psi_j^n)d\theta| \\
&\lesssim |\delta_x^+\psi(x_j,t_n)|\int_0^1 |\phi_{1,j}(\theta) - \phi_{2,j}(\theta)|d\theta \\
&\quad + |\phi_{2,j}(\theta)|^2\int_0^1 |\delta_x^+\psi(x_j,t_n) - \delta_x^+\psi_j^n|d\theta \\
&\lesssim |\psi(x_{j+1},t_n) - \psi_{j+1}^n| + |\psi(x_j,t_n) - \psi_j^n| + |\delta_x^+\psi(x_j,t_n) - \delta_x^+\psi_j^n|.
\end{aligned} \tag{4.3.36}
$$

Similarly for the second term, $(\cdot)^2$ is locally Lipschitz, therefore

$$
\begin{aligned}
&|\int_0^1 (\phi_{1,j}(\theta))^2\delta_x^+\overline{\psi(x_j,t_n)} - (\phi_{2,j}(\theta))^2\delta_x^+\overline{\psi_j^n}d\theta| \\
&\lesssim |\psi(x_{j+1},t_n) - \psi_{j+1}^n| + |\psi(x_j,t_n) - \psi_j^n| + |\delta_x^+\psi(x_j,t_n) - \delta_x^+\psi_j^n|, \quad j \in \mathcal{T}_M.
\end{aligned} \tag{4.3.37}
$$

Combining these two estimates, noticing Lemma 4.2 and 4.3, we have

$$
\begin{aligned}
&\|\delta_x^+(f(\psi(x_j,t_n)) - f(\psi_j^n))\|_{l^2} \\
&\lesssim \|\psi(x_j,t_n) - \psi_j^n\|_{l^2} + \|\delta_x^+\psi(x_j,t_n) - \delta_x^+\psi_j^n\|_{l^2} \\
&\lesssim \|I_M\psi(x,t_n) - I_M\psi^n\|_{L^2} + \|\nabla I_M\psi(x,t_n) - \nabla I_M\psi^n\|_{L^2} \\
&\lesssim \|I_M\psi(x,t_n) - P_M\psi(x,t_n)\|_{L^2} + \|e_M^n\|_{L^2} \\
&\quad + \|\nabla I_M\psi(x,t_n) - \nabla P_M\psi(x,t_n)\|_{L^2} + \|\nabla e_M^n\|_{L^2} \\
&\lesssim \|e_M^n\|_{H^1} + h^{m-1}.
\end{aligned} \tag{4.3.38}
$$

Therefore by Lemma 4.3, for the H^1 semi norm we have

$$
\begin{aligned}
\|\nabla(I_M(f(\psi(t_n))) - I_M(f(\psi^n)))\|_{L^2} &\lesssim \|\delta_x^+(f(\psi(x_j,t_n)) - f(\psi_j^n))\|_{l^2} \\
&\lesssim \|e_M^n\|_{H^1} + h^{m-1},
\end{aligned} \tag{4.3.39}
$$

and combining the L^2 norm estimates, we prove

$$
\|I_M(f(\psi(t_n))) - I_M(f(\psi^n))\|_{H^1} \lesssim \|e_M^n\|_{H^1} + h^{m-1}. \tag{4.3.40}
$$

With this result, we have for $n \geq 1$,

$$\begin{aligned}
&\|I_M(\delta_t^- f(\psi(t_n))) - I_M(\delta_t^- f(\psi^n))\|_{H^1} \\
&\leq \tau^{-1}(\|I_M(f(\psi(t_n))) - I_M(f(\psi^n))\|_{H^1} \\
&\quad + \|I_M(f(\psi(t_{n-1}))) - I_M(f(\psi^{n-1}))\|_{H^1}) \\
&\lesssim \tau^{-1}(\|e_M^n\|_{H^1} + \|e_M^{n-1}\|_{H^1} + h^{m-1}).
\end{aligned} \tag{4.3.41}$$

Submit the above two estimates into (4.3.32),

$$\|\eta^{n,\pm}(x)\|_{H_1}^2 \lesssim \varepsilon^4\tau^2(\|e_M^n\|_{H^1}^2 + \|e_M^{n-1}\|_{H^1}^2 + h^{2m-2}), \tag{4.3.42}$$

thus estimates (4.3.29) are proved. □

Now, having Lemma 4.4 and Lemma 4.5 proved, we are ready to prove Theorem 4.1.

Proof of the main result. To estimate $e^n(x)$, by Lemma 4.1, $|\|e^n(x)\|_{H^1} - \|e_M^n(x)\|_{H^1}| \lesssim h^{m-1}+$, so it suffices to estimate the H^1 norm of $e_M^n(x)$.

First consider the case $n = 0$ and $n = 1$. When $n = 0$, $e_M^0(x) = P_M\psi_0(x) - I_M\psi_0(x)$, so $\|e_M^0(x)\|_{H^1} \lesssim h^{m-1}$. When $n = 1$, we have the decomposition

$$\begin{aligned}
\widetilde{(e_M^1)}_l =&\widetilde{(\xi^0)}_l + c_l^0(\widehat{(\psi_0)}_l - \widetilde{(\psi_0)}_l) + d_l^0(\widehat{(\psi_1)}_l - \widetilde{(\psi_1)}_l), \\
=&e^{i\beta_l^+\tau}\widetilde{(e_M^{0,+})}_l + e^{i\beta_l^-\tau}\widetilde{(e_M^{0,-})}_l + e^{i\beta_l^+\tau}\widetilde{(\xi^{0,+})}_l \\
&- e^{i\beta_l^-\tau}\widetilde{(\xi^{0,-})}_l + e^{i\beta_l^+\tau}\widetilde{(\eta^{0,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\eta^{0,-})}_l,
\end{aligned} \tag{4.3.43}$$

as $\widetilde{(\eta^{0,\pm})}_l = 0$, where $e_M^{0,\pm}(x) = \sum_{l\in\mathcal{T}_M}\widetilde{(e_M^{0,\pm})}_l e^{i\mu_l(x-a)} \in X_M$ defined as

$$\begin{aligned}
\widetilde{(e_M^{0,+})}_l &= -\beta_l^{-1}(\beta_l^-(\widehat{(\psi_0)}_l - \widetilde{(\psi_0)}_l) + i(\widehat{(\psi_1)}_l - \widetilde{(\psi_1)}_l)), \\
\widetilde{(e_M^{0,-})}_l &= \beta_l^{-1}(\beta_l^+(\widehat{(\psi_0)}_l - \widetilde{(\psi_0)}_l) + i(\widehat{(\psi_1)}_l - \widetilde{(\psi_1)}_l)),
\end{aligned} \tag{4.3.44}$$

so $\widetilde{(e_M^0)}_l = \widetilde{(e_M^{0,+})}_l + \widetilde{(e_M^{0,-})}_l$. Because $\beta_l^{-1}\beta_l^{\pm}, \beta_l^{-1} \lesssim 1$ for all $l \in \mathcal{T}_m$, by Bessel's equality

$$\begin{aligned}
\|e_M^{0,\pm}(x)\|_{H^1} &\lesssim \|P_M\psi_0 - I_M\psi_0\|_{H^1} + \|P_M\psi_1 - I_M\psi_1\|_{H^1} \\
&\lesssim h^{m-1},
\end{aligned} \tag{4.3.45}$$

so

$$\begin{aligned}\|e_M^1(x)\|_{H^1} &\lesssim \|e_M^{0,+}(x)\|_{H^1} + \|e_M^{0,-}(x)\|_{H^1} + \|\xi^{0,+}(x)\|_{H^1} + \|\xi^{0,-}(x)\|_{H^1} \\ &\lesssim h^{m-1} + \varepsilon^2\tau^3.\end{aligned} \tag{4.3.46}$$

For the l^∞ norm, by 1D discrete Sobolev inequality,

$$\|e^n(x)\|_{L^\infty}^2 \lesssim \|e^n(x)\|_{L^2}\|\nabla e^n(x)\|_{L^2} \lesssim \|e^n(x)\|_{H^1}^2, \tag{4.3.47}$$

and

$$\|\psi^n\|_\infty \le \|\psi(x,t_n)\|_{L^\infty} + \|e^n(x)\|_{L^\infty} \le M_1 + \|e^n(x)\|_{L^\infty}. \tag{4.3.48}$$

For $n = 0, 1$, we have proved $\|e^n(x)\|_{H^1} \lesssim h^{m-1} + \|e_M^n(x)\|_{H^1} \lesssim h^{m-1} + \varepsilon^2\tau^3$, so there exists $h_0, \tau_0 > 0$, when $0 < h < h_0, 0 < \tau < \tau_0$,

$$\|\psi^n\|_\infty \le M_1 + 1, \quad n = 0, 1, \tag{4.3.49}$$

thus (4.3.3) holds for $n = 0, 1$.

We then adopt mathematical induction. Assume estimates (4.3.3) holds for all $0 \le m \le n \le \frac{T_\varepsilon}{\tau} - 1$, and for all $0 \le m \le n$ the following error decomposition holds

$$\begin{aligned}\widetilde{(e_M^m)}_l =& e^{i\beta_l^+ m\tau}\widetilde{(e_M^{0,+})}_l + e^{i\beta_l^- m\tau}\widetilde{(e_M^{0,-})}_l \\ &+ \sum_{k=0}^{m-1}\Bigg(e^{i\beta_l^+(m-k)\tau}\widetilde{(\xi^{k,+})}_l - e^{i\beta_l^-(m-k)\tau}\widetilde{(\xi^{k,-})}_l \\ &+ e^{i\beta_l^+(m-k)\tau}\widetilde{(\eta^{k,+})}_l - e^{i\beta_l^-(m-k)\tau}\widetilde{(\eta^{k,-})}_l\Bigg),\end{aligned} \tag{4.3.50}$$

we will prove (4.3.3) and (4.3.50) holds for $n + 1$.

For any $a, b \in \mathbb{C}$, $k \ge 0$, we have the equality

$$\begin{aligned}&(e^{i\beta_l^+\tau} + e^{i\beta_l^-\tau})(e^{i\beta_l^+k\tau}a + e^{i\beta_l^-k\tau}b) - e^{i(\beta_l^+ + \beta_l^-)\tau}(e^{i\beta_l^+(k-1)\tau}a + e^{i\beta_l^-(k-1)\tau}b) \\ &= e^{i\beta_l^+(k+1)\tau}a + e^{i\beta_l^-(k+1)\tau}b.\end{aligned} \tag{4.3.51}$$

Then in (4.3.26), by the definition of c_l and d_l (4.2.21), combined with the decomposition of ξ and η and apply the above equality, we know

$$\begin{aligned}
\widetilde{(e_M^{n+1})}_l =&(e^{i\beta_l^+\tau}+e^{i\beta_l^-\tau})\widetilde{(e_M^n)}_l - e^{i(\beta_l^++\beta_l^-)\tau}\widetilde{(e_M^{n-1})}_l\\
&+e^{i\beta_l^+\tau}\widetilde{(\xi^{n,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\xi^{n,-})}_l - e^{i(\beta_l^++\beta_l^-)\tau}(\widetilde{(\xi^{n-1,+})}_l-\widetilde{(\xi^{n-1,-})}_l)\\
&+e^{i\beta_l^+\tau}\widetilde{(\eta^{n,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\eta^{n,-})}_l - e^{i(\beta_l^++\beta_l^-)\tau}(\widetilde{(\eta^{n-1,+})}_l-\widetilde{(\eta^{n-1,-})}_l)\\
=&e^{i\beta_l^+(n+1)\tau}\widetilde{(e_M^{0,+})}_l + e^{i\beta_l^-(n+1)\tau}\widetilde{(e_M^{0,-})}_l\\
&+\sum_{k=0}^{n-2}\Bigg(e^{i\beta_l^+(n+1-k)\tau}\widetilde{(\xi^{k,+})}_l - e^{i\beta_l^-(n+1-k)\tau}\widetilde{(\xi^{k,-})}_l\\
&+e^{i\beta_l^+(n+1-k)\tau}\widetilde{(\eta^{k,+})}_l - e^{i\beta_l^-(n+1-k)\tau}\widetilde{(\eta^{k,-})}_l\Bigg)\\
&+(e^{i\beta_l^+\tau}+e^{i\beta_l^-\tau})(e^{i\beta_l^+\tau}\widetilde{(\xi^{n-1,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\xi^{n-1,-})}_l)\\
&-e^{i(\beta_l^++\beta_l^-)\tau}(\widetilde{(\xi^{n-1,+})}_l-\widetilde{(\xi^{n-1,-})}_l)\\
&+(e^{i\beta_l^+\tau}+e^{i\beta_l^-\tau})(e^{i\beta_l^+\tau}\widetilde{(\eta^{n-1,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\eta^{n-1,-})}_l)\\
&-e^{i(\beta_l^++\beta_l^-)\tau}(\widetilde{(\eta^{n-1,+})}_l-\widetilde{(\eta^{n-1,-})}_l)\\
&+e^{i\beta_l^+\tau}\widetilde{(\xi^{n,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\xi^{n,-})}_l + e^{i\beta_l^+\tau}\widetilde{(\eta^{n,+})}_l - e^{i\beta_l^-\tau}\widetilde{(\eta^{n,-})}_l\\
=&e^{i\beta_l^+(n+1)\tau}\widetilde{(e_M^{0,+})}_l + e^{i\beta_l^-(n+1)\tau}\widetilde{(e_M^{0,-})}_l\\
&+\sum_{k=0}^{n}\Bigg(e^{i\beta_l^+(n+1-k)\tau}\widetilde{(\xi^{k,+})}_l - e^{i\beta_l^-(n+1-k)\tau}\widetilde{(\xi^{k,-})}_l\\
&+e^{i\beta_l^+(n+1-k)\tau}\widetilde{(\eta^{k,+})}_l - e^{i\beta_l^-(n+1-k)\tau}\widetilde{(\eta^{k,-})}_l\Bigg),
\end{aligned}\tag{4.3.52}$$

i.e. the decomposition (4.3.50) still holds for $n+1$. Then by Cauchy inequality,

$$\begin{aligned}
|\widetilde{(e_M^{n+1})}_l|^2 \le 6\Bigg(&|\widetilde{(e_M^{0,+})}_l|^2+|\widetilde{(e_M^{0,-})}_l|^2\\
&+(n+1)\sum_{k=0}^{n}(|\widetilde{(\xi^{k,+})}_l|^2+|\widetilde{(\xi^{k,-})}_l|^2+|\widetilde{(\eta^{k,+})}_l|^2+|\widetilde{(\eta^{k,-})}_l|^2)\Bigg),
\end{aligned}\tag{4.3.53}$$

knowing the estimates from Lemma 4.4 and 4.5, by Bessel's equality, for $1 \le n \le \frac{T_0\varepsilon^{-\beta}}{\tau}$,

$$\begin{aligned}\|e_M^{n+1}(x)\|_{H^1}^2 \le & 6\Big(\|e_M^{0,+}(x)\|_{H^1}^2 + \|e_M^{0,-}(x)\|_{H^1}^2 + (n+1)\sum_{k=0}^{n}\big(\|\xi^{k,+}(x)\|_{H^1}^2 \\ & + \|\xi^{k,-}(x)\|_{H^1}^2 + \|\eta^{k,+}(x)\|_{H^1}^2 + \|\eta^{k,-}(x)\|_{H^1}^2\big)\Big) \\ \le & C_1 h^{2m-2} + C_2(n+1)^2\varepsilon^4\tau^2(\tau^4 + h^{2m-2}) \\ & + C_3(n+1)\varepsilon^4\tau^2\sum_{k=0}^{n}(\|e_M^k\|_{H^1}^2 + h^{2m-2}) \\ \le & C_0(\varepsilon^{4-2\beta}\tau^4 + h^{2m-2}) + C_3\varepsilon^{4-\beta}\tau\sum_{k=0}^{n}\|e_M^k\|_{H^1}^2.\end{aligned} \tag{4.3.54}$$

By the condition $0 \le \beta \le 2$ and $0 < \varepsilon \le 1$, we apply discrete Gronwall's inequality to get

$$\|e_M^{n+1}(x)\|_{H^1}^2 \le C_{T_0}(\varepsilon^{4-2\beta}\tau^4 + h^{2m-2}), \quad 1 \le n \le \frac{T_0\varepsilon^{-\beta}}{\tau}, \tag{4.3.55}$$

C_{T_0} is a constant independent of τ, h, ε and β. Therefore by Lemma 4.1, $\|e^{n+1}(x)\|_{H^1} \lesssim \varepsilon^{2-\beta}\tau^2 + h^{m-1}$ By triangle inequality and 1D discrete Sobolev inequality, we can choose h_0 and τ_0 small enough such that $0 < h < h_0, 0 < \tau < \tau_0$,

$$\|\psi^{n+1}\|_{l^\infty} \le \|\psi(x,t_n)\|_{L^\infty} + \|e^{n+1}(x)\|_{L^\infty} \le 1. \tag{4.3.56}$$

We have proved the induction hypothesis holds for $n+1$, thus finished the proof for the theorem. □

4.4 Numerical results

4.4.1 Convergence tests

In this section we present numerical results for the NPI-FP scheme (4.2.24) for the NLSW (4.1.3) with weak nonlinearity. In our following numerical tests, we choose $\alpha = 1$, the computation domain to be $\Omega = [a,b] = [-\pi,\pi]$, and the initial data

$$\psi_0(x) = \frac{1}{2+\cos^2(x)+\sin(x)}, \quad \psi_1(x) = \frac{1}{2+\sin^2(x)+\cos(x)}, \quad x \in [-\pi,\pi]. \tag{4.4.1}$$

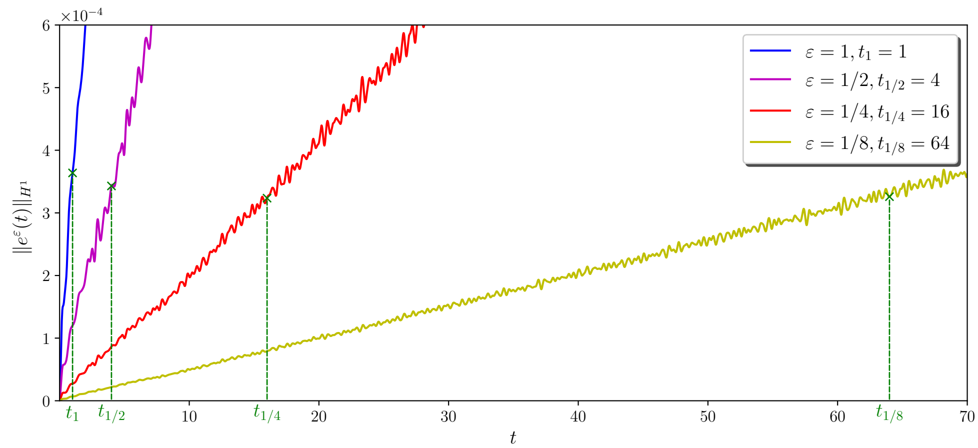

Figure 4.1: Long-time errors $\|e^{\varepsilon,\tau}(t)\|_{H^1}$ with different ε.

The numerical approximations are computed on the time interval $[0, \varepsilon^{-\beta}T_0]$ with $0 \leq \beta \leq 2$. $T_0 = 1$ is fixed. We study the following three cases with different β:

Case I. Fixed time dynamics up to the time at $O(1)$, i.e. $\beta = 0$.

Case II. Intermediate long-time dynamics up to the time at $O(\varepsilon^{-1})$, i.e. $\beta = 1$.

Case III. Long-time dynamics up to the time at $O(\varepsilon^{-2})$, i.e. $\beta = 2$.

The "exact" solution is computed using the proposed scheme with a very fine mesh $h_e = \pi/64$ and very small time step $\tau_e = 5 \times 10^{-4}$. The errors are defined as $e^n \in Y_M$ and $e^n(x) \in X_M$, with $e_j^n = \psi(x_j, t_n) - \psi_j^n$ and $e^n(x) = \psi(x, t_n) - I_M\psi^n(x)$. Denote $T_{\varepsilon,\beta} = T_0\varepsilon^{-\beta}$. For given ε, τ and h, we measure the H^1 norm of $e^{\varepsilon,h,\tau}(x, t = T_{\varepsilon,\beta}) := e^n(x)$ where $n = T_{\varepsilon,\beta}/\tau$ as the error.

Figure 4.1 shows the long-time error $\|e^{\varepsilon,\tau}(t)\|_{H^1}$ at time t. The numerical approximation is computed with $h = \pi/32$ and $\tau = 5 \times 10^{-3}$. From the graphs we can observe that the error can be uniformly bounded for all $0 < \varepsilon \leq 1$ up to time $t = O(\varepsilon^{-\beta^2})$.

For the spatial errors, we fix the time step $\tau = 5 \times 10^{-4}$, so error in time discretization can be ignored. The results are displayed in Table 4.1, and clearly shows that EWI-FP is uniformly spectral accurate in h for any $0 < \varepsilon \leq 1$ and $0 \leq \beta \leq 2$.

For the temporal errors, we choose $h = \pi/64$ such that the spatial error can be neglected. Table 4.2, 4.3 and 4.4 show the temporal errors with different τ for $\beta = 0$, $\beta = 1$ and $\beta = 2$ respectively. From the results we can observe: in time, for any fixed

$\|e^{\varepsilon,h}(t=T_0/\varepsilon^\beta)\|_{H^1}$		$h=\pi/4$	$h=\pi/8$	$h=\pi/16$	$h=\pi/32$
$\beta=0$	$\varepsilon=1$	1.81E-1	5.69E-3	8.84E-5	7.01E-10
	$\varepsilon=1/2$	1.28E-1	6.57E-3	5.95E-5	6.43E-10
	$\varepsilon=1/2^2$	1.08E-1	7.53E-3	5.27E-5	6.34E-10
	$\varepsilon=1/2^3$	1.04E-1	7.74E-3	5.10E-5	6.29E-10
	$\varepsilon=1/2^4$	1.02E-1	7.79E-3	5.05E-5	6.27E-10
$\beta=1$	$\varepsilon=1$	1.81E-1	5.69E-3	8.84E-5	7.01E-10
	$\varepsilon=1/2$	1.28E-1	7.39E-3	3.28E-5	1.22E-10
	$\varepsilon=1/2^2$	8.86E-2	1.05E-2	3.89E-5	2.29E-10
	$\varepsilon=1/2^3$	3.94E-2	1.20E-2	6.05E-5	5.17E-10
	$\varepsilon=1/2^4$	7.66E-2	6.84E-3	6.42E-6	4.07E-10
$\beta=2$	$\varepsilon=1$	1.81E-1	5.69E-3	8.84E-5	7.01E-10
	$\varepsilon=1/2$	8.70E-2	1.22E-2	5.04E-5	2.50E-10
	$\varepsilon=1/2^2$	8.60E-2	8.43E-3	9.12E-6	4.10E-10
	$\varepsilon=1/2^3$	1.04E-1	4.64E-3	3.43E-5	5.74E-10
	$\varepsilon=1/2^4$	1.15E-1	1.14E-2	5.78E-5	2.81E-10

Table 4.1: Spatial error analysis for EWI-FP, with different β and ε.

ε, the EWI-FP is uniformly second order accurate. In addition, the temporal error is of $O(\varepsilon^2\tau^2)$ for the fixed time dynamics ($\beta=1$) up to time at $O(1)$, and $O(\varepsilon\tau^2)$ for the intermediate long-time dynamics ($\beta=1$) up to time at $O(\varepsilon^{-1})$, and $O(\tau^2)$ for the long-time dynamics $\beta=2$ up to time at $O(\varepsilon^{-2})$.

To better show the convergence rate for temporal error, Figure 4.2, 4.3 and 4.4 presents the temporal convergence rate curves of different τ and ε, for $\beta=0,1,2$ correspondingly. The order τ^2 and $\varepsilon^{2-\beta}$ curves are also presented in those figures for reference. These figures confirms the $O(\tau^2\varepsilon^{2-\beta})$ convergence rate at time $O(\varepsilon^{-\beta})$.

In conclusion, the numerical results confirm the error bounds given in the Theorem 4.1, and suggest they are optimal.

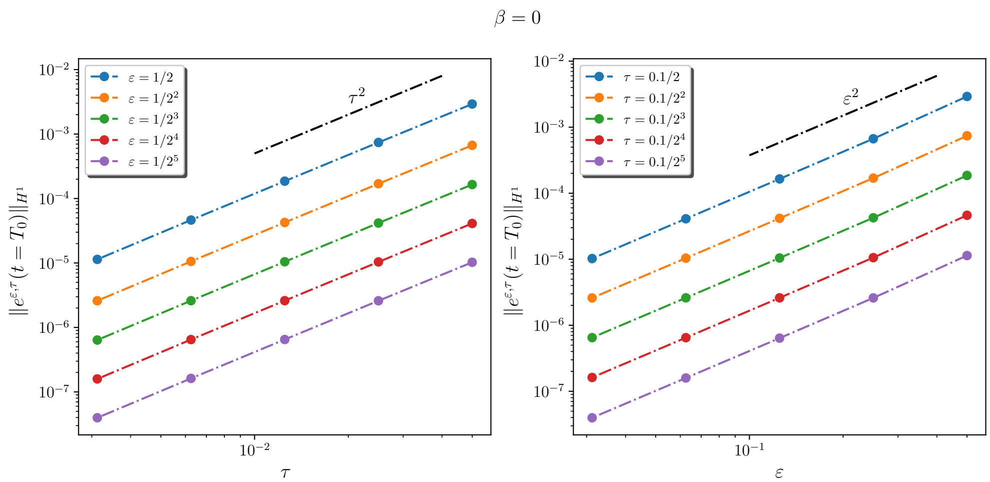

Figure 4.2: The convergence rate of $\|e^{\varepsilon,\tau}(t = T_{\varepsilon,\beta})\|_{H^1}$ with different ε and τ for $\beta = 0$.

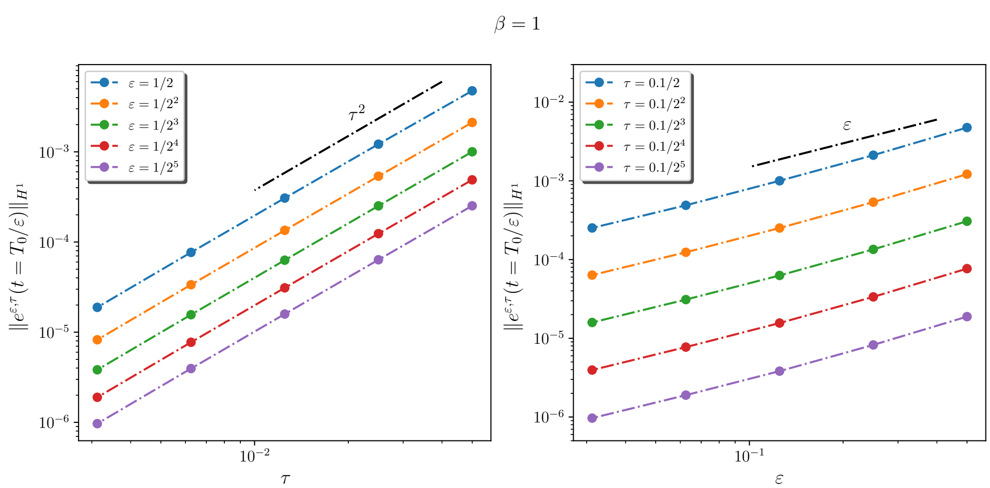

Figure 4.3: The convergence rate of $\|e^{\varepsilon,\tau}(t = T_{\varepsilon,\beta})\|_{H^1}$ with different ε and τ for $\beta = 1$.

$\|e^{\varepsilon,\tau}(t=T_0)\|_{H^1}$	$\tau=0.1$	$\tau=0.1/2$	$\tau=0.1/2^2$	$\tau=0.1/2^3$	$\tau=0.1/2^4$	$\tau=0.1/2^5$
$\varepsilon=1$	6.78E-2	1.68E-2	4.24E-3	1.07E-3	2.66E-4	6.54E-5
rate	-	2.01	1.99	1.99	2.00	2.03
$\varepsilon=1/2$	1.12E-2	2.92E-3	7.40E-4	1.86E-4	4.63E-5	1.14E-5
rate	-	1.94	1.98	1.99	2.00	2.03
$\varepsilon=1/2^2$	2.55E-3	6.69E-4	1.69E-4	4.24E-5	1.06E-5	2.59E-6
rate	-	1.93	1.98	2.00	2.00	2.03
$\varepsilon=1/2^3$	6.27E-4	1.65E-4	4.17E-5	1.04E-5	2.60E-6	6.38E-7
rate	-	1.93	1.98	2.00	2.01	2.03
$\varepsilon=1/2^4$	1.56E-4	4.10E-5	1.04E-5	2.60E-6	6.48E-7	1.59E-7
rate	-	1.93	1.98	2.00	2.01	2.03
$\varepsilon=1/2^5$	3.90E-5	1.02E-5	2.59E-6	6.50E-7	1.62E-7	3.97E-8
rate	-	1.93	1.98	2.00	2.01	2.03

Table 4.2: Temporal error analysis for EWI-FP when $\beta=0$ with different and ε. The convergence rate is computed as $\log_2(\|e^{\varepsilon,2\tau}(t=T_{\varepsilon,\beta})\|_{H^1}/\|e^{\varepsilon,\tau}(t=T_{\varepsilon,\beta})\|_{H^1})$.

$\|e^{\varepsilon,\tau}(t=T_0/\varepsilon)\|_{H^1}$	$\tau=0.1$	$\tau=0.1/2$	$\tau=0.1/2^2$	$\tau=0.1/2^3$	$\tau=0.1/2^4$	$\tau=0.1/2^5$
$\varepsilon=1$	6.78E-2	1.68E-2	4.24E-3	1.07E-3	2.66E-4	6.54E-5
rate	-	2.01	1.99	1.99	2.00	2.03
$\varepsilon=1/2$	1.81E-2	4.75E-3	1.22E-3	3.07E-4	7.67E-5	1.89E-5
rate	-	1.93	1.97	1.99	2.00	2.02
$\varepsilon=1/2^2$	8.14E-3	2.12E-3	5.37E-4	1.35E-4	3.36E-5	8.24E-6
rate	-	1.94	1.98	1.99	2.00	2.03
$\varepsilon=1/2^3$	3.88E-3	1.00E-3	2.52E-4	6.29E-5	1.56E-5	3.83E-6
rate	-	1.95	1.99	2.00	2.01	2.03
$\varepsilon=1/2^4$	1.88E-3	4.89E-4	1.24E-4	3.10E-5	7.73E-6	1.90E-6
rate	-	1.94	1.98	2.00	2.01	2.03
$\varepsilon=1/2^5$	9.67E-4	2.52E-4	6.36E-5	1.59E-5	3.95E-6	9.68E-7
rate	-	1.94	1.99	2.00	2.01	2.03

Table 4.3: Temporal error analysis for EWI-FP when $\beta=1$ with different and ε. The convergence rate is computed as $\log_2(\|e^{\varepsilon,2\tau}(t=T_{\varepsilon,\beta})\|_{H^1}/\|e^{\varepsilon,\tau}(t=T_{\varepsilon,\beta})\|_{H^1})$.

$\|e^{\varepsilon,\tau}(t=T_0/\varepsilon^2)\|_{H^1}$	$\tau=0.1$	$\tau=0.1/2$	$\tau=0.1/2^2$	$\tau=0.1/2^3$	$\tau=0.1/2^4$	$\tau=0.1/2^5$
$\varepsilon=1$	6.78E-2	1.68E-2	4.24E-3	1.07E-3	2.66E-4	6.54E-5
rate	-	2.01	1.99	1.99	2.00	2.03
$\varepsilon=1/2$	3.35E-2	8.41E-3	2.12E-3	5.31E-4	1.32E-4	3.24E-5
rate	-	1.99	1.99	2.00	2.00	2.03
$\varepsilon=1/2^2$	3.15E-2	7.96E-3	2.01E-3	5.04E-4	1.26E-4	3.08E-5
rate	-	1.98	1.99	2.00	2.00	2.03
$\varepsilon=1/2^3$	3.19E-2	8.03E-3	2.03E-3	5.08E-4	1.27E-4	3.10E-5
rate	-	1.99	1.99	2.00	2.00	2.03
$\varepsilon=1/2^4$	3.42E-2	8.43E-3	2.10E-3	5.25E-4	1.31E-4	3.20E-5
rate	-	2.02	2.00	2.00	2.01	2.03
$\varepsilon=1/2^5$	3.39E-2	8.33E-3	2.07E-3	5.16E-4	1.28E-4	3.13E-5
rate	-	2.03	2.01	2.01	2.01	2.03

Table 4.4: Temporal error analysis for EWI-FP when $\beta=2$ with different and ε. The convergence rate is computed as $\log_2(\|e^{\varepsilon,2\tau}(t=T_{\varepsilon,\beta})\|_{H^1}/\|e^{\varepsilon,\tau}(t=T_{\varepsilon,\beta})\|_{H^1})$.

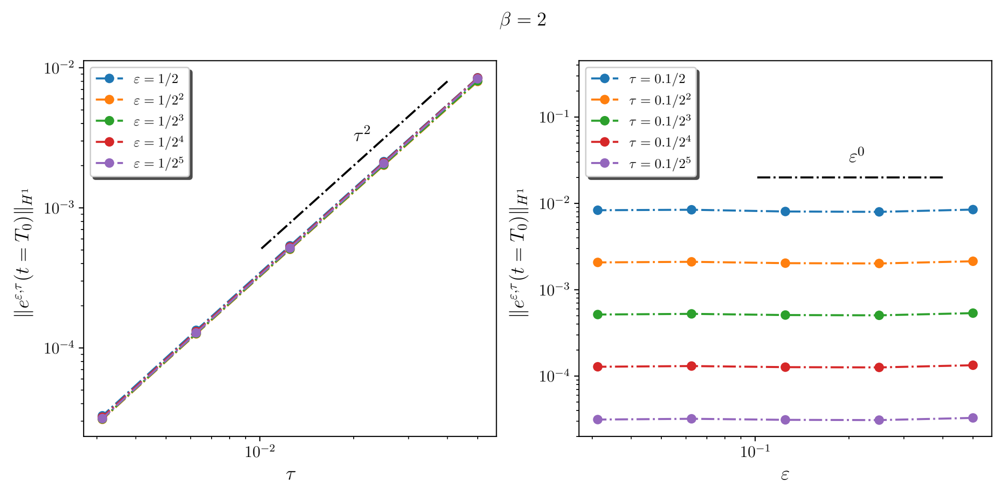

Figure 4.4: The convergence rate of $\|e^{\varepsilon,\tau}(t=T_{\varepsilon,\beta})\|_{H^1}$ with different ε and τ for $\beta=2$.

4.4.2 Long-time dynamics of NLSW

Our EWI-FP (4.2.24) can be easily generalized to the 2D NLSW equation with weak nonlinearity on torus as follows (denote $\psi:=\psi(x,y,t)$, $\Omega=(a_x,b_x)\times(a_y,b_y)$):

$$\begin{cases} i\partial_t\psi-\alpha\partial_{tt}\psi+\nabla^2\psi-\varepsilon^2|\psi|^2\psi=0,\ (x,y)\in\Omega,\ t>0,\\ \psi(x,y,0)=\psi_0(x,y),\ \partial_t\psi(x,y,0)=\psi_1(x,y),\ (x,y)\in\overline{\Omega},\\ \psi(a_x,y,t)=\psi(b_x,y,t),\ \partial_x\psi(a_x,y,t)=\partial_x\psi(b_x,y,t),\ y\in(a_y,b_y),\ t\geq 0,\\ \psi(x,a_y,t)=\psi(x,b_y,t),\ \partial_y\psi(x,a_y,t)=\partial_y\psi(x,b_y,t),\ x\in(a_y,b_y),\ t\geq 0.\end{cases} \tag{4.4.2}$$

In this subsection, we will show numerical simulations for the dynamics of the density $|\psi(x,y,t)|^2$ of the equation (4.4.2). For the following simulations, we choose the torus to be $\Omega = [-\pi,\pi]\times[-\pi,\pi]$, $\alpha = 1/4$ and $\beta = 2$. The initial wave and velocity are chosen as

$$\psi_0(x,y) = \frac{1}{4+\cos^2(x)+\cos^2(y)}, \quad \psi_1(x,y) = \sin(x)+\sin(y).$$

The following Figures 4.5, 4.6, 4.7 and 4.8 show the contour maps of $|\psi(x,y,t)|^2$ at different times with the given conditions and different ε. The ε is chosen as $\varepsilon = 0, 1/2, 1/4, 1/8$ respectively for Figures 4.5, 4.6, 4.7 and 4.8. The time points are kT_0/ε^β, where $T_0 = 0.2$ and $k = 0,1,2,3,4,5$.

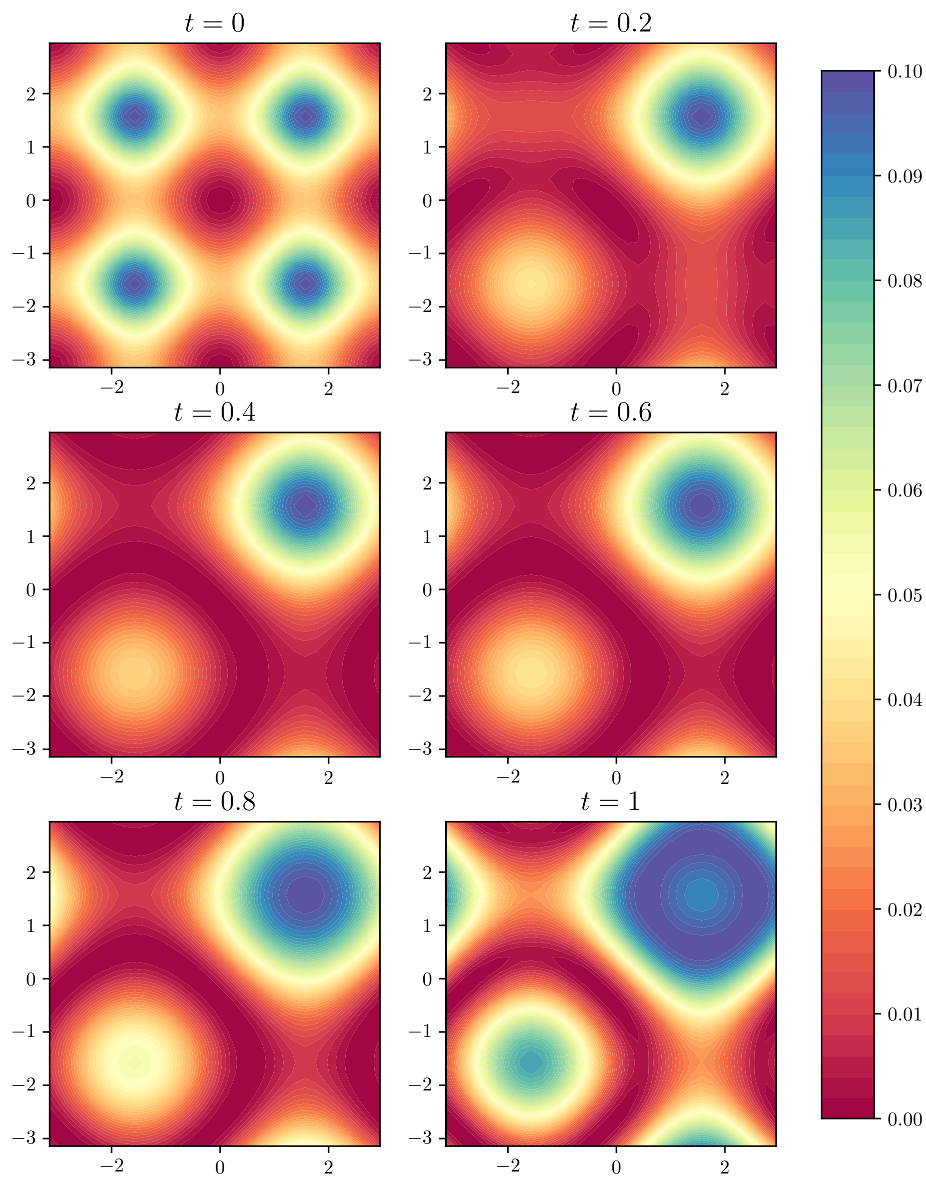

Figure 4.5: Contour map of of $|\psi(x, y, t)|^2$ at different times when $\varepsilon = 1$.

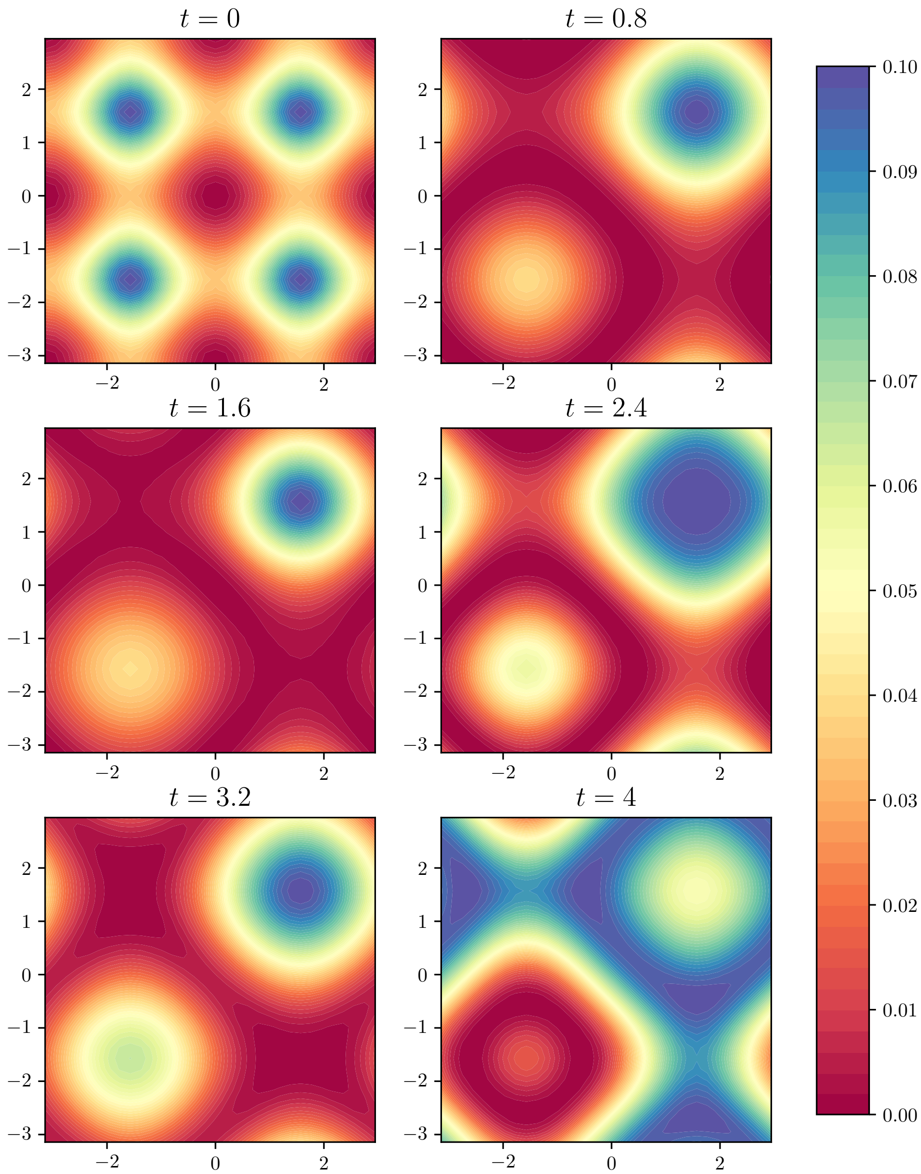

Figure 4.6: Contour map of of $|\psi(x, y, t)|^2$ at different times when $\varepsilon = 1/2$.

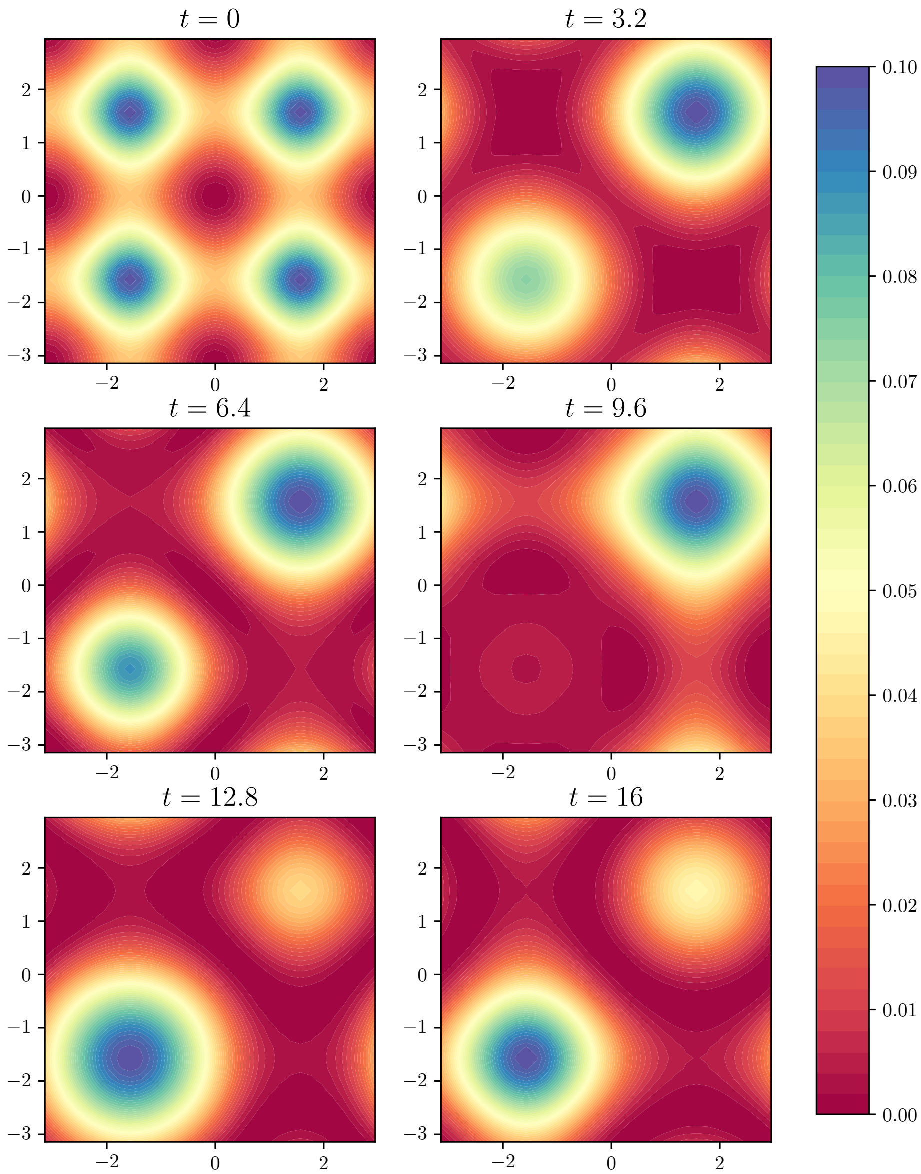

Figure 4.7: Contour map of of $|\psi(x, y, t)|^2$ at different times when $\varepsilon = 1/4$.

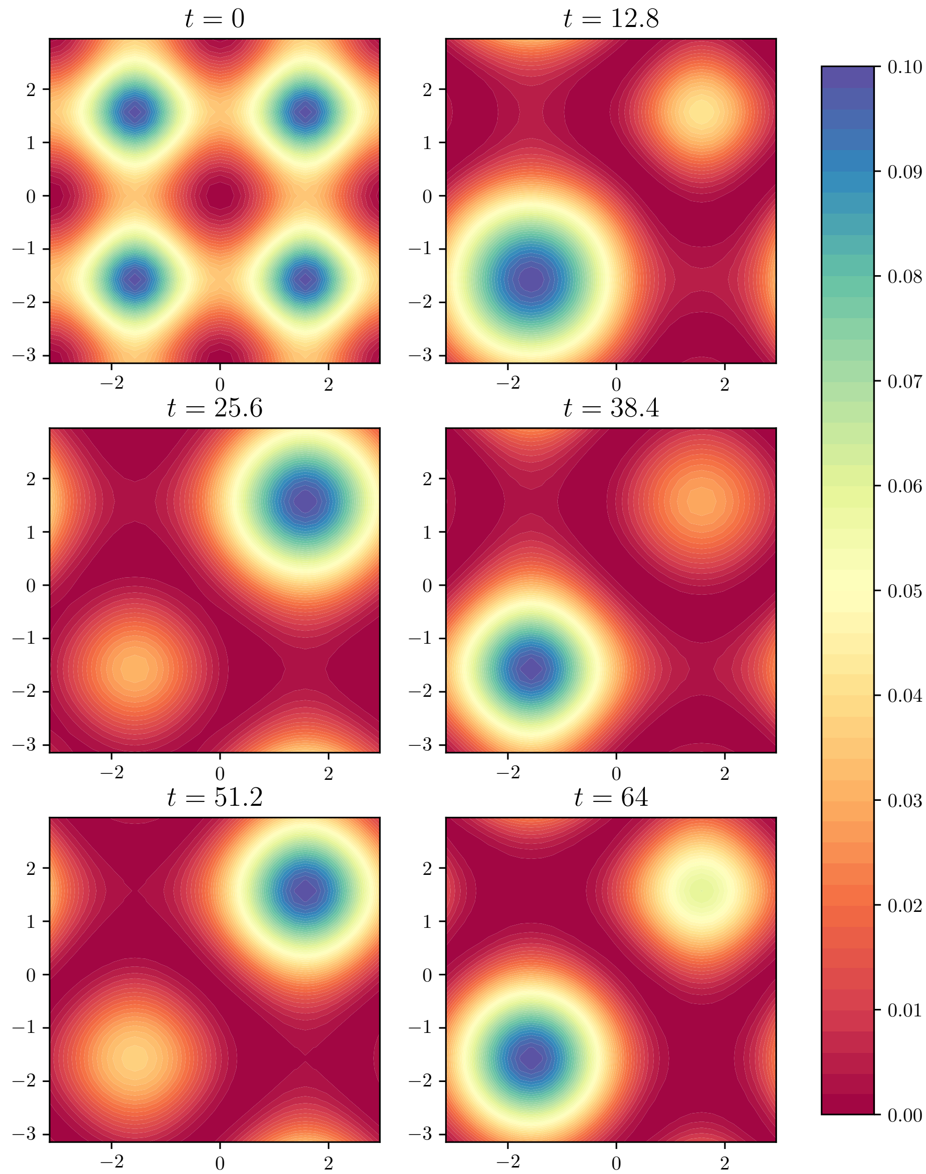

Figure 4.8: Contour map of of $|\psi(x, y, t)|^2$ at different times when $\varepsilon = 1/8$.

Chapter 5

Conclusions and Future Works

This thesis is devoted to study the multiscale methods for the Nonlinear Schrödinger Equation with Wave Operator (NLSW). The numerical schemes. Several multiscale methods for the NLSW and related equations are presented, including the NLSW, the ODE system arises from a spatial discretization of the NLSW, and the NLSW with a weak nonlinearity up to long-time. The error bounds are presented and rigorously proved. The main work of the thesis is summarized as follows, and possible future topics are also listed.

1. Nested Picard Integrators for Oscillatory ODEs

In this chapter, we have constructed and analyzed a uniformly second order accurate nested Picard integrator for an oscillatory complex ordinary differential system involving a parameter $\varepsilon \in (0, 1]$. The ODE system arises from a spatial discretization of the NLSW after applying suitable spatial discretization such as finite difference. The initial data can be categorized into well-prepared case and ill-prepared case, and for both ill-prepared case $0 \leq \alpha < 2$ and well-prepared case $\alpha \geq 2$, it was rigorously proved that the method is uniformly second order in time w.r.t. $\varepsilon \in (0, 1]$, and for fixed ε, the method converges with third order accuracy in time step τ as $\tau \to 0$. Numerical results confirmed the uniform accuracy. The NPI method could also be applied to related NLSW, and is discussed in detail in the next chapter.

2. Nested Picard Integrators for NLSW

In this chapter, we have presented a NPI-SP method for the nonlinear Schrödinger equation with wave operator with a small parameter $\varepsilon \in (0,1]$ describing the perturbation strength. The difficulty of achieving uniform second order in time is the unboundedness of $\partial_{tt}\psi(x,t)$ for ill-prepared initial data. We have applied the idea of nested Picard integrator for temporal discretization to overcome this difficulty. Using sine pseudospectral method for spatial discretization, the uniform spectral accuracy in mesh size h and the uniform $O(\tau^2)$ convergence rate in time step τ of NPI-SP in H^1 norm are proved rigorously. This improves the convergence results of EWI-SP in previous works. Numerical results confirms the theoretical estimates. The third order convergence in time step τ as $\tau \to 0$, similar to the ODE case in the previous chapter are also observed numerically.

3. An EWI-FP Method for Long-time Dynamics of NLSW

We have proposed an EWI-FP method for the nonlinear Schrödinger equation with wave operator and a with weak nonlinearity in this chapter. This equation with $O(1)$ initial data can be reformulated as the following NLSW with $O(1)$ nonlinearity and small initial data. An efficient and accurate EWI-FP scheme is proposed by applying exponential wave integrator for temporal discretization and Fourier pseudospectral method for spatial discretization. Uniform error bounds of the EWI-FP method are rigorously carried out up to the time $t = T_0/\varepsilon^\beta$ with $0 \le \beta \le 2$ and T_0 fixed. Numerical results confirms the uniform spectral accuracy in mesh size h and the uniform $O(\varepsilon^{-\beta}\tau^2)$ convergence rate in time step τ and its optimality, and applications in higher dimension cases are presented.

Some possible future projects are listed as follows.

- Solve the nonlinear Schrödinger equation with wave operator (NLSW) (1.2.1) with initial data (1.2.6), involving singular initial data, i.e. $-2 < \alpha < 0$ in (1.2.6).

- Increase the number of nested Picard iterations to achieve higher order accuracy in time.

- Propose NPI methods for coupled NLSW [16, 17].

- Propose Lawson-type EWI methods [19, 81, 82] for NLSW .

- Compare different numerical methods for NLSW.

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List of Publications

[1] Y. Cai and Y. Guo, "Uniformly accurate nested Picard integrators for a system of oscillatory ordinary differential equations", *BIT Numer. Math.*, pp. 1–38, 2021.

[2] Y. Cai and Y. Guo, "Uniform and optimal error estimate of a nested picard integrator for the nonlinear Schrödinger equation with wave operator", preprint.

[3] W. Bao and Y. Guo, "Uniform error estimate of a exponential wave integrator for the long-time dynamics of the nonlinear Schrödinger equation with wave operator and weak nonlinearity", in preparation.