A CONSTRUCTIVE LOW-REGULARITY INTEGRATOR FOR THE 1D CUBIC NONLINEAR SCHRÖDINGER EQUATION UNDER THE NEUMANN BOUNDARY CONDITION

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Abstract. A new harmonic analysis technique by using the Littlewood–Paley dyadic decomposition is developed for constructing low-regularity integrators for the one-dimensional cubic nonlinear Schrödinger equation in a bounded domain under the Neumann boundary condition, when the frequency analysis based on the Fourier series cannot be used. In particular, a low-regularity integrator is constructively designed through the consistency analysis by the Littlewood–Paley decomposition of the solution, in order to have almost first-order convergence (up to a logarithmic factor) in the L^2 norm for H^1 initial data. A spectral method in space, using fast Fourier transform with $O(N\ln N)$ operations at every time level, is constructed without requiring any CFL condition, where N is the degrees of freedom in the spatial discretization. The proposed fully discrete method is proved to have an L^2-norm error bound of $O(\tau[\ln(1/\tau)]^2+N^{-1})$ for H^1 initial data, where τ is the time stepsize.

1. Introduction

Classical time discretization methods for the nonlinear Schrödinger (NLS) equation typically requires the initial data to be in $H^{\gamma+2m}$ in order to have mth-order convergence in H^γ (for sufficiently large $\gamma>0$), where $H^{\gamma+2m}$ denotes the conventional Sobolev space and m is a positive integer. This requirement is optimal for the Strang splitting methods [5, 18], the Lie splitting method [9], and classical exponential integrators [7]. The finite difference methods generally require more regularity of the initial data, i.e., one temporal derivative on the solution generally requires the initial data to have two spatial derivatives to satisfy certain compatibility conditions; see [24, 26].

Recently, a low-regularity type exponential integrator was introduced in [8, 21] to reduce the regularity requirement in solving nonlinear dispersive equations under periodic boundary conditions. For $\gamma>\frac{d}{2}$, where d denotes the dimension of space, such low-regularity integrators can have first-order convergence in H^γ for initial data in $H^{\gamma+1}$. In one dimension, a low-regularity integrator was proposed in [27] with first-order convergence in H^γ for initial data in H^γ when $\gamma>\frac{3}{2}$. These results imply that it is possible to develop first-order convergent numerical methods when the regularity of the solution is strictly below H^2. A second-order low-regularity integrator for the NLS equation was constructed in [10], which requires the initial data to be in $H^{\gamma+2}$ and $H^{\gamma+3}, \gamma>\frac{d}{2}$ when $d=1$ and $d\geq 2$, respectively.

The techniques were also used in developing low-regularity integrators for other nonlinear dispersive equations, including the nonlinear Dirac equations and the KdV equations; see [16, 21, 22, 25, 28, 29]. Lower-order convergence of the numerical solution when the regularity of the solution is below H^1 was analyzed by using the discrete Bourgain spaces introduced in [20]. A fully discrete low-regularity integrator for the NLS equation with a Fourier spectral method in space was constructed in [15], with computational cost $O(N\ln N)$ at every time level and has first-order convergence (up to a logarithmic factor) in both time and space for H^1 initial data, where N is the degree of freedom in the spatial discretization. All these results require periodic boundary conditions, as the numerical methods were constructed by using the twisted-variable techniques based on the Fourier series expansion of the solution in the Duhamel formula.

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Under general boundary conditions (including periodic, Dirichlet and Neumann boundary conditions), a general framework of low-regularity integrators was introduced in [23] based on the semigroup techniques without using Fourier series expansion of the solution. In one dimension, it is shown that the numerical solution of the NLS equation can have first-order convergence when the initial data is in $H^{\frac{5}{4}}$. Generalisations of these schemes have been completed in recent works by using combinatorial objects that are decorated trees for writing low regularity schemes for a large class of PDEs; see [2, 3]. Under the Dirichlet or Neumann boundary condition, the following results still remain open:

- The construction of a first-order low-regularity integrator which only requires the initial data to be in H^1;
- The extension to fully discrete low-regularity integrators under the same regularity requirement.

Note that the harmonic analysis techniques in [15] is on the frequency domain and therefore significantly relies on the following property of the eigenfunctions of periodic Laplacian:

$$e^{ik_1x}e^{ik_2x} = e^{i(k_1+k_2)x} \quad \text{for } k_1, k_2 \in \mathbb{N},$$

while this property does not hold for the eigenfunctions of the Neumann Laplacian, i.e.,

$$\cos(k_1x)\cos(k_2x) \neq \cos[(k_1+k_2)x] \quad \text{for } k_1, k_2 \geq 1.$$

As a result, the frequency analysis techniques in [15] can not be used under the Neumann boundary condition.

The objective of this article is to fill in this gap for the one-dimensional NLS equation under the Neumann boundary condition, by constructing a fully discrete low-regularity integrator which has computational cost $O(N \ln N)$ at every time level and first-order convergence (up to a logarithmic factor) in both time and space for H^1 initial data. We shall construct and analyze a new method by developing new harmonic analysis techniques on the physical domain, utilizing the Littlewood–Paley dyadic decomposition of the solution. More specifically, in the variation-of-constants formula

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda \int_0^\tau e^{i(\tau-s)\partial_x^2}[|u(t_n+s)|^2 u(t_n+s)]\mathrm{d}s,$$

we approximate the function $u(t_n+s)$ by $e^{is\partial_x^2}u(t_n)$ as usual and therefore obtain the following expression of the solution:

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda \int_0^\tau e^{i(\tau-s)\partial_x^2}[e^{-is\partial_x^2}\bar{u}(t_n)e^{is\partial_x^2}u(t_n)e^{is\partial_x^2}u(t_n)]\mathrm{d}s + R_1^n.$$

The remainder R_1^n can be estimated as usual, with $\|R_1^n\|_{H^1} \leq C\tau^2\|u\|^5_{L^\infty(0,T;H^1)}$. This is the same as starting stage in the construction of the low-regularity integrators in [2, 15, 23]. <u>The main idea of this article is</u> to rewrite the above formula into the following form:

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda \int_0^\tau B^n(s, u(t_n))\mathrm{d}s + R_1^n$$

with

$$B^n(s, u(t_n)) = e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}v(s)\big] \quad \text{and} \quad v(s) = e^{-is\partial_x^2}\big(e^{is\partial_x^2}u(t_n)\big)^2,$$

and then decompose $B^n(s, u(t_n))$ into the following three parts:

$$B^n(s, u(t_n)) = B_1^n(s, u(t_n)) + e^{i\tau\partial_x^2}B_2^n(s, u(t_n)) + r_2^n(s)$$

with

$$\begin{aligned} B_1^n(s, u(t_n)) &= e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}v(0)\big]; \\ B_2^n(s, u(t_n)) &= \bar{u}(t_n)\,(v(s) - v(0)) \\ r_2^n(s) &= e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}(v(s) - v(0))\big] - e^{i\tau\partial_x^2}\big[\bar{u}(t_n)(v(s) - v(0))\big], \end{aligned}$$

where $r_2^n(s)$ is a remainder to be dropped in the numerical scheme. In this decomposition, $B_1^n(s, u(t_n))$ is an approximation of $B^n(s, u(t_n))$ by the commutator technique in [23], i.e., approximating $v(s) = e^{-is\partial_x^2}\big(e^{is\partial_x^2}u(t_n)\big)^2$ by $v(0)$ in the expression of $B^n(s, u(t_n))$ yields $B_1^n(s, u(t_n))$

with the remainder

$$e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}(v(s)-v(0))\big].$$

We further approximate this remainder by $e^{i\tau\partial_x^2}B_2^n(s,u(t_n))$. This leads to the new remainder $R_2^n=\int_0^\tau r_2^n(s)\mathrm{d}s$. This further approximation, as well as the discovery of the closed forms of

$$\int_0^\tau B_1^n(s,u(t_n))\mathrm{d}s \quad\text{and}\quad \int_0^\tau B_2^n(s,u(t_n))\mathrm{d}s, \tag{1.1}$$

is inspired by the frequency analysis in [15]. The resulting remainder $R_2^n=\int_0^\tau r_2^n(s)\mathrm{d}s$ can be estimated by distributing the derivatives more equally to the functions in the product through the analysis using the Littlewood-Paley decomposition. The technical parts of this article are the derivation of the closed forms for the two integrals in (1.1), the error analysis for the time discretization by the Littlewood-Paley decomposition, as well as the construction and analysis of the spatial discretization with rigorous error estimates.

The construction of the low-regularity integrators in [2, 23] treat general nonlinearities by using the fundamental theorem of calculus and by exploring the cancellation of the highest-order derivative using commutators, while the low-regularity integrator constructed in this article is constructively designed based on more detailed analysis of a specific form of nonlinearities, such as the cubic nonlinearity in the NLS equation, by combining the commutator approach in [23] and the frequency analysis in [15] (as mentioned above), as well as the error analysis using the Littlewood–Paley decomposition. As a result, the scheme constructed in this article can further weaken the regularity condition for a specific form of nonlinearity, while the schemes in [2, 23] work well for more general nonlinearities.

In the construction of spatial discretization, several techniques are introduced to resolve the incompatibility between the low-regularity integrator and the Neumann boundary condition. These techniques can also be used for the construction of spatial discretization methods for other low-regularity integrators under the Neumann boundary condition.

The rest of this article is organised as follows. The fully discrete low-regularity integrator and the main theorem are presented in Section 2. The construction of the time discretization method and the analysis of its consistency error are presented in Section 4. The construction of the spatial discretization method and the analysis of its consistency error are presented in section Section 5. The stability and error analysis for the fully discrete method are presented in Section 6. Numerical results are provided in Section 7 to support the theoretical analysis and to illustrate the performance of the proposed numerical method.

2. The main results

Let H^s, $s\in\mathbb{R}$, be the conventional Sobolev space of functions on the domain $\Omega=(0,\pi)$. We consider the one-dimensional cubic NLS equation

$$\begin{cases} i\partial_t u(t,x)+\partial_x^2 u(t,x)=\lambda|u(t,x)|^2u(t,x) & \text{for } x\in\Omega \text{ and } t\in(0,T],\\ \partial_x u(t,x)=0 & \text{for } x\in\partial\Omega \text{ and } t\in(0,T],\\ u(0,x)=u^0(x) & \text{for } x\in\Omega, \end{cases} \tag{2.1}$$

on the bounded domain Ω, where $\lambda=-1$ and 1 correspond to the focusing and defocusing cases, respectively.

Let S_N and C_N be the finite-dimensional subspaces of $L^2(\Omega)$ defined by

$$S_N=\Big\{f\in L^2: f=\sum_{k=1}^N \hat{f}_k\sin(kx)\Big\} \quad\text{and}\quad C_N=\Big\{f\in L^2: f=\sum_{k=0}^N \hat{f}_k\cos(kx)\Big\},$$

and denote by ∂_x^{-2} the inverse of the Neumann Laplacian in the sense of Fourier cosine multiplier on Ω. For any $f=\sum_{k=0}^N\hat{f}_k\cos(kx)$, with the Fourier cosine coefficients $\hat{f}_k$, $k=0,\dots,N$, stored in the computer, one can easily compute the Fourier cosine coefficients of $\partial_x^{-2}f\in C_N$ and

$e^{is\partial_x^2} f \in C_N$ by

$$\partial_x^{-2} f := -\sum_{k=1}^{N} k^{-2} \hat{f}_k \cos(kx) \quad \text{and} \quad e^{is\partial_x^2} f := \sum_{k=0}^{N} e^{-isk^2} \hat{f}_k \cos(kx) \tag{2.2}$$

and the Fourier sine coefficients of $\partial_x f \in S_N$ by

$$\partial_x f = -\sum_{k=1}^{N} k \hat{f}_k \sin(kx). \tag{2.3}$$

If $f, g \in S_N$ then the $fg \in C_{2N} \cap H_0^1$. And if $f, g \in C_N$ then the $fg \in C_{2N}$.

Let $I_N : H^1 \to C_N$ be the trigonometric cosine interpolation operator, i.e., $I_N f$ is obtained by first extending f to be an even function on the torus $[-\pi, \pi]$ and then applying the standard $(2N+1)$-term trigonometric interpolation on the torus; see [15, eq. (2.5)]. The trigonometric interpolation of the even function would yield a cosine series which, restricted to $\Omega = (0, \pi)$, is the function $I_N f$. To be more precise, given $f \in H^1(0, \pi)$, we denote its even extension as $\widetilde{f} \in \{u \in H^1(-\pi, \pi) : u(-\pi) = u(\pi)\} \cong H^1(\mathbb{T})$. Then $I_N : H^1(0, \pi) \to C_N$ is defined as

$$I_N f(x) := \sum_{k=-N}^{N} e^{ikx} \widetilde{f}_k \quad \text{for } \widetilde{f}_k = \frac{1}{2N+1} \sum_{n=-N}^{N} e^{-ikx_n} \widetilde{f}(x_n)$$

where

$$x_n = \frac{2\pi n}{2N+1} \quad \text{for } n = -N, ..., N.$$

Since $\widetilde{f}$ is an even function, we have $\widetilde{f}_k = \widetilde{f}_{-k}$, and this leads to $I_N f \in C_N$. Furthermore we define the averaging operator

$$Sf := \frac{1}{\pi} \int_\Omega f(x) \mathrm{d}x \tag{2.4}$$

and the projection operator

$$\Pi_N f := \sum_{k=0}^{N} \hat{f}_k \cos(kx) \quad \text{for } f = \sum_{k=0}^{\infty} \hat{f}_k \cos(kx).$$

Let $t_n = n\tau$, $n = 0, 1, \ldots, L$, be a sequence of time levels with stepsize τ and $L = [T/\tau]$. The fully discrete low-regularity integrator for (2.1) constructed in this paper is defined as follows: Let $u_N^0 = I_N u^0$, and for given $u_N^n \in C_N$ compute $u_N^{n+1} \in C_N$ by

$$u_N^{n+1} = e^{i\tau\partial_x^2} u_N^n + \widehat{A}_1^N(\tau, u_N^n) - \widehat{A}_1^N(0, u_N^n) + e^{i\tau\partial_x^2} \widehat{A}_2^N(\tau, u_N^n) - e^{i\tau\partial_x^2} \widehat{A}_2^N(0, u_N^n), \tag{2.5}$$

where

$$\begin{aligned} \widehat{A}_1^N(s, u_N^n) = &\frac{1}{2}\lambda e^{i(\tau-s)\partial_x^2} \Pi_N \partial_x^{-2} \partial_x \left[\partial_x \partial_x^{-2} e^{-is\partial_x^2} \bar{u}_N^n \, e^{is\partial_x^2} \Pi_N(u_N^n u_N^n)\right] \\ &- is\lambda S[\overline{u}_N^n \Pi_N(u_N^n u_N^n)] \\ &- is\lambda S\overline{u}_N^n \Pi_N(e^{i\tau\partial_x^2}(u_N^n u_N^n) - S(u_N^n u_N^n)), \end{aligned} \tag{2.6}$$

$$\begin{aligned} \widehat{A}_2^N(s, u_N^n) = &\frac{\lambda}{2} \Pi_N \left[\bar{u}_N^n \, e^{-is\partial_x^2} \Pi_N \left(\partial_x \partial_x^{-2} e^{is\partial_x^2} u_N^n\right)^2\right] \\ &+ is\lambda \Pi_N \left(\overline{u}_N^n \Pi_N(u_N^n u_N^n)\right) \\ &- 2is\lambda S u_N^n \Pi_N(|u_N^n|^2) \\ &+ is\lambda (S u_N^n)^2 \overline{u}_N^n. \end{aligned} \tag{2.7}$$

The construction of the method is presented in Section 4. From (2.5)–(2.7) we see that the method only requires computing several functions of the following two types:

- $\partial_x^{-2} f$, $\partial_x f$ and $e^{\pm i\tau\partial_x^2} f$ for some function $f \in C_{2N}$,
- fg, fh, and hk for some functions $f, g \in C_N$, and $h, k \in S_N$.

The coefficients of Fourier cosine series of the first type of functions can be computed exactly by (2.2)–(2.3). The coefficients of Fourier sine series of the second type of functions can be computed exactly by using the $(4N+1)$-point fast Fourier transform (FFT). For example, we can extend f and h to be odd and even functions on the torus $(-\pi, \pi)$ and then apply the $(4N+1)$-point FFT (first evaluate, then do trigonometric interpolation at $(4N+1)$ equidistant points) to compute the Fourier coefficients of the odd function fh exactly. Hence, the computational cost is $O(N \ln N)$ at every time level.

The convergence of the proposed fully discrete method in (2.5) is presented in the following theorem.

Theorem 2.1. *If $u^0 \in H^1$ then there exist positive constants τ_0, N_0 and C such that for $\tau \le \tau_0$ and $N \ge N_0$ the numerical solution given by* (2.5) *has the following error bound:*

$$\max_{1\le n\le L} \|u(t_n,\cdot) - u_N^n\|_{L^2} \le C\big(\tau[\ln(1/\tau)]^2 + N^{-1}\big), \tag{2.8}$$

where $L := \lfloor T/\tau \rfloor$ and the constants τ_0, N_0 and C depend only on T and $\|u^0\|_{H^1}$.

The rest of this paper is devoted to the construction of the method (2.5) and the proof of Theorem 2.1.

3. Preliminary results

In this section, we introduce the basic notation and harmonic analysis results to be used in the construction and analysis of the numerical method.

3.1. Notation

Let H^s be the conventional Sobolev space on $\Omega = (0, \pi)$, with $L^2 = H^0$. The sesquilinear inner product and norm on L^2 are denoted by

$$(f, g) = \int_\Omega f(x)\overline{g(x)}\,\mathrm{d}x \quad \text{and} \quad \|f\|_{L^2} = \sqrt{(f, f)},$$

respectively. Moreover we define the dotted Sobolev space on $\Omega = (0, \pi)$ as

$$\dot{H}^s(\Omega) = \Big\{ \sum_{k=0}^{\infty} \hat{f}_k \cos(kx) : |\hat{f}_0|^2 + \sum_{k=1}^{\infty} |k|^{2s} \big|\hat{f}_k\big|^2 < \infty \Big\}, \tag{3.1}$$

and we will specify its norm in the next section.

3.2. Eigenfunctions expansion and the $\dot{H}^s$ norm

We consider the Neumann Laplacian $\Delta : D(A) \to L^2$, where $A = -\Delta$ has the following domain:

$$D(A) = \{v \in H^2 : \partial_x v(x) = 0 \ \text{ at } \ x = 0, \pi\}.$$

Any $f \in L^2$ can be expanded into a series of the eigenfunctions of A, i.e.,

$$f = \sum_{k=0}^{\infty} \hat{f}_k \cos(kx) \quad \text{with} \quad \hat{f}_k = \frac{2}{\pi} \int_\Omega f(x) \cos(kx)\mathrm{d}x. \tag{3.2}$$

It is straightforward to verify that

$$\begin{aligned}
\partial_x f &= -\sum_{k=1}^{\infty} k \hat{f}_k \sin(kx) && \text{for } f \in H^1 = D(A^{\frac12}),\\
\partial_x^2 f &= -\sum_{k=1}^{\infty} k^2 \hat{f}_k \cos(kx) && \text{for } f \in D(A),\\
\partial_x^2 \partial_x^{-2} f = Pf &:= \sum_{k=1}^{\infty} \hat{f}_k \cos(kx) && \text{for } f \in L^2
\end{aligned}$$

where

$$Pf = f - Sf, \quad \text{with } S \text{ defined in (2.4).}$$

and

$$\|f\|_{H^s}^2 \sim |\hat{f}_0|^2 + \sum_{k=1}^{\infty} |k|^{2s} |\hat{f}_k|^2 \quad \text{for } f \in \dot{H}^s \text{ and } s = 0, 1, 2, \tag{3.3}$$

where $\dot{H}^0 = L^2$, $\dot{H}^1 = H^1$ and $\dot{H}^2 = D(A)$.

Following [19, Definition 2.1, 2.3], we define the complex interpolation spaces as below. Let D be the strip $\{z = x + iy \in \mathbb{C} : 0 \le x \le 1\}$ and X, Y be two Banach spaces. Let $\mathcal{F}(X, Y)$ be the space of all functions $f : D \to X + Y$ such that

(i) f is holomorphic in the interior of D and continuous and bounded up to its boundary, with values in $X + Y$.

(ii) $t \mapsto f(it) \in C_b(\mathbb{R}; X), t \mapsto f(1 + it) \in C_b(\mathbb{R}; Y)$, and

$$\|f\|_{\mathcal{F}(X,Y)} = \max\{\sup_{t\in\mathbb{R}} \|f(it)\|_X, \sup_{t\in\mathbb{R}} \|f(1 + it)\|_Y\} < +\infty.$$

Then the complex interpolation space $(X, Y)_{[\theta]}$, with $\theta \in [0, 1]$, is defined through the traces on the real axis of the functions in $\mathcal{F}(X, Y)$, i.e., $(X, Y)_{[\theta]} := \{f(\theta) : f \in \mathcal{F}(X, Y)\}$ with the following quotient norm:

$$\|a\|_{(X,Y)_{[\theta]}} := \inf_{f\in\mathcal{F}(X,Y), f(\theta)=a} \|f\|_{\mathcal{F}(X,Y)}.$$

For $s \in [0, 2]$, $\dot{H}^s$ coincides with the complex interpolation space $(L^2, \dot{H}^2)_{[s/2]}$, with the following norm:

$$\|f\|_{\dot{H}^s} = \left(|\hat{f}_0|^2 + \sum_{k=1}^{\infty} |k|^{2s} |\hat{f}_k|^2\right)^{\frac{1}{2}} \quad \text{for } f \in \dot{H}^s. \tag{3.4}$$

This is equivalent to the conventional H^s norm, but has the following useful property (with equality instead of equivalence):

$$\|e^{it\partial_x^2} f\|_{\dot{H}^s} = \|f\|_{\dot{H}^s}. \tag{3.5}$$

Property (3.5) will be used in the stability estimates for the numerical method.

3.3. Littlewood–Paley type decomposition

We denote by $\mathbb{N}$ the set of nonnegative integers. For $N \in \mathbb{N}$ and $f = \sum_{k=0}^{\infty} \hat{f}_k \cos(kx)$, we define the following several projection operators on L^2:

$$\Pi_N f := \sum_{k=0}^{N} \hat{f}_k \cos(kx), \quad \Pi_{>N} f := f - \Pi_N f \quad \text{and} \quad P_N f := \Pi_{2N} f - \Pi_N f,$$

with $P_0 f := \Pi_1 f$. The following estimates are consequences of (3.3).

Lemma 3.1. *For $s = 0, 1, 2$, the following inequalities hold:*

$$\left\|\Pi_N f\right\|_{H^s} \lesssim N^s \|f\|_{L^2} \qquad \text{for } f \in L^2, \tag{3.6}$$

$$\left\|\Pi_{>N} f\right\|_{L^2} \lesssim N^{-s} \|f\|_{H^s} \quad \text{for } f \in \dot{H}^s, \tag{3.7}$$

$$\left\|P_N f\right\|_{H^s} \lesssim N^s \|f\|_{L^2} \qquad \text{for } f \in L^2. \tag{3.8}$$

If we denote by $\mathbb{N}_d = \{0\} \cup \{2^k : k \in \mathbb{N}\}$ the set of dyadic integers, then the following Littlewood–Paley type dyadic decomposition holds:

$$f = \sum_{N\in\mathbb{N}_d} P_N f \quad \text{for } f \in L^2. \tag{3.9}$$

and

$$\|f\|_{\dot{H}^s}^2 = \sum_{N\in\mathbb{N}_d} \|P_N f\|_{\dot{H}^s}^2 \quad \text{for } f \in \dot{H}^s \quad \text{for } s \in [0, 2]. \tag{3.10}$$

The following Kato–Ponce inequality and Gagliardo–Nirenberg interpolation inequality will be used in the analysis of the consistency error.

Lemma 3.2 (The Kato–Ponce inequality [11]). *If $s > \frac{1}{2}$ then*

$$\|fg\|_{H^s} \lesssim \|f\|_{H^s}\|g\|_{H^s} \quad \forall\, f, g \in H^s.$$

Lemma 3.3 (Gagliardo–Nirenberg interpolation inequality [1]).

$$\|f\|_{L^\infty} \lesssim \|f\|_{L^2}^{\frac{1}{2}}\|f\|_{H^1}^{\frac{1}{2}} \quad \forall\, f \in H^1.$$

Remark 3.4. *A powerful general Leibniz rule for fractional Laplacian operators has been recently established in the deep work of Li [?]. See also [?] for a remarkable new effective maximum principle which is developed for the first time for general spectral methods.*

3.4. Accuracy of trigonometric interpolation

The following trigonometric interpolation error estimate will be used in the construction of the spatial discretization.

Lemma 3.5 (Trigonometric interpolation error). *Let $f \in \dot H^\beta$ with $\beta \in [0,2]$. Then the following estimate holds for $N \ge 1$:*

$$\big\|f - I_N f\big\|_{H^\alpha} \lesssim N^{\alpha-\beta}\big\|f\big\|_{H^\beta} \quad \textit{if}\ \ 0 \le \alpha \le \beta\,.$$

Proof. If $f \in \dot H^\beta$ with $\beta \in [0,2]$, then its even extension $\tilde f$ is in $H^\beta(\mathbb{T})$, where $\mathbb{T}$ is the one-dimensional torus $[-\pi,\pi]$ that identifies the two endpoints $-\pi$ and π. For the function $\tilde f \in H^\beta(\mathbb{T})$ the trigonometric interpolation $\tilde I_N$ on the torus $[-\pi,\pi]$ has the following standard error bound (see [12, Theorem 11.8]):

$$\big\|\tilde f - \tilde I_N \tilde f\big\|_{H^\alpha(\mathbb{T})} \lesssim N^{\alpha-\beta}\big\|\tilde f\big\|_{H^\beta(\mathbb{T})} \lesssim N^{\alpha-\beta}\big\|f\big\|_{H^\beta} \quad \text{when}\ \ 0 \le \alpha \le \beta.$$

Since $I_N f$ is defined as the restriction of $\tilde I_N \tilde f$ to $\Omega = (0,\pi)$ (see the definition in Section 2), the above estimate implies the desired result of Lemma 3.5. □

3.5. Global well-posedness of NLS equation (2.1) in $\dot H^1 \cong H^1$

The Neumann boundary condition does not make sense when we consider low regularity solution, say H^1. Thus we need to find a suitable substitute function space. The space $\dot H^s$, defined by Fourier cosine multipliers, is an appropriate candidate in the sense that for large s, $s \ge 2$ for example, the derivative of the cosine Fourier series, which is a sine Fourier series, converges uniformly and thus vanishes at the boundary. Therefore, the functions in $\dot H^2$ satisfy the Neumann boundary condition. By the complex interpolation theory, see [6, Theorem 2.3] with the identifications $L^2 \cong B^0_{2,2}$ and $\dot H^2 = D(A) \cong B^2_{2,2,\mathcal{B}}$ therein, the following relation holds:

$$\begin{aligned}
&\dot H^s = (L^2, \dot H^2)_{[s/2]} = (B^0_{2,2}, B^2_{2,2,\mathcal{B}})_{[s/2]} = B^s_{2,2,\mathcal{B}} && \text{for}\ \ s \in (3/2, 2],\\
&\dot H^s = (L^2, \dot H^2)_{[s/2]} = H^s && \text{for}\ \ s \in [0, 3/2),
\end{aligned}$$

where $B^s_{p,q,\mathcal{B}}(\Omega) := \{u \in B^s_{p,q}(\Omega) : \partial_x u(x) = 0 \text{ at } x = 0,\pi\}$ with $s > 1 + 1/p$ denoting the subset of Besov space on $\Omega = (0,\pi)$ with gradient vanishing on the boundary. In particular, the functions in $\dot H^s$, with $s > 3/2$, satisfies the Neumann boundary condition. Similar results for real interpolation spaces with boundary conditions can be found in [17].

Analogous to unbounded domain and torus cases, we have the following global well-posedness result.

Theorem 3.6. *For $u^0 \in H^1$, there exists a unique solution $u \in C([0,T]; \dot H^1)$, with any $T > 0$, satisfying the integral equation:*

$$u(t) = e^{it\partial_x^2}u^0 - i\lambda \int_0^t e^{i(t-s)\partial_x^2}\big(|u(s)|^2 u(s)\big)\mathrm{d}s. \tag{3.11}$$

Proof. By the norm equivalence of H^s and $\dot{H}^s$ with $s \in [0,2]$, we know that $\dot{H}^1$ is an algebra under pointwise product. Follow the standard arguments in [4], then the local existence and uniqueness of solution follow directly from Banach fixed point theorem. Moreover the maximal local existence time $T_{loc} = T_{loc}(\|u^0\|_{\dot{H}^1})$ depends only on the $\dot{H}^1$ norm of the initial data.

Furthermore the global existence is a consequence of mass and energy conservation. Since the cubic nonlinearity is L^2 subcritical in one dimension, the global existence holds unconditionally for both focusing and defocusing cases. □

4. Construction and analysis of the time-stepping method

In this section we construct the numerical method through analysing the consistency error in approximating the Duhamel formula.

4.1. Construction of the time-stepping method

From Theorem 3.6 we know that the NLS equation (2.1), with initial value $u^0 \in H^1$, has a unique solution $u \in C([0,T]; H^1)$ satisfying Duhamel's formula:

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda \int_0^\tau e^{i(\tau-s)\partial_x^2}[|u(t_n+s)|^2 u(t_n+s)]\mathrm{d}s. \tag{4.1}$$

Moreover, the solution satisfies the mass conservation law

$$\frac{1}{\pi}\int_\Omega |u(t,x)|^2\,dx = \frac{1}{\pi}\int_\Omega |u^0(x)|^2\,dx \quad \text{for } t > 0. \tag{4.2}$$

For the simplicity of notation, we denote the mass of the solution by

$$M := \frac{1}{\pi}\int_\Omega |u^0(x)|^2\,dx. \tag{4.3}$$

Through approximating the function $u(t_n+s)$ in the integral of (4.1) by $e^{is\partial_x^2}u(t_n)$, we obtain

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda \int_0^\tau e^{i(\tau-s)\partial_x^2}[e^{-is\partial_x^2}\bar{u}(t_n)e^{is\partial_x^2}u(t_n)e^{is\partial_x^2}u(t_n)]\mathrm{d}s + R_1^n, \tag{4.4}$$

with

$$R_1^n := i\lambda \int_0^\tau e^{i(\tau-s)\partial_x^2}\big[|e^{is\partial_x^2}u(t_n)|^2 e^{is\partial_x^2}u(t_n) - |u(t_n+s)|^2 u(t_n+s)\big]\mathrm{d}s. \tag{4.5}$$

The remainder R_1^n will be dropped in the numerical scheme. By using the Kato–Ponce inequality in Lemma 3.2, it is straightforward to verify that for $\alpha \in (\frac{1}{2}, 1]$

$$\|R_1^n\|_{H^\alpha} \lesssim \int_0^\tau (\|u(t_n+s)\|_{H^\alpha}^2 + \|e^{is\partial_x^2}u(t_n)\|_{H^\alpha}^2)\|e^{is\partial_x^2}u(t_n) - u(t_n+s)\|_{H^\alpha}\mathrm{d}s.$$

The term $\|e^{is\partial_x^2}u(t_n) - u(t_n+s)\|_{H^1}$ can be estimated by applying Lemma 3.2 to (4.1), i.e.,

$$\begin{aligned}\|u(t_{n+1}) - e^{i\tau\partial_x^2}u(t_n)\|_{H^1} &\lesssim \left\| \int_0^\tau e^{i(\tau-s)\partial_x^2}[|u(t_n+s)|^2 u(t_n+s)]\mathrm{d}s \right\|_{H^1} \\ &\lesssim \tau\|u\|_{C([0,T];H^1)}^3. \end{aligned} \tag{4.6}$$

The two estimates above imply that

$$\|R_1^n\|_{H^1} \lesssim \tau^2\|u\|_{L^\infty(0,T;H^1)}^5. \tag{4.7}$$

We further rewrite (4.4) as

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda \int_0^\tau B^n(s, u(t_n))\mathrm{d}s + R_1^n$$

with

$$B^n(s,u(t_n)) = e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}v(s)\big] \quad \text{and} \quad v(s) = e^{-is\partial_x^2}\big(e^{is\partial_x^2}u(t_n)\big)^2. \tag{4.8}$$

The motivation for the definition of $v(s)$ will become clear in Section 4.4 in the analysis of the consistency error, i.e., this choice of definition allows us to explore more cancellation in estimating the remainder of the numerical scheme. With the above definition, we have

$$\begin{aligned}B^n(s,u(t_n)) =& e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}v(0)\big]\\ &+ e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}(v(s)-v(0))\big]\\ =&: B_1^n(s,u(t_n)) + e^{i\tau\partial_x^2}B_2^n(s,u(t_n)) + r_2^n(s)\end{aligned} \tag{4.9}$$

with

$$\begin{aligned}B_1^n(s,u(t_n)) &= e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}v(0)\big];\\ B_2^n(s,u(t_n)) &= \bar{u}(t_n)\,(v(s)-v(0))\\ r_2^n(s) &= e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}(v(s)-v(0))\big] - e^{i\tau\partial_x^2}\big[\bar{u}(t_n)(v(s)-v(0))\big],\end{aligned}$$

and therefore

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) - i\lambda\int_0^\tau B_1^n(s,u(t_n))\mathrm{d}s - i\lambda\int_0^\tau e^{i\tau\partial_x^2}B_2^n(s,u(t_n))\mathrm{d}s + R_1^n + R_2^n, \tag{4.10}$$

with

$$R_2^n = -i\lambda\int_0^\tau r_2^n(s)\mathrm{d}s. \tag{4.11}$$

We shall approximate (4.10) by integrating $B_1^n(s,u(t_n))$ and $B_2^n(s,u(t_n))$ analytically, and dropping the remainders R_1^n and R_2^n.

The remainder R_1^n is already estimated in (4.7). From the definition of $r_2^n(s)$ in (4.9), i.e.,

$$r_2^n(s) = e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\, e^{is\partial_x^2}(v(s)-v(0))\big] - e^{i\tau\partial_x^2}\big[\bar{u}(t_n)(v(s)-v(0))\big],$$

it is easy to see that

$$\|R_2^n\|_{H^1} \lesssim \int_0^\tau \|r_2^n(s)\|_{H^1}\mathrm{d}s \lesssim \tau\|u\|^3_{L^\infty(0,T;H^1)}. \tag{4.12}$$

This estimate is, however, not sufficient to prove the first-order convergence of the numerical solution. A higher-order estimate of $\|R_2^n\|_{L^2}$ is presented in Lemma 4.5 and Section 4.4 by using the bilinear Littlewood–Paley decomposition.

4.2. The anti-derivative of $B_1^n(s,u(t_n))$

To proceed to the construction of anti-derivatives, we need the following two lemmas to justify the afterward calculus of Fréchet derivatives.

Lemma 4.1. *For any $f\in \dot{H}^1\cong H^1$, the Fréchet derivative $\frac{d}{ds}e^{is\partial_x^2}f$ exists in $(H^1)'$, i.e., the dual space of H^1, and it holds that*

$$\frac{d}{ds}e^{is\partial_x^2}f = (-i\partial_x e^{is\partial_x^2}f, \partial_x\cdot) \in (H^1)'. \tag{4.13}$$

Proof. We first construct $g(s) := \sum\limits_{k=0}^\infty e^{-isk^2}(-ik^2)\widehat{f}_k \in (H^1)'$. Then for any $\phi\in H^1$ we have

$$\begin{aligned}(g,\phi) &= \sum_{k=0}^\infty e^{-isk^2}(-ik^2)\widehat{f}_k\overline{\widehat{\phi}}_k\\ &= \sum_{k=0}^\infty e^{-isk^2}(-ik)\widehat{f}_k k\overline{\widehat{\phi}}_k\\ &= -i(\partial_x e^{is\partial_x^2}f, \partial_x\phi),\end{aligned} \tag{4.14}$$

thus $g = (-i\partial_x e^{is\partial_x^2}f, \partial_x\cdot)\in (H^1)'$.

By definition, it suffices to show the following limit exists and is zero

$$
\begin{aligned}
&\lim_{h\to 0}\sup_{\|v\|_{H^1}\le 1}\left(\frac{e^{i(s+h)\partial_x^2}-e^{is\partial_x^2}}{h}f-g,v\right)_{L^2}\\
&=\lim_{h\to 0}\sup_{\|v\|_{H^1}\le 1}\lim_{N\to+\infty}\sum_{k=0}^{N}\left(\frac{e^{-i(s+h)k^2}-e^{-isk^2}}{h}+e^{-isk^2}ik^2\right)\widehat{f}_k\overline{\widehat{v}}_k\\
&=\lim_{h\to 0}\sup_{\|v\|_{H^1}\le 1}\Big(\sum_{k=0}^{K}+\sum_{k=K+1}^{\infty}\Big)(1-e^{-i\xi_{h,k}k^2})e^{-isk^2}ik\widehat{f}_k k\overline{\widehat{v}}_k \text{ for some } |\xi_{h,k}|\le |h|. \qquad (4.15)
\end{aligned}
$$

We can choose K large enough such that the residual term is small (uniformly w.r.t. h and v). On the other hand, for the first $K+1$ sums, a sufficiently small h can be chosen so that $e^{-i\xi_{h,k}k^2}-1$ is small (uniformly w.r.t. v and $k=0,...,K$). These altogether show that the limit exists and is zero. This proves that $\lim_{h\to 0}\frac{e^{i(s+h)\partial_x^2}-e^{is\partial_x^2}}{h}f=g$ in $(H^1)'$. □

Lemma 4.2. *The following Fréchet derivative exists in L^2 and the identity*

$$
\begin{aligned}
\frac{d}{ds}\partial_x^{-2}\partial_x[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\overline{u}(t_n)e^{is\partial_x^2}v(0)] =&-i(1-S)\big[e^{-is\partial_x^2}\overline{u}(t_n)\,e^{is\partial_x^2}v(0)\big]\\
&+i(1-S)\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\overline{u}(t_n)\,\partial_x e^{is\partial_x^2}v(0)\big]\\
&+iS\overline{u}(t_n)(e^{is\partial_x^2}v(0)-Sv(0)) \qquad (4.16)
\end{aligned}
$$

holds, where the averaging operator S is defined in (2.4).

Proof. Take difference quotient and we obtain

$$
\begin{aligned}
&\frac{1}{h}\partial_x^{-2}\partial_x[\partial_x\partial_x^{-2}e^{-i(s+h)\partial_x^2}\overline{u}(t_n)e^{i(s+h)\partial_x^2}v(0)]-\frac{1}{h}\partial_x^{-2}\partial_x[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\overline{u}(t_n)e^{is\partial_x^2}v(0)]\\
=&\partial_x^{-2}\partial_x[\partial_x\partial_x^{-2}\frac{e^{-i(s+h)\partial_x^2}-e^{-is\partial_x^2}}{h}\overline{u}(t_n)e^{i(s+h)\partial_x^2}v(0)]+\partial_x^{-2}\partial_x[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\overline{u}(t_n)\frac{e^{i(s+h)\partial_x^2}-e^{is\partial_x^2}}{h}v(0)].\\
&\qquad (4.17)
\end{aligned}
$$

To simplify the notation, we use $A(\phi,h)\xrightarrow[h]{\phi}B(\phi,h)$ to denote the relation $\lim_{h\to 0}\sup_{\|\phi\|_{L^2}\le 1}|A(\phi,h)-B(\phi,h)|=0$. Thus upon testing (4.17) by ϕ, we have

$$
\begin{aligned}
&-\big(\partial_x\partial_x^{-2}\frac{e^{-i(s+h)\partial_x^2}-e^{-is\partial_x^2}}{h}\overline{u}(t_n)e^{i(s+h)\partial_x^2}v(0),\partial_x\partial_x^{-2}\phi\big)\\
&-\big(\partial_x\partial_x^{-2}e^{-is\partial_x^2}\overline{u}(t_n)\frac{e^{i(s+h)\partial_x^2}-e^{is\partial_x^2}}{h}v(0),\partial_x\partial_x^{-2}\phi\big)\\
=&+\big(\frac{e^{-i(s+h)\partial_x^2}-e^{-is\partial_x^2}}{h}\overline{u}(t_n),\partial_x^{-2}\partial_x[e^{-i(s+h)\partial_x^2}\overline{v}(0)\partial_x\partial_x^{-2}\phi]\big)\\
&-\big(\frac{e^{i(s+h)\partial_x^2}-e^{is\partial_x^2}}{h}v(0),\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)\partial_x\partial_x^{-2}\phi\big)\\
\xrightarrow[h]{\phi}&+i\big(\partial_x e^{-is\partial_x^2}\overline{u}(t_n),\partial_x\partial_x^{-2}\partial_x[e^{-is\partial_x^2}\overline{v}(0)\partial_x\partial_x^{-2}\phi]\big)\\
&+i\big(\partial_x e^{is\partial_x^2}v(0),\partial_x[\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)\partial_x\partial_x^{-2}\phi]\big)\quad \text{(c.f. proof of Lemma 4.1)}\\
=&-i\big(e^{-is\partial_x^2}\overline{u}(t_n),(1-S)\partial_x[e^{-is\partial_x^2}\overline{v}(0)\partial_x\partial_x^{-2}\phi]\big)\\
&+i\big(\partial_x e^{is\partial_x^2}v(0),(1-S)e^{is\partial_x^2}u(t_n)\partial_x\partial_x^{-2}\phi+\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
=&-i\big(e^{-is\partial_x^2}\overline{u}(t_n),\partial_x e^{-is\partial_x^2}\overline{v}(0)\partial_x\partial_x^{-2}\phi+e^{-is\partial_x^2}\overline{v}(0)(1-S)\phi\big)\\
&-i\big(e^{is\partial_x^2}v(0),\partial_x e^{is\partial_x^2}u(t_n)\partial_x\partial_x^{-2}\phi+(1-S)e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
&+i\big(\partial_x e^{is\partial_x^2}v(0),\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)(1-S)\phi\big),
\end{aligned}
$$

where in the first and last equality we have used integration by parts. This is legitimate in view of the boundary condition $(\partial_x\partial_x^{-2}f)(z)=0$ at $z=0$ and $z=\pi$ for any $f\in L^2$. We have also used the relation $S(\partial_x g)=0$ with $g\in H_0^1$. By using integration by parts again, we obtain

$$\begin{aligned}
&-i\big(e^{-is\partial_x^2}\overline{u}(t_n),\partial_x e^{-is\partial_x^2}\overline{v}(0)\partial_x\partial_x^{-2}\phi+e^{-is\partial_x^2}\overline{v}(0)(1-S)\phi\big)\\
&-i\big(e^{is\partial_x^2}v(0),\partial_x e^{is\partial_x^2}u(t_n)\partial_x\partial_x^{-2}\phi+(1-S)e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
&+i\big(\partial_x e^{is\partial_x^2}v(0),\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
=&+i\big(\partial_x e^{-is\partial_x^2}\overline{u}(t_n),e^{-is\partial_x^2}\overline{v}(0)\partial_x\partial_x^{-2}\phi\big)\\
&-i\big(e^{is\partial_x^2}v(0),\partial_x e^{is\partial_x^2}u(t_n)\partial_x\partial_x^{-2}\phi+(1-S)e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
&+i\big(\partial_x e^{is\partial_x^2}v(0),\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
=&-i\big(e^{is\partial_x^2}v(0),(1-S)e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
&+i\big(\partial_x e^{is\partial_x^2}v(0),\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)(1-S)\phi\big)\\
=&-\big(i(1-S)\big[e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big],\phi\big)\\
&+\big(i(1-S)\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,\partial_x e^{is\partial_x^2}v(0)\big],\phi\big)\\
&+\big(iS\bar{u}(t_n)(e^{is\partial_x^2}v(0)-Sv(0)),\phi\big),\quad\text{(use the relation } (u,Sv)=(Su,v))
\end{aligned}$$

which, by definition, is exactly what we want to prove. □

Now we are in a position to construct the anti-derivatives.

Lemma 4.3.

$$-\int_0^\tau i\lambda B_1^n(s,u(t_n))\mathrm{d}s=A_1(\tau,u(t_n))-A_1(0,u(t_n)),\tag{4.18}$$

where

$$\begin{aligned}
A_1(s,u(t_n)):=&\frac{1}{2}\lambda e^{i(\tau-s)\partial_x^2}\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big]\\
&-is\lambda S\big[\bar{u}(t_n)\,v(0)\big]-is\lambda S\bar{u}(t_n)(e^{i\tau\partial_x^2}v(0)-Sv(0)).
\end{aligned}\tag{4.19}$$

Proof. In order to find an anti-derivative of $B_1^n(s,u(t_n))$ we consider the function

$$\widetilde{A}_1(s,u(t_n)):=\frac{1}{2}\lambda e^{i(\tau-s)\partial_x^2}\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big],\tag{4.20}$$

whose L^2 Fréchet derivative satisfies the following identity:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}s}\widetilde{A}_1(s,u(t_n))\\
&=-\frac{1}{2}i\lambda e^{i(\tau-s)\partial_x^2}\partial_x^2\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big] &\text{(4.21a)}\\
&\quad+\frac{1}{2}i\lambda e^{i(\tau-s)\partial_x^2}\frac{d}{ds}\big[\partial_x^{-2}\partial_x\big(\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big)\big]. &\text{(4.21b)}
\end{aligned}$$

For the terms in (4.21), applying lemma 4.2 we have that

$$\begin{aligned}
\text{(4.21a)}=&-\frac{1}{2}i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big]\\
=&-\frac{1}{2}i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[(1-S)e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big]\\
&-\frac{1}{2}i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar{u}(t_n)\,\partial_x e^{is\partial_x^2}v(0)\big]\\
=&-\frac{1}{2}i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}v(0)\big]\\
&+\frac{1}{2}i\lambda S\bar{u}(t_n)\big(e^{i\tau\partial_x^2}v(0)-Sv(0)\big)
\end{aligned}$$

$$
\begin{aligned}
&\quad - \frac{1}{2} i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[\partial_x\partial_x^{-2} e^{-is\partial_x^2}\bar u(t_n)\, \partial_x e^{is\partial_x^2} v(0)\big] \\
(4.21\text{b}) = &- \frac{1}{2} i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2} v(0)\big] \\
&+ \frac{1}{2} i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[\partial_x\partial_x^{-2} e^{-is\partial_x^2}\bar u(t_n)\, \partial_x e^{is\partial_x^2} v(0)\big] \\
&+ \frac{1}{2} i\lambda S\bar u(t_n)(e^{i\tau\partial_x^2} v(0) - Sv(0)).
\end{aligned}
$$

Collecting two equalities above, we obtain

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s}\widetilde{A}_1(s,u(t_n)) = &- i\lambda e^{i(\tau-s)\partial_x^2}(1-S)\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2} v(0)\big] \\
&+ i\lambda S\bar u(t_n)(e^{i\tau\partial_x^2} v(0) - Sv(0)) \\
= &- i\lambda e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2} v(0)\big] \\
&+ i\lambda S\big[\bar u(t_n)\, v(0)\big] + i\lambda S\bar u(t_n)(e^{i\tau\partial_x^2} v(0) - Sv(0)) \\
= &- i\lambda B_1^n(s,u(t_n)) \\
&+ i\lambda S\big[\bar u(t_n)\, v(0)\big] + i\lambda S\bar u(t_n)(e^{i\tau\partial_x^2} v(0) - Sv(0)).
\end{aligned} \tag{4.22}
$$

Integrating this equality yields

$$
\begin{aligned}
&- \int_0^\tau i\lambda B_1^n(s,u(t_n))\mathrm{d}s \\
&= \widetilde{A}_1(\tau,u(t_n)) - \widetilde{A}_1(0,u(t_n)) - i\tau\lambda S\big[\bar u(t_n)\, v(0)\big] - i\tau\lambda S\bar u(t_n)(e^{i\tau\partial_x^2} v(0) - Sv(0)).
\end{aligned} \tag{4.23}
$$

This implies (4.18) in view of the definition of $A_1(s,u(t_n))$ in (4.19). □

4.3. The anti-derivative of $B_2^n(s,u(t_n))$

Lemma 4.4.

$$
-i\lambda \int_0^\tau B_2^n(s,u(t_n))\mathrm{d}s = A_2(\tau,u(t_n)) - A_2(0,u(t_n)), \tag{4.24}
$$

where

$$
\begin{aligned}
A_2(s,u(t_n)) := &\frac{\lambda}{2}\big[\bar u(t_n) e^{-is\partial_x^2}\big(\partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\big)^2\big] + is\lambda|u(t_n)|^2 u(t_n) \\
&- 2is\lambda|u(t_n)|^2 Su(t_n) + is\lambda[Su(t_n)]^2\bar u(t_n).
\end{aligned} \tag{4.25}
$$

Proof. We consider the derivative of the function

$$
\widetilde{A}_2(s,u(t_n)) = \frac{\lambda}{2}\big[\bar u(t_n) e^{-is\partial_x^2}\big(\partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\big)^2\big], \tag{4.26}
$$

which satisfies the following identity:

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s}\widetilde{A}_2(s,u(t_n)) = &i\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\big(\partial_x\partial_x^{-2}\partial_x^2 e^{is\partial_x^2} u(t_n)\, \partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\big)\big] \\
&- \frac{i}{2}\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\partial_x^2\big(\partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\, \partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\big)\big] \\
= &i\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\big(\partial_x e^{is\partial_x^2} u(t_n)\, \partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\big)\big] \\
&- i\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\big(\partial_x e^{is\partial_x^2} u(t_n)\, \partial_x\partial_x^{-2} e^{is\partial_x^2} u(t_n)\big)\big] \\
&- i\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\big((1-S) e^{is\partial_x^2} u(t_n)\, (1-S) e^{is\partial_x^2} u(t_n)\big)\big] \\
= &- i\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\big((1-S) e^{is\partial_x^2} u(t_n)\, (1-S) e^{is\partial_x^2} u(t_n)\big)\big] \qquad (4.27) \\
= &- i\lambda\big[\bar u(t_n) e^{-is\partial_x^2}\big(e^{is\partial_x^2} u(t_n)\, e^{is\partial_x^2} u(t_n)\big)\big] \\
&+ 2i\lambda|u(t_n)|^2 Su(t_n) - i\lambda[Su(t_n)]^2\bar u(t_n) \\
= &- i\lambda B_2^n(s,u(t_n)) - i\lambda|u(t_n)|^2 u(t_n) + 2i\lambda|u(t_n)|^2 Su(t_n) - i\lambda[Su(t_n)]^2\bar u(t_n).
\end{aligned}
$$

Integrating the identity above and using the definition in (4.25)–(4.26), we obtain (4.24). □

Therefore,

$$u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) + A_1(\tau, u(t_n)) - A_1(0, u(t_n)) \\ + e^{i\tau\partial_x^2}[A_2(\tau, u(t_n)) - A_2(0, u(t_n))] + R_1^n + R_2^n. \tag{4.28}$$

In the next subsection we shall prove the following result.

Lemma 4.5.

$$\|R_2^n\|_{L^2} \lesssim \tau^2[\ln(1/\tau)]^2\|u(t_n)\|_{H^1}^3.$$

In view of (4.7) and Lemma 4.5, dropping R_1^n and R_2^n from (4.28) yields a temporally semidiscrete low-regularity integrator with first-order consistency error (up to a logarithmic factor):

$$u^{n+1} = e^{i\tau\partial_x^2}u^n + A_1(\tau, u^n)) - A_1(0, u^n) + e^{i\tau\partial_x^2}[A_2(\tau, u^n) - A_2(0, u^n)], \tag{4.29}$$

where the expressions of $A_1(s, u^n)$ and $A_2(s, u^n)$ are defined in (4.19) and (4.25), respectively. The spatial discretization of the semidiscrete method (4.29) is presented in Section 5.

4.4. Proof of Lemma 4.5

The main difficulty in the construction of temporally semidiscrete low-regularity integrator is the analysis of the remainder R_2^n defined in (4.11). In this subsection, we present estimates for $\|R_2^n\|_{L^2}$ by using the Littlewood–Paley dyadic decomposition of $u(t_n)$, i.e.,

$$u(t_n) = \sum_{N\in\mathbb{N}_d} P_N u(t_n).$$

By using such a dyadic decomposition, we rewrite $v(s) = e^{-is\partial_x^2}(e^{is\partial_x^2}u(t_n)e^{is\partial_x^2}u(t_n))$ as

$$\begin{aligned} v(s) = &\sum_{N_1,N_2} e^{-is\partial_x^2}\big(e^{is\partial_x^2}P_{N_1}u(t_n)\cdot e^{is\partial_x^2}P_{N_2}u(t_n)\big) \\ =&\,(2\sum_{N_1>N_2} + \sum_{N_1=N_2})e^{-is\partial_x^2}\big(e^{is\partial_x^2}P_{N_1}u(t_n)\cdot e^{is\partial_x^2}P_{N_2}u(t_n)\big) \quad \text{(symmetry between } N_1 \text{ and } N_2) \\ =&\,(2\sum_{N_1>N_2} + \sum_{N_1=N_2})v_{N_1,N_2}(s), \end{aligned} \tag{4.30}$$

where

$$v_{N_1,N_2}(s) := e^{-is\partial_x^2}\big(e^{is\partial_x^2}P_{N_1}u(t_n)\cdot e^{is\partial_x^2}P_{N_2}u(t_n)\big).$$

The summation in (4.30) is over all dyadic integers $N_1, N_2 \in \mathbb{N}_d$ satisfying the conditions under the summation symbol (the same below). Substituting (4.30) into the expression

$$r_2^n(s) = e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}(v(s)-v(0))\big] - e^{i\tau\partial_x^2}\big[\bar{u}(t_n)(v(s)-v(0))\big],$$

we have

$$\begin{aligned} e^{-i\tau\partial_x^2}r_2^n(s) =&\,(2\sum_{N_1>N_2} + \sum_{N_1=N_2})\Big\{e^{-is\partial_x^2}\Big[e^{-is\partial_x^2}\bar{u}(t_n)\,e^{is\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big] \\ &- \Big[\bar{u}(t_n)\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big]\Big\} \\ :=&\,(2\sum_{N_1>N_2} + \sum_{N_1=N_2})\big(r^1_{N_1,N_2}(s) + r^2_{N_1,N_2}(s)\big), \end{aligned} \tag{4.31}$$

where

$$\begin{aligned} r^1_{N_1,N_2}(s) =&\,e^{-is\partial_x^2}\Big[e^{-is\partial_x^2}\Pi_{N_2}\bar{u}(t_n)\,e^{is\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big] \\ &- \Big[\Pi_{N_2}\bar{u}(t_n)\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big], \\ r^2_{N_1,N_2}(s) =&\,e^{-is\partial_x^2}\Big[e^{-is\partial_x^2}\Pi_{>N_2}\bar{u}(t_n)\,e^{is\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big] \end{aligned}$$

$$-\Big[\Pi_{>N_2}\bar{u}(t_n)\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big].$$

We shall prove the following results.

$$\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}+\big\|r^2_{N_1,N_2}(s)\big\|_{L^2}\lesssim|N_1|^{-1}|N_2|^{-\frac12}\|u(t_n)\|^3_{H^1}, \tag{4.32}$$

$$\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}+\big\|r^2_{N_1,N_2}(s)\big\|_{L^2}\lesssim\tau\|u(t_n)\|^3_{H^1}. \tag{4.33}$$

Assuming for a moment that (4.32)–(4.33) hold, the geometric average between (4.32) and (4.33) yields

$$\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}+\big\|r^2_{N_1,N_2}(s)\big\|_{L^2}\lesssim\tau^{1-\theta}|N_1|^{-\theta}|N_2|^{-\frac{\theta}{2}}\|u(t_n)\|^3_{H^1}\quad\forall\,\theta\in[0,1],$$

which furthermore implies that

$$\begin{aligned}\big\|r^n_2(s)\big\|_{L^2}=&\big\|e^{-i\tau\partial_x^2}r^n_2(s)\big\|_{L^2}\\ \lesssim&\sum_{N_1\ge N_2}\big(\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}+\big\|r^2_{N_1,N_2}(s)\big\|_{L^2}\big)\\ \lesssim&\sum_{N_1\ge N_2}\tau^{1-\theta}|N_1|^{-\theta}|N_2|^{-\frac{\theta}{2}}\|u(t_n)\|^3_{H^1}\\ \lesssim&\sum_{N_2}\frac{\tau^{1-\theta}}{1-2^{-\theta}}|N_2|^{-\frac{3\theta}{2}}\|u(t_n)\|^3_{H^1}\\ \lesssim&\frac{\tau^{1-\theta}}{(1-2^{-\theta})(1-2^{-3\theta/2})}\|u(t_n)\|^3_{H^1}\\ \lesssim&\frac{\tau^{1-\theta}}{(1-2^{-\theta})^2}\|u(t_n)\|^3_{H^1}.\end{aligned}$$

As a result, we have

$$\big\|R^n_2\big\|_{L^2}\lesssim\int_0^\tau\big\|r^n_2(s)\big\|_{L^2}\mathrm{d}s\lesssim\frac{\tau^{2-\theta}}{(1-2^{-\theta})^2}\|u(t_n)\|^3_{H^1}\quad\forall\,\theta\in(0,1].$$

Choosing $\theta=1/\ln(1/\tau)$ in the inequality above, we obtain the desired result of Lemma 4.5:

$$\big\|R^n_2\big\|_{L^2}\lesssim\tau^2[\ln(1/\tau)]^2\|u(t_n)\|^3_{H^1}.$$

It remains to prove (4.32)–(4.33).

Proof of (4.32): By the Sobolev and Hölder inequalities, we have

$$\begin{aligned}\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}\lesssim&(\|e^{-is\partial_x^2}\Pi_{N_2}u(t_n)\|_{L^\infty}+\|\Pi_{N_2}u(t_n)\|_{L^\infty})\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\|_{L^2}\\ \lesssim&\|u(t_n)\|_{H^1}\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\|_{L^2}\\ \lesssim&\|u(t_n)\|_{H^1}\big\|e^{-is\partial_x^2}(e^{is\partial_x^2}P_{N_1}u(t_n)\cdot e^{is\partial_x^2}P_{N_2}u(t_n))-P_{N_1}u(t_n)\cdot P_{N_2}u(t_n)\big\|_{L^2}\\ \lesssim&\|u(t_n)\|_{H^1}\|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{L^2}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{L^\infty}\\ &+\|u(t_n)\|_{H^1}\|P_{N_1}u(t_n)\|_{L^2}\|P_{N_2}u(t_n)\|_{L^\infty})\\ \lesssim&\|u(t_n)\|_{H^1}\|P_{N_1}u(t_n)\|_{L^2}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|^{\frac12}_{H^1}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|^{\frac12}_{L^2}\\ &+\|u(t_n)\|_{H^1}\|P_{N_1}u(t_n)\|_{L^2}\|P_{N_2}u(t_n)\|^{\frac12}_{H^1}\|P_{N_2}u(t_n)\|^{\frac12}_{L^2}\\ \lesssim&\|u(t_n)\|_{H^1}\|P_{N_1}u(t_n)\|_{L^2}\|P_{N_2}u(t_n)\|^{\frac12}_{H^1}\|P_{N_2}u(t_n)\|^{\frac12}_{L^2}\\ \lesssim&|N_1|^{-1}|N_2|^{-\frac12}\|u(t_n)\|^3_{H^1},\end{aligned}$$

and similarly

$$\begin{aligned}\big\|r^2_{N_1,N_2}(s)\big\|_{L^2}\lesssim&(\|e^{-is\partial_x^2}\Pi_{>N_2}u(t_n)\|_{L^\infty}+\|\Pi_{>N_2}u(t_n)\|_{L^\infty})\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\|_{L^2}\\ \lesssim&(\|e^{-is\partial_x^2}\Pi_{>N_2}u(t_n)\|_{H^1}+\|\Pi_{>N_2}u(t_n)\|_{H^1})\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\|_{L^2}\\ \lesssim&\|u(t_n)\|_{H^1}\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\|_{L^2}\end{aligned}$$

$$\lesssim |N_1|^{-1}|N_2|^{-\frac{1}{2}}\|u(t_n)\|_{H^1}^3,$$

where the last inequality follows in the same way as that for $\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}$.

Proof of (4.33) *for* $\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}$: We rewrite $r^1_{N_1,N_2}(s)$ as

$$\begin{aligned}
r^1_{N_1,N_2}(s) =& \int_0^s \frac{\mathrm{d}}{\mathrm{d}\rho}\Big\{e^{-i\rho\partial_x^2}\Big[e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\, e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big]\Big\}\mathrm{d}\rho\\
=& -i\int_0^s \Big\{e^{-i\rho\partial_x^2}\partial_x^2\Big[e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\, e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big]\Big\}\mathrm{d}\rho\\
& -i\int_0^s \Big\{e^{-i\rho\partial_x^2}\Big[\partial_x^2 e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\, e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big]\Big\}\mathrm{d}\rho\\
& +i\int_0^s \Big\{e^{-i\rho\partial_x^2}\Big[e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\, \partial_x^2 e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big]\Big\}\mathrm{d}\rho.
\end{aligned}$$

By denoting $f=e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)$, $g=e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)$, and using the identity

$$-(fg)''-f''g+fg''=(-f''g-2f'g'-fg'')-f''g+fg''=-2f''g-2f'g',$$

we obtain

$$\begin{aligned}
r^1_{N_1,N_2}(s) =& -2i\int_0^s \Big\{e^{-i\rho\partial_x^2}\Big[\partial_x^2 e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\, e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\Big]\Big\}\mathrm{d}\rho\\
& -2i\int_0^s \Big\{e^{-i\rho\partial_x^2}\Big[\partial_x e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\, \partial_x\big[e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\big]\Big]\Big\}\mathrm{d}\rho.
\end{aligned}$$

By using the Sobolev interpolation inequality in Lemma 3.3, we have

$$\begin{aligned}
\big\|r^1_{N_1,N_2}(s)\big\|_{L^2} \lesssim& \int_0^s \big\|\partial_x^2 e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\big\|_{L^2}\big\|e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\big\|_{L^\infty}\mathrm{d}\rho\\
& +\int_0^s \big\|\partial_x e^{-i\rho\partial_x^2}\Pi_{N_2}\bar u(t_n)\big\|_{L^\infty}\big\|\partial_x\big[e^{i\rho\partial_x^2}\big(v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big)\big]\big\|_{L^2}\mathrm{d}\rho\\
\lesssim& \int_0^s \big\|\Pi_{N_2}\bar u(t_n)\big\|_{H^2}\big\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big\|_{L^2}^{\frac{1}{2}}\big\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big\|_{H^1}^{\frac{1}{2}}\mathrm{d}\rho\\
& +\int_0^s \big\|\Pi_{N_2}\bar u(t_n)\big\|_{H^1}^{\frac{1}{2}}\big\|\Pi_{N_2}\bar u(t_n)\big\|_{H^2}^{\frac{1}{2}}\big\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big\|_{H^1}\mathrm{d}\rho\\
\lesssim& \int_0^s N_2\big\|u(t_n)\big\|_{H^1}\big\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big\|_{L^2}^{\frac{1}{2}}\big\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big\|_{H^1}^{\frac{1}{2}}\mathrm{d}\rho\\
& +\int_0^s N_2^{\frac{1}{2}}\big\|u(t_n)\big\|_{H^1}\big\|v_{N_1,N_2}(s)-v_{N_1,N_2}(0)\big\|_{H^1}\mathrm{d}\rho, \qquad (4.34)
\end{aligned}$$

where the last inequality follows from using (3.6). By using the Sobolev interpolation inequality again, we have

$$\begin{aligned}
&\big\|v_{N_1,N_2}(s)\big\|_{H^1}\\
&=\big\|e^{is\partial_x^2}P_{N_1}u(t_n)\, e^{is\partial_x^2}P_{N_2}u(t_n)\big\|_{H^1}\\
&\lesssim \|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{H^1}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{L^\infty}+\|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{L^\infty}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{H^1}\\
&\lesssim \|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{H^1}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{H^1}^{\frac{1}{2}}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{L^2}^{\frac{1}{2}}\\
&\quad+\|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{L^2}^{\frac{1}{2}}\|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{H^1}^{\frac{1}{2}}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{H^1}\\
&\lesssim N_2^{-\frac{1}{2}}\|u(t_n)\|_{H^1}^2 \quad \text{(here we have used (3.7) and } N_1\ge N_2)
\end{aligned}$$

and

$$\begin{aligned}
\big\|v_{N_1,N_2}(s)\big\|_{L^2} &= \big\|e^{is\partial_x^2}P_{N_1}u(t_n)\, e^{is\partial_x^2}P_{N_2}u(t_n)\big\|_{L^2}\\
&\lesssim \|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{L^2}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{L^\infty}\\
&\lesssim \|e^{is\partial_x^2}P_{N_1}u(t_n)\|_{L^2}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{L^2}^{\frac{1}{2}}\|e^{is\partial_x^2}P_{N_2}u(t_n)\|_{H^1}^{\frac{1}{2}}
\end{aligned}$$

$$\lesssim N_2^{-\frac{3}{2}}\|u(t_n)\|_{H^1}^2 \quad \text{(here we have used (3.7) and } N_1\geq N_2).$$

Setting $s=0$ in the two estimates above yields

$$N_2\big\|v_{N_1,N_2}(0)\big\|_{L^2}+\big\|v_{N_1,N_2}(0)\big\|_{H^1}\lesssim N_2^{-\frac{1}{2}}\|u(t_n)\|_{H^1}^2.$$

By substituting the three estimates above into (4.34), we obtain

$$\big\|r^1_{N_1,N_2}(s)\big\|_{L^2}\lesssim\int_0^s\|u(t_n)\|_{H^1}^3\mathrm{d}\rho\lesssim\tau\|u(t_n)\|_{H^1}^3 \quad \text{for } s\in[0,\tau].$$

Proof of (4.33) *for* $\big\|r^2_{N_1,N_2}(s)\big\|_{L^2}$: We rewrite $r^2_{N_1,N_2}(s)$ by

$$r^2_{N_1,N_2}(s)=e^{-is\partial_x^2}\Big[e^{-is\partial_x^2}\Pi_{>N_2}\bar u(t_n)\,e^{is\partial_x^2}\int_0^s\frac{\mathrm{d}}{\mathrm{d}\rho}v_{N_1,N_2}(\rho)\mathrm{d}\rho\Big] \tag{4.35}$$

$$-\Pi_{>N_2}\bar u(t_n)\int_0^s\frac{\mathrm{d}}{\mathrm{d}\rho}v_{N_1,N_2}(\rho)\mathrm{d}\rho. \tag{4.36}$$

It is easy to verify that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\rho}v_{N_1,N_2}(\rho)&=\frac{\mathrm{d}}{\mathrm{d}\rho}\Big(e^{-i\rho\partial_x^2}\big(e^{i\rho\partial_x^2}P_{N_1}u(t_n)\cdot e^{i\rho\partial_x^2}P_{N_2}u(t_n)\big)\Big)\\&=-\,2ie^{-i\rho\partial_x^2}\big(\partial_xe^{i\rho\partial_x^2}P_{N_1}u(t_n)\,\partial_xe^{i\rho\partial_x^2}P_{N_2}u(t_n)\big),\end{aligned}$$

where the last equality uses the identity $(fg)''-f''g-fg''=2f'g'$ with $f=e^{i\rho\partial_x^2}P_{N_1}u(t_n)$ and $g=e^{i\rho\partial_x^2}P_{N_2}u(t_n)$. Hence,

$$\begin{aligned}\Big\|\frac{\mathrm{d}}{\mathrm{d}\rho}v_{N_1,N_2}(\rho)\Big\|_{L^2}&\lesssim\big\|\partial_xe^{i\rho\partial_x^2}P_{N_1}u(t_n)\big\|_{L^2}\big\|\partial_xe^{i\rho\partial_x^2}P_{N_2}u(t_n))\big\|_{L^\infty}\\&\lesssim\big\|\partial_xe^{i\rho\partial_x^2}P_{N_1}u(t_n)\big\|_{L^2}\big\|\partial_xe^{i\rho\partial_x^2}P_{N_2}u(t_n))\big\|_{L^2}^{\frac12}\big\|\partial_xe^{i\rho\partial_x^2}P_{N_2}u(t_n))\big\|_{H^1}^{\frac12}\\&\lesssim\big\|P_{N_1}u(t_n)\big\|_{H^1}\big\|P_{N_2}u(t_n)\big\|_{H^1}^{\frac12}\big\|P_{N_2}u(t_n)\big\|_{H^2}^{\frac12}\\&\lesssim N_2^{\frac12}\|u(t_n)\|_{H^1}^2.\end{aligned}$$

Since

$$\|e^{-is\partial_x^2}\Pi_{>N_2}\bar u(t_n)\|_{L^\infty}\lesssim\|e^{-is\partial_x^2}\Pi_{>N_2}\bar u(t_n)\|_{L^2}^{\frac12}\|e^{-is\partial_x^2}\Pi_{>N_2}\bar u(t_n)\|_{H^1}^{\frac12}\lesssim N_2^{-\frac12}\|u(t_n)\|_{H^1},$$

substituting the two estimates above into (4.35) yields

$$\|r^2_{N_1,N_2}(s)\|_{L^2}\lesssim\int_0^sN_2^{-\frac12}\|u(t_n)\|_{H^1}N_2^{\frac12}\|u(t_n)\|_{H^1}^2\mathrm{d}\rho\lesssim\tau\big\|u(t_n)\big\|_{H^1}^3 \quad \text{for } s\in[0,\tau].$$

The proof of Lemma 4.5 is complete. □

5. Spatial discretization of the low-regularity integrator

In this section, we construct a spectral method for the spatial discretization of (4.29) with computational cost $O(N\ln N)$ at every time level and first-order accuracy for H^1 initial data. Our spectral method is based on approximating the following two terms in (4.28),

$$A_1(\tau,u(t_n))-A_1(0,u(t_n)) \quad \text{and} \quad A_2(\tau,u(t_n))-A_2(0,u(t_n)),$$

by truncated cosine series that can be computed by FFT. For simplicity, we still use the notation $v(s)=e^{-is\partial_x^2}(e^{is\partial_x^2}u(t_n))^2$ defined in (4.8).

5.1. Approximation to $A_1(\tau,u(t_n))$.

Since $B_1^n(s,u(t_n))=e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\,e^{is\partial_x^2}v(0)\big]$ is in H^1 for $s\in[0,\tau]$, it follows from (4.18) that

$$A_1(\tau,u(t_n))-A_1(0,u(t_n))=-\int_0^\tau i\lambda B_1^n(s,u(t_n))\mathrm{d}s\in H^1.$$

In view of the expression

$$A_1(s,u(t_n)) = \frac{1}{2}\lambda e^{i(\tau-s)\partial_x^2}\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}v(0)\big] - is\lambda S\big[\bar u(t_n)\, v(0)\big] - is\lambda S\bar u(t_n)(e^{i\tau\partial_x^2}v(0) - Sv(0)),$$

we define

$$A_1^N(s,u(t_n)) = \frac{1}{2}\lambda e^{i(\tau-s)\partial_x^2}\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}\Pi_N v(0)\big] - is\lambda S\big[\bar u(t_n)\,\Pi_N v(0)\big] - is\lambda S\bar u(t_n)(e^{i\tau\partial_x^2}v(0) - Sv(0)), \tag{5.1}$$

and approximate $A_1(\tau,u(t_n)) - A_1(0,u(t_n))$ by

$$\Pi_N[A_1^N(\tau,u(t_n)) - A_1^N(0,u(t_n))]. \tag{5.2}$$

Remark 5.1. Before proving the error in approximating $A_1(\tau,u(t_n)) - A_1(0,u(t_n))$ with (5.2), we drop a comment on the construction of this approximation. Since $u(t_n)^2 \in H^1$, it follows that (see Lemma 3.1)

$$\|u(t_n)^2 - \Pi_N(u(t_n)^2)\|_{L^2} \lesssim N^{-1}\|u(t_n)^2\|_{H^1} \lesssim N^{-1}\|u(t_n)\|_{H^1}^2. \tag{5.3}$$

In practical computation, $\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}(u(t_n)^2)$ would be approximated by $w = \partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u^n\, e^{is\partial_x^2}\Pi_N[(u^n)^2]$, where $u^n \in C_N$ is a cosine series with frequency bounded by N, and therefore $\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u^n$ is a sine series with frequency bounded by N. Since w is the product between the sine series $\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u^n$ and the cosine series $e^{is\partial_x^2}\Pi_N[(u^n)^2]$, it follows that w is a sine series with frequency bounded by $2N$. As a result, $\partial_x^{-2}\partial_x w$ can be computed as a cosine series.

Now we prove that (5.2) indeed approximates $A_1(\tau,u(t_n)) - A_1(0,u(t_n))$ with a desired error bound, i.e.,

$$\big\|A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1^N(\tau,u(t_n)) - A_1^N(0,u(t_n))]\big\|_{L^2} \lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3. \tag{5.4}$$

This can be proved by decomposing the error into the following two parts:

$$\begin{aligned}
&\big\|A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1^N(\tau,u(t_n)) - A_1^N(0,u(t_n))]\big\|_{L^2}\\
\lesssim&\big\|A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1(\tau,u(t_n)) - A_1(0,u(t_n))]\big\|_{L^2}\\
&+ \big\|\Pi_N[A_1(\tau,u(t_n)) - A_1(0,u(t_n))] - \Pi_N[A_1^N(\tau,u(t_n)) - A_1^N(0,u(t_n))]\big\|_{L^2}\\
\lesssim&\big\|A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1(\tau,u(t_n)) - A_1(0,u(t_n))]\big\|_{L^2}\\
&+ \big\|[A_1(\tau,u(t_n)) - A_1^N(\tau,u(t_n))] - [A_1(0,u(t_n)) - A_1^N(0,u(t_n))]\big\|_{L^2}.
\end{aligned} \tag{5.5}$$

The two parts on the right-hand side of (5.5) are estimated below.

First, by using the identity in (4.18) we have

$$\begin{aligned}
&A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1(\tau,u(t_n)) - A_1(0,u(t_n))]\\
&= -\int_0^\tau i\lambda B_1^n(s,u(t_n))\mathrm{d}s + \Pi_N\int_0^\tau i\lambda B_1^n(s,u(t_n))\mathrm{d}s\\
&= -i\lambda\int_0^\tau (1-\Pi_N)B_1^n(s,u(t_n))\mathrm{d}s\\
&= -i\lambda\int_0^\tau (1-\Pi_N)\Big(e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}v(0)\big]\Big)\mathrm{d}s.
\end{aligned} \tag{5.6}$$

Since the function $w = e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}v(0)\big]$ is in H^1, it follows from Lemma 3.1 that

$$\|(1-\Pi_N)w\|_{L^2} \lesssim N^{-1}\|w\|_{H^1}$$

and therefore

$$\|A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1(\tau,u(t_n)) - A_1(0,u(t_n))]\|_{L^2}$$

$$\lesssim \int_0^\tau N^{-1}\big\|e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}v(0)\big]\big\|_{H^1}\mathrm{d}s$$
$$\lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3. \tag{5.7}$$

Second, since

$$\begin{aligned}&A_1(s,u(t_n)) - A_1^N(s,u(t_n))\\ &=\frac12\lambda e^{i(\tau-s)\partial_x^2}\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}(1-\Pi_N)v(0)\big]\\ &\quad - is\lambda S\big[\bar u(t_n)\,(1-\Pi_N)v(0)\big]\end{aligned} \tag{5.8}$$

it follows that

$$\begin{aligned}&A_1(\tau,u(t_n)) - A_1^N(\tau,u(t_n)) - [A_1(0,u(t_n)) - A_1^N(0,u(t_n))]\\ &=\int_0^\tau \bigg[\frac{\mathrm{d}}{\mathrm{d}s}\frac12\lambda e^{i(\tau-s)\partial_x^2}\partial_x^{-2}\partial_x\big[\partial_x\partial_x^{-2}e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}(1-\Pi_N)(u(t_n)^2)\big]\bigg]\mathrm{d}s\\ &\quad - i\tau\lambda S\big[\bar u(t_n)\,(1-\Pi_N)v(0)\big]\\ &= -i\lambda\int_0^\tau e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}(1-\Pi_N)(u(t_n)^2)\big]\mathrm{d}s\\ &\quad + i\tau\lambda S\overline{u}(t_n)\big(e^{i\tau\partial_x^2}(1-\Pi_N)v(0) - S(1-\Pi_N)v(0)\big),\end{aligned} \tag{5.9}$$

where we have used formula (4.22) with $v(0)$ replaced by $(1-\Pi_N)\big(u(t_n)^2\big)$. Since $S(1-\Pi_N)v(0)=0$, it follows that

$$\begin{aligned}&\big\|A_1(\tau,u(t_n)) - A_1^N(\tau,u(t_n)) - [A_1(0,u(t_n)) - A_1^N(0,u(t_n))]\big\|_{L^2}\\ &\lesssim \int_0^\tau \|e^{-is\partial_x^2}\bar u(t_n)\|_{L^\infty}\|(1-\Pi_N)(u(t_n)^2)\|_{L^2}\mathrm{d}s\\ &\quad + i\tau\lambda|S\overline{u}(t_n)|\|(1-\Pi_N)v(0)\|_{L^2}\\ &\lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3.\end{aligned} \tag{5.10}$$

Finally, substituting (5.7) and (5.10) into (5.5) yields the desired error bound in (5.4).

5.2. Approximation to $A_2(\tau,u(t_n))$.

In order to approximately compute the expression

$$\begin{aligned}A_2(s,u(t_n)) =& \frac{\lambda}{2}\big[\bar u(t_n)e^{-is\partial_x^2}\big(\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)\big)^2\big] + is\lambda\big[|u(t_n)|^2u(t_n)\big]\\ &- 2is\lambda\big[|u(t_n)|^2Su(t_n)\big] + is\lambda\big[(Su(t_n))^2\overline{u}(t_n)\big],\end{aligned}$$

by truncated Fourier cosine series and FFT, we define an approximation of $A_2(s,u(t_n))$ by

$$\begin{aligned}A_2^N(s,u(t_n)) :=& \frac{\lambda}{2}\big[\bar u(t_n)\, e^{-is\partial_x^2}\Pi_N\big(\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n)\big)^2\big] + is\lambda\big[\bar u(t_n)\,\Pi_N\big(u(t_n)^2\big)\big]\\ &- 2is\lambda\big[|u(t_n)|^2Su(t_n)\big] + is\lambda\big[(Su(t_n))^2\overline{u}(t_n)\big]\end{aligned} \tag{5.11}$$

and approximate $A_2(\tau,u(t_n)) - A_2(0,u(t_n))$ by

$$\Pi_N[A_2^N(\tau,u(t_n)) - A_2^N(0,u(t_n))]. \tag{5.12}$$

We shall prove the following error bound for this approximation:

$$\begin{aligned}&\big\|A_2(\tau,u(t_n)) - A_2(0,u(t_n)) - \Pi_N[A_2^N(\tau,u(t_n)) - A_2^N(0,u(t_n))]\big\|_{L^2}\\ &\lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3.\end{aligned} \tag{5.13}$$

The proof of (5.13) is divided into the following several parts.

First, by using the triangle inequality, we decompose the left-hand side of (5.13) into

$$\begin{aligned}&\big\|A_2(\tau,u(t_n)) - A_2(0,u(t_n)) - \Pi_N[A_2^N(\tau,u(t_n)) - A_2^N(0,u(t_n))]\big\|_{L^2}\\ &\lesssim \big\|A_2(\tau,u(t_n)) - A_2(0,u(t_n)) - \Pi_N[A_2(\tau,u(t_n)) - A_2(0,u(t_n))]\big\|_{L^2}\end{aligned}$$

$$
\begin{aligned}
&\quad + \big\|\Pi_N[A_2(\tau,u(t_n)) - A_2(0,u(t_n))] - \Pi_N[A_2^N(\tau,u(t_n)) - A_2^N(0,u(t_n))]\big\|_{L^2} \\
&\lesssim \big\|(1-\Pi_N)[A_2(\tau,u(t_n)) - A_2(0,u(t_n))]\big\|_{L^2} \\
&\quad + \big\|[A_2(\tau,u(t_n)) - A_2^N(\tau,u(t_n))] - [A_2(0,u(t_n)) - A_2^N(0,u(t_n))]\big\|_{L^2}. \qquad (5.14)
\end{aligned}
$$

Analogous to (5.7), we have

$$
\begin{aligned}
&\|(1-\Pi_N)[A_2(\tau,u(t_n)) - A_2(0,u(t_n))]\|_{L^2} \\
&\lesssim \int_0^\tau N^{-1}\big\|e^{i(\tau-s)\partial_x^2}\overline{u}(t_n)(v(s)-v(0))\big\|_{H^1}\mathrm{d}s \\
&\lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3. \qquad (5.15)
\end{aligned}
$$

Second, we note that

$$
\begin{aligned}
&A_2(s,u(t_n)) - A_2^N(s,u(t_n)) \\
&= \frac{1}{2}\lambda\big[\overline{u}(t_n)e^{-is\partial_x^2}(1-\Pi_N)(\partial_x\partial_x^{-2}e^{is\partial_x^2}u(t_n))^2\big] \\
&\quad + is\lambda u(t_n)(1-\Pi_N)|u(t_n)|^2. \qquad (5.16)
\end{aligned}
$$

By using formula (4.27) with an additional operator $1-\Pi_N$, we obtain

$$
\begin{aligned}
&\frac{d}{ds}(A_2(s,u(t_n)) - A_2^N(s,u(t_n))) \\
&= -i\lambda\big[\overline{u}(t_n)e^{-is\partial_x^2}(1-\Pi_N)[(1-S)e^{is\partial_x^2}u(t_n)]^2 \\
&\quad + i\lambda\overline{u}(t_n)(1-\Pi_N)\big(u(t_n)^2\big) \\
&= -i\lambda\big[\overline{u}(t_n)e^{-is\partial_x^2}(1-\Pi_N)[e^{is\partial_x^2}u(t_n)]^2\big] \\
&\quad + 2i\lambda Su(t_n)\overline{u}(t_n)(1-\Pi_N)u(t_n) \\
&\quad + i\lambda u(t_n)(1-\Pi_N)|u(t_n)|^2. \qquad (5.17)
\end{aligned}
$$

Therefore, we obtain

$$
\begin{aligned}
&\big\|A_2(\tau,u(t_n)) - A_2^N(\tau,u(t_n)) - [A_2(0,u(t_n)) - A_2^N(0,u(t_n))]\big\|_{L^2} \\
&\lesssim \int_0^\tau \|\frac{d}{ds}(A_2(s,u(t_n)) - A_2^N(s,u(t_n)))\|_{L^2}\mathrm{d}s \\
&\lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3. \qquad (5.18)
\end{aligned}
$$

Substituting (5.15)–(5.18) into (5.14) yields the desired estimate (5.13).

5.3. The fully discrete method

In view of the error bounds in (5.4) and (5.13), we can rewrite (4.28) as

$$
\begin{aligned}
u(t_{n+1}) = e^{i\tau\partial_x^2}u(t_n) &+ \Pi_N[A_1^N(\tau,u(t_n))) - A_1^N(0,u(t_n))] \\
&+ e^{i\tau\partial_x^2}\Pi_N[A_2^N(\tau,u(t_n)) - A_2^N(0,u(t_n))] \\
&+ R_1^n + R_2^n + R_3^n, \qquad (5.19)
\end{aligned}
$$

where the remainders R_1^n, R_2^n and

$$
\begin{aligned}
R_3^n &= A_1(\tau,u(t_n)) - A_1(0,u(t_n)) - \Pi_N[A_1^N(\tau,u(t_n)) - A_1^N(0,u(t_n))] \\
&\quad + e^{i\tau\partial_x^2}[A_2(\tau,u(t_n)) - A_2(0,u(t_n))] - e^{i\tau\partial_x^2}\Pi_N[A_2^N(\tau,u(t_n)) - A_2^N(0,u(t_n))] \qquad (5.20)
\end{aligned}
$$

satisfy the following estimates:

$$
\begin{aligned}
&\|R_1^n\|_{L^2} + \|R_2^n\|_{L^2} \lesssim \tau^2\|u(t_n)\|_{H^1}^5 + \tau^2[\ln(1/\tau)]^2\|u(t_n)\|_{H^1}^3, \\
&\|R_3^n\|_{L^2} \lesssim \tau N^{-1}\|u(t_n)\|_{H^1}^3. \qquad (5.21)
\end{aligned}
$$

By dropping the remainders R_1^n, R_2^n and R_3^n in (5.19), we define the following fully discrete method: For given $u_N^n \in C_N$, compute $u_N^{n+1} \in C_N$ by

$$u_N^{n+1} = e^{i\tau\partial_x^2} u_N^n + \Pi_N[A_1^N(\tau, u_N^n)) - A_1^N(0, u_N^n)] + e^{i\tau\partial_x^2}\Pi_N[A_2^N(\tau, u_N^n) - A_2^N(0, u_N^n)], \quad (5.22)$$

where the expressions of $A_1^N(s, u_N^n)$ and $A_2^N(s, u_N^n)$ are defined in (5.1) and (5.11), respectively. The method (5.22) can be equivalently written as (2.5), where $\widehat{A}_1^N(s, u_N^n) = \Pi_N A_1^N(s, u_N^n)$ and $\widehat{A}_2^N(s, u_N^n) = \Pi_N A_2^N(s, u_N^n)$ are written into a form which is more convenient for computation.

6. Proof of Theorem 2.1

We define a nonlinear functional $\Phi_\tau^N : H^1 \to H^1$ which satisfies $u_N^{n+1} = \Phi_\tau^N(u_N^n)$ for the numerical solutions u^n defined in (5.22), i.e.,

$$\Phi_\tau^N(u) := e^{i\tau\partial_x^2} u + \Pi_N[A_1^N(\tau, u) - A_1^N(0, u)] + e^{i\tau\partial_x^2}\Pi_N[A_2^N(\tau, u) - A_2^N(0, u)]. \quad (6.1)$$

The proof of the convergence is based on the following two results:

$$\big\|u(t_{n+1}) - \Phi_\tau^N(u(t_n))\big\|_{L^2} \le C\big(\tau^2[\ln(1/\tau)]^2 + \tau N^{-1}\big), \quad (6.2)$$

$$\big\|\Phi_\tau^N(u_N^n) - \Phi_\tau^N(u(t_n))\big\|_{L^2} \le (1 + C\tau)\|u_N^n - u(t_n)\|_{L^2} + C\tau N^{-1}, \quad (6.3)$$

where the constant C depends only on T and $\|u\|_{C([0,T];H^1)}$. Estimates (6.2) and (6.3) can be regarded as the local truncation error and the stability estimate, respectively. By using these estimates and the triangle inequality, we have

$$\begin{aligned}\|u_N^{n+1} - u(t_{n+1})\|_{L^2} &= \|\Phi_\tau^N(u_N^n) - u(t_{n+1})\|_{L^2} \\ &\le \|\Phi_\tau^N(u_N^n) - \Phi_\tau^N(u(t_n))\|_{L^2} + \|\Phi_\tau^N(u(t_n)) - u(t_{n+1})\|_{L^2} \\ &\le (1 + C\tau)\|u_N^n - u(t_n)\|_{L^2} + C\big(\tau^2[\ln(1/\tau)]^2 + \tau N^{-1}\big).\end{aligned}$$

Then iterating this inequality yields the desired error bound in (2.8).

The proof of the local truncation error (6.2) is relatively simple. From (5.19)–(5.21) we immediately see that

$$\big\|u(t_{n+1}) - \Phi_\tau^N(u(t_n))\big\|_{L^2} \lesssim \|R_1^n\|_{L^2} + \|R_2^n\|_{L^2} + \|R_3^n\|_{L^2} \le C(\tau^2[\ln(1/\tau)]^2 + \tau N^{-1}),$$

which implies (6.2).

The proof the stability estimate (6.3) is presented in Section 6.3, which requires the boundedness of numerical solutions in H^1 uniformly with respect to the stepsize τ, while the proof of such H^1 estimate requires the boundedness of numerical solutions in H^γ for some $\gamma \in (\frac{1}{2}, 1)$. The proof of such H^γ and H^1 estimates are presented in the next two subsections, respectively.

6.1. Boundedness of numerical solutions in H^γ for $\gamma \in (\frac{1}{2}, 1)$

In this subsection we prove the following lemma.

Lemma 6.1. *Let $u^0 \in H^1$, $L := \lfloor T/\tau \rfloor$ and $\gamma \in (\frac{1}{2}, 1)$. Then there exist positive constants τ_0, N_0 and C depending only on $\|u^0\|_{H^1}$, T and γ, such that for $\tau \le \tau_0$ and $N \ge N_0$ the numerical solution given by* (5.22) *has the following error bound:*

$$\max_{1\le n\le L} \|u(t_n, \cdot) - u_N^n\|_{H^\gamma} \le C(\tau[\ln(1/\tau)]^2 + N^{-1})^{1-\gamma}, \quad (6.4)$$

$$\max_{1\le n\le L} \|u_N^n\|_{H^\gamma} \le C. \quad (6.5)$$

Proof. By using the triangle inequality it is easy to see that (6.5) is a consequence of (6.4). Therefore, it suffices to prove (6.4).

We prove the following bound for the local truncation error:

$$\big\|u(t_{n+1}) - \Phi_\tau^N(u(t_n))\big\|_{H^\gamma} \lesssim \tau(\tau[\ln(1/\tau)]^2 + N^{-1})^{1-\gamma}. \quad (6.6)$$

Indeed, from (5.19)–(5.21) we see that

$$\big\|u(t_{n+1}) - \Phi_\tau^N(u(t_n))\big\|_{H^1} \lesssim \|R_1^n\|_{H^1} + \|R_2^n\|_{H^1} + \|R_3^n\|_{H^1} \lesssim \tau + \|R_3^n\|_{H^1}, \quad (6.7)$$

where we have used the estimates of $\|R_1^n\|_{H^1}$ and $\|R_2^n\|_{H^1}$ in (4.7) and (4.12), respectively. The bound for $\|R_3^n\|_{H^1}$ can be obtained by estimating each term in (5.20). For example, by using the identities (4.18) and (4.24) we have

$$\begin{aligned}\|A_1(\tau,u(t_n))-A_1(0,u(t_n))\|_{H^1} = \left\|\int_0^\tau i\lambda B_1^n(s,u(t_n))\mathrm{d}s\right\|_{H^1} &\lesssim \tau \sup_{s\in[0,\tau]}\|B_1^n(s,u(t_n))\|_{H^1}\\ &\lesssim \tau\|u\|^3_{L^\infty(0,T;H^1)} \end{aligned}\tag{6.8}$$

and

$$\begin{aligned}\|A_2(\tau,u(t_n))-A_2(0,u(t_n))\|_{H^1} = \left\|\int_0^\tau i\lambda B_2^n(s,u(t_n))\mathrm{d}s\right\|_{H^1} &\lesssim \tau \sup_{s\in[0,\tau]}\|B_2^n(s,u(t_n))\|_{H^1}\\ &\lesssim \tau\|u\|^3_{L^\infty(0,T;H^1)}. \end{aligned}\tag{6.9}$$

The term $\|A_1^N(\tau,u(t_n))-A_1^N(0,u(t_n))\|_{H^1}$ in (5.20) can be estimated by applying H^1 norm to (5.9) and using (6.8). The term $\|A_2^N(\tau,u(t_n))-A_2^N(0,u(t_n))\|_{H^1}$ in (5.20) can be estimated similarly. Substituting these estimates into (5.20) yields

$$\|R_3^n\|_{H^1}\lesssim \tau, \tag{6.10}$$

which together with (6.7) implies the following bound for the local truncation error:

$$\left\|u(t_{n+1})-\Phi_\tau^N(u(t_n))\right\|_{H^1}\lesssim\tau. \tag{6.11}$$

Then (6.6) can be obtained by using the Sobolev interpolation between (6.2) and (6.11).

Second, we prove the following stability estimate in the H^γ norm:

$$\left\|\Phi_\tau^N(u_N^n)-\Phi_\tau^N(u(t_n))\right\|_{H^\gamma}\le(1+C\tau)\|u_N^n-u(t_n)\|_{H^\gamma}+C\tau\|u_N^n-u(t_n)\|^3_{H^\gamma}. \tag{6.12}$$

From the definition of $\Phi_\tau^N(u)$ in (6.1) we see that

$$\begin{aligned}&\Phi_\tau^N(u_N^n)-\Phi_\tau^N(u(t_n))\\ &=e^{i\tau\partial_x^2}(u_N^n-u(t_n))\\ &\quad+\Pi_N[A_1^N(\tau,u_N^n)-A_1^N(0,u_N^n)-(A_1^N(\tau,u(t_n))-A_1^N(0,u(t_n)))]\\ &\quad+e^{i\tau\partial_x^2}\Pi_N[A_2^N(\tau,u_N^n)-A_2^N(0,u_N^n)-(A_2^N(\tau,u(t_n))-A_2^N(0,u(t_n)))]\\ &=:J_1+\Pi_NJ_2+e^{i\tau\partial_x^2}\Pi_NJ_3.\end{aligned}\tag{6.13}$$

By using the equivalent norm in (3.4) and its property (3.5), we have

$$\|J_1\|_{\dot H^\gamma}=\|u(t_n)-u_N^n\|_{\dot H^\gamma}. \tag{6.14}$$

In order to estimate $\|J_2\|_{H^\gamma}$, we use identities (5.9) and (4.18) , which implies that

$$\begin{aligned}&-[A_1^N(\tau,u(t_n))-A_1^N(0,u(t_n))]\\ &=\Big(A_1(\tau,u(t_n))-A_1^N(\tau,u(t_n))-[A_1(0,u(t_n))-A_1^N(0,u(t_n))]\Big)-[A_1(\tau,u(t_n))-A_1(0,u(t_n))]\\ &=-i\lambda\int_0^\tau e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\,e^{is\partial_x^2}(1-\Pi_N)(u(t_n)^2)\big]\mathrm{d}s\\ &\quad+i\tau\lambda S\overline{u}(t_n)e^{i\tau\partial_x^2}(1-\Pi_N)[u(t_n)^2]\\ &\quad+i\lambda\int_0^\tau e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\,e^{is\partial_x^2}(u(t_n)^2)\big]\mathrm{d}s\\ &=+i\lambda\int_0^\tau e^{i(\tau-s)\partial_x^2}\big[e^{-is\partial_x^2}\bar u(t_n)\,e^{is\partial_x^2}\Pi_N(u(t_n)^2)\big]\mathrm{d}s\\ &\quad+i\tau\lambda S\overline{u}(t_n)e^{i\tau\partial_x^2}(1-\Pi_N)[u(t_n)^2]\\ &=:J_{21}(u(t_n))+J_{22}(u(t_n)).\end{aligned}\tag{6.15}$$

By using this expression we obtain that

$$J_2 = \sum_{k=1}^{2} [J_{2k}(u(t_n)) - J_{2k}(u_N^n)]. \tag{6.16}$$

It is straightforward to show that

$$\|J_{2k}(u(t_n)) - J_{2k}(u_N^n)\|_{H^\gamma} \lesssim \tau(\|u(t_n)\|_{H^\gamma}^2 + \|u_N^n\|_{H^\gamma}^2)\|u(t_n) - u_N^n\|_{H^\gamma} \quad \text{for } k = 1, 2. \tag{6.17}$$

Substituting the estimates of $\|J_{2k}(u(t_n)) - J_{2k}(u_N^n)\|_{H^\gamma}$, $k = 1, 2$, into (6.16) yields that

$$\|J_2\|_{H^\gamma} \lesssim \tau\|u(t_n) - u_N^n\|_{H^\gamma}(\|u(t_n)\|_{H^\gamma}^2 + \|u_N^n\|_{H^\gamma}^2). \tag{6.18}$$

Note that $\|e^{i\tau\partial_x^2}\Pi_N J_3\|_{H^\gamma} \lesssim \|J_3\|_{H^\gamma}$ for $\gamma \in (\frac{1}{2}, 1)$. The term $\|J_3\|_{H^\gamma}$ can be estimated similarly as $\|J_2\|_{H^\gamma}$ by using identity (5.16) and (5.17), which implies that

$$\begin{aligned}
&-[A_2^N(\tau, u(t_n)) - A_2^N(0, u(t_n))] \\
=&\big[A_2(\tau, u(t_n)) - A_2(0, u(t_n))\big] - [A_2^N(\tau, u(t_n)) - A_2^N(0, u(t_n))] - \big[A_2(\tau, u(t_n)) - A_2(0, u(t_n))\big] \\
=& - i\lambda \int_0^\tau \overline{u}(t_n)e^{-is\partial_x^2}(1 - \Pi_N)[e^{is\partial_x^2}u(t_n)]^2 \mathrm{d}s \\
&+ 2i\tau\lambda e^{is\partial_x^2} S u(t_n)\overline{u}(t_n)(1 - \Pi_N)u(t_n) \\
&+ i\tau\lambda\overline{u}(t_n)(1 - \Pi_N)[u(t_n)^2] \\
&+ i\lambda \int_0^\tau \overline{u}(t_n)e^{-is\partial_x^2}[e^{is\partial_x^2}u(t_n)]^2 \mathrm{d}s \\
=& + i\lambda \int_0^\tau \overline{u}(t_n)e^{-is\partial_x^2}\Pi_N[e^{is\partial_x^2}u(t_n)]^2 \mathrm{d}s \\
&+ 2i\tau\lambda e^{is\partial_x^2} S u(t_n)\overline{u}(t_n)(1 - \Pi_N)u(t_n) \\
&+ i\tau\lambda\overline{u}(t_n)(1 - \Pi_N)[u(t_n)^2] \\
=:& J_{31}(u(t_n)) + J_{32}(u(t_n)) + J_{33}(u(t_n)),
\end{aligned} \tag{6.19}$$

By using this expression we see that

$$J_3 = \sum_{k=1}^{3} [J_{3k}(u(t_n)) - J_{3k}(u_N^n)]. \tag{6.20}$$

Similarly as the estimates for $\|J_{2k}(u(t_n)) - J_{2k}(u_N^n)\|_{H^\gamma}$, it is straightforward to verify that

$$\|J_{3k}(u(t_n)) - J_{3k}(u_N^n)\|_{H^\gamma} \lesssim \tau(\|u(t_n)\|_{H^\gamma}^2 + \|u_N^n\|_{H^\gamma}^2)\|u(t_n) - u_N^n\|_{H^\gamma} \qquad \text{for } k = 1, 2, 3.$$

Hence we obtain

$$\|J_3\|_{H^\gamma} \lesssim \tau\|u(t_n) - u_N^n\|_{H^\gamma}(\|u(t_n)\|_{H^\gamma}^2 + \|u_N^n\|_{H^\gamma}^2). \tag{6.21}$$

Then, substituting the estimates of $\|J_1\|_{\dot H^\gamma}$, $\|J_2\|_{H^\gamma}$ and $\|J_3\|_{H^\gamma}$ into (6.13) and using the equivalence between $\|\cdot\|_{\dot H^\gamma}$ and $\|\cdot\|_{H^\gamma}$, we obtain

$$\begin{aligned}
\|\Phi_\tau^N(u_N^n) - \Phi_\tau^N(u(t_n))\|_{\dot H^\gamma} &\le [1 + C\tau(\|u(t_n)\|_{\dot H^\gamma}^2 + \|u_N^n\|_{\dot H^\gamma}^2)]\|u(t_n) - u_N^n\|_{\dot H^\gamma} \\
&\le (1 + C\tau)\|u(t_n) - u_N^n\|_{\dot H^\gamma} + C\tau\|u(t_n) - u_N^n\|_{\dot H^\gamma}^3.
\end{aligned} \tag{6.22}$$

Hence, from (6.6) and (6.22) we obtain that (using the triangle inequality)

$$\begin{aligned}
&\|u(t_{n+1}) - u_N^{n+1}\|_{\dot H^\gamma} \\
&\le (1 + C\tau)\|u(t_n) - u_N^n\|_{\dot H^\gamma} + C\tau\|u(t_n) - u_N^n\|_{\dot H^\gamma}^3 + C\tau(\tau[\ln(1/\tau)]^2 + N^{-1})^{1-\gamma}.
\end{aligned}$$

By using the discrete Gronwall's inequalities, Lemma 3.5 and the equivalence between $\|\cdot\|_{\dot H^\gamma}$ and $\|\cdot\|_{H^\gamma}$, we obtain for sufficiently small τ and sufficiently large N

$$\|u(t_{n+1}) - u_N^{n+1}\|_{H^\gamma} \lesssim (\tau[\ln(1/\tau)]^2 + N^{-1})^{1-\gamma}.$$

This completes the proof of Lemma 6.1. □

6.2. Boundedness of numerical solutions in H^1

Lemma 6.2. *Let $u^0 \in H^1$ and $L := \lfloor T/\tau \rfloor$. Then there exist positive constants τ_0, N_0 and C depending only on $\|u^0\|_{H^1}$ and T, such that for $\tau \le \tau_0$ and $N \ge N_0$ the numerical solution given by* (5.22) *has the following error bound:*

$$\max_{1\le n\le L} \|u_N^n\|_{H^1} \le C. \tag{6.23}$$

Proof. Let $\eta_N^n = u(t_n) - u_N^n$. We need to prove the following results:

$$\|J_2\|_{H^1} \lesssim \tau \|\eta_N^n\|_{H^1}, \tag{6.24}$$

$$\|J_3\|_{H^1} \lesssim \tau \|\eta_N^n\|_{H^1}. \tag{6.25}$$

If (6.24)–(6.25) hold, substituting the two estimates above into (6.13) would yield

$$\|\Phi_\tau^N(u_N^n) - \Phi_\tau^N(u(t_n))\|_{\dot H^1} \le \|\eta_N^n\|_{\dot H^1} + C\tau \|\eta_N^n\|_{\dot H^1}, \tag{6.26}$$

and therefore (since $u_N^{n+1} = \Phi_\tau^N(u_N^n)$)

$$\|u_N^{n+1} - \Phi_\tau^N(u(t_n))\|_{\dot H^1} \le \|\eta_N^n\|_{\dot H^1} + C\tau \|\eta_N^n\|_{\dot H^1}. \tag{6.27}$$

From (6.11) we also know that

$$\|u(t_{n+1}) - \Phi_\tau^N(u(t_n))\|_{H^1} \lesssim \tau. \tag{6.28}$$

By using the triangle inequality, we have

$$\begin{aligned}
\|\eta_N^{n+1}\|_{\dot H^1} &= \|u(t_{n+1}) - u_N^{n+1}\|_{\dot H^1} \\
&\le \|u(t_{n+1}) - \Phi_\tau^N(u(t_n))\|_{\dot H^1} + \|u_N^{n+1} - \Phi_\tau^N(u(t_n))\|_{\dot H^1} \\
&\le \|\eta_N^n\|_{\dot H^1} + C\tau \|\eta_N^n\|_{\dot H^1} + C\tau.
\end{aligned} \tag{6.29}$$

By using Gronwall's inequality, we obtain

$$\max_{1\le n\le L} \|\eta_N^n\|_{\dot H^1} \lesssim 1. \tag{6.30}$$

This proves the desired result in (6.23). It remains to prove (6.24)–(6.25).

We prove (6.24) by using the expression in (6.16). From Lemma 6.1 we already know that $\max\limits_{1\le n\le L} \|u_N^n\|_{H^\gamma} \lesssim 1$ for any $\gamma \in (\frac12, 1)$. By using this result with any fixed $\gamma \in (\frac12, 1)$, from the expression of $J_{21}(u)$ in (6.15) we derive that

$$\begin{aligned}
&\|J_{21}(u(t_n)) - J_{21}(u_N^n)\|_{H^1} \\
&\lesssim \int_0^\tau \big\|e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}\Pi_N[u(t_n)^2] - e^{-is\partial_x^2}\bar u_N^n\, e^{is\partial_x^2}\Pi_N[(u_N^n)^2]\big\|_{H^1}\mathrm{d}s \\
&\lesssim \int_0^\tau \big\|e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}\Pi_N[u(t_n)^2] - e^{-is\partial_x^2}(\bar u(t_n) - \bar\eta_N^n)\, e^{is\partial_x^2}\Pi_N[(u(t_n) - \eta_N^n)^2]\big\|_{H^1}\mathrm{d}s \\
&\lesssim \int_0^\tau \big\|e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}\Pi_N[u(t_n)\eta_N^n]\big\|_{H^1}\mathrm{d}s \\
&\quad + \int_0^\tau \big\|e^{-is\partial_x^2}\bar u(t_n)\, e^{is\partial_x^2}\Pi_N[(\eta_N^n)^2]\big\|_{H^1}\mathrm{d}s \\
&\quad + \int_0^\tau \big\|e^{-is\partial_x^2}\bar\eta_N^n\, e^{is\partial_x^2}\Pi_N[u(t_n)^2]\big\|_{H^1}\mathrm{d}s \\
&\quad + \int_0^\tau \big\|e^{-is\partial_x^2}\bar\eta_N^n\, e^{is\partial_x^2}\Pi_N[u(t_n)\eta_N^n]\big\|_{H^1}\mathrm{d}s \\
&\quad + \int_0^\tau \big\|e^{-is\partial_x^2}\bar\eta_N^n\, e^{is\partial_x^2}\Pi_N[(\eta_N^n)^2]\big\|_{H^1}\mathrm{d}s \\
&\lesssim \int_0^\tau \|\eta_N^n\|_{H^1}\mathrm{d}s + \int_0^\tau \|\eta_N^n\|_{H^\gamma}\|\eta_N^n\|_{H^1}\mathrm{d}s + \int_0^\tau \|\eta_N^n\|_{H^1}\mathrm{d}s \\
&\quad + \int_0^\tau (\|\eta_N^n\|_{H^1}\|u(t_n)\eta_N^n\|_{H^\gamma} + \|\eta_N^n\|_{H^\gamma}\|u(t_n)\eta_N^n\|_{H^1})\mathrm{d}s
\end{aligned}$$

$$+\int_0^\tau (\|\eta_N^n\|_{H^1}\|(\eta_N^n)^2\|_{H^\gamma} + \|\eta_N^n\|_{H^\gamma}\|(\eta_N^n)^2\|_{H^1})\mathrm{d}s$$
$$\lesssim \tau\|\eta_N^n\|_{H^1}. \tag{6.31}$$

The other terms $\|J_{22}(u(t_n)) - J_{22}(u_N^n)\|_{H^1}$ can also be estimated similarly as $\|J_{21}(u(t_n)) - J_{21}(u_N^n)\|_{H^1}$ by using the expressions in (6.15), by expressing u_N^n as $u(t_n) - \eta_N^n$ and apply the following result: for any product of three functions f, g, h,

$$\|fgh\|_{H^1} \le \|f\|_{H^1}\|g\|_{H^\gamma}\|h\|_{H^\gamma} + \|f\|_{H^\gamma}\|g\|_{H^1}\|h\|_{H^\gamma} + \|f\|_{H^\gamma}\|g\|_{H^\gamma}\|h\|_{H^1}. \tag{6.32}$$

Namely, the H^1 norm only acts on one term in a product, and the other two terms involving H^γ norm would be bounded according to Lemma 6.1. In this way, the following results can be shown:

$$\sum_{k=1}^{2} \|J_{2k}(u(t_n)) - J_{2k}(u_N^n)\|_{H^1} \lesssim \tau\|\eta_N^n\|_{H^1}. \tag{6.33}$$

This proves (6.24), and (6.25) can be proved similarly by using identity (6.19). □

6.3. Stability estimates

Similarly as the H^γ-norm estimates in (6.18)–(6.21), by using the expressions in (6.16) and (6.20) it is straightforward to verify that

$$\|J_2\|_{L^2} \lesssim \tau(\|u(t_n)\|_{H^\gamma}^2 + \|u_N^n\|_{H^\gamma}^2)\|u(t_n) - u_N^n\|_{L^2}, \tag{6.34}$$
$$\|J_3\|_{L^2} \lesssim \tau(\|u(t_n)\|_{H^\gamma}^2 + \|u_N^n\|_{H^\gamma}^2)\|u(t_n) - u_N^n\|_{L^2}, \tag{6.35}$$

which holds for any fixed $\gamma \in (\frac{1}{2}, 1)$. Therefore, we have

$$\|J_2\|_{L^2} + \|\Pi_N J_3\|_{L^2} \lesssim \tau N^{-1} + \tau\|u(t_n) - u_N^n\|_{L^2}. \tag{6.36}$$

Note that (6.14) still holds for $s = 0$, i.e.,

$$\|J_1\|_{L^2} = \|u(t_n) - u_N^n\|_{L^2}. \tag{6.37}$$

By substituting the estimates of $\|J_1\|_{L^2}$, $\|J_2\|_{L^2}$ and $\|\Pi_N J_3\|_{L^2}$ into (6.13) we obtain the desired stability estimate in (6.3). This completes the proof of Theorem 2.1. □

7. Numerical examples

Example 7.1. We consider the NLS equation (2.1) with $\lambda = -1$. The initial value is given by

$$u^0(x) = \sum_{k=1}^{\infty} \frac{\cos(kx)}{|k|^{0.51+\alpha}}, \tag{7.1}$$

which satisfies that $u^0 \in H^\alpha$ and $u^0 \notin H^{\alpha-0.01}$. For $\alpha = 1, 2$, we solve the problem by the proposed method (2.5) and denote by $u_{\tau,N}$ the numerical solution with time stepsize τ and degrees of freedom N (in the spatial discretization). We compare the numerical solution with the reference solution $u_{\tau,N}^{\mathrm{ref}}$, which is computed by using the following general low-regularity integrator proposed in [23] (with spatial discretization by the trigonometric interpolation):

$$u_N^{n+1} = e^{i\tau\partial_x^2}u_N^n - i\lambda e^{i\tau\partial_x^2} I_N\big[I_N(u_N^n u_N^n)\big(\tau S\bar{u}_N^n + \frac{i}{2}(e^{-i2\tau\partial_x^2} - 1)\partial_x^{-2}\bar{u}_N^n\big)\big]. \tag{7.2}$$

The time stepsize of the reference solution is set to $\tau_{\mathrm{ref}} = 2^{-16}$. Further decreasing the time stepsize in the reference solution does not affect the numerical results.

We present the temporal discretization errors $\|u_{\tau,N} - u_{\tau_{\mathrm{ref}},N}^{\mathrm{ref}}\|_{L^2}$ for both H^2 and H^1 initial data with sufficiently large N in Tables 1–2, which show that the errors from the spatial discretization is negligibly small in observing the temporal convergence rates, i.e., almost first-order convergent as $\tau \to 0$. This is consistent with the theoretical result proved in Theorem 2.1.

TABLE 1. Temporal discretization error $\|u_{\tau,N} - u^{\text{ref}}_{\tau_{\text{ref}},N}\|_{L^2}$ at $T = 1$ with $\alpha = 2$ in (7.1) (for H^2 initial data).

	$N = 2^8$	$N = 2^9$	$N = 2^{10}$
$\tau = 2^{-6}$	8.466E–03	8.466E–03	8.466E–03
$\tau = 2^{-7}$	4.271E–03	4.271E–03	4.271E–03
$\tau = 2^{-8}$	2.157E–03	2.157E–03	2.157E–03
convergence rate	$O(\tau^{0.99})$	$O(\tau^{0.99})$	$O(\tau^{0.99})$

TABLE 2. Temporal discretization error $\|u_{\tau,N} - u^{\text{ref}}_{\tau_{\text{ref}},N}\|_{L^2}$ at $T = 1$ with $\alpha = 1$ in (7.1) (for H^1 initial data).

	$N = 2^8$	$N = 2^9$	$N = 2^{10}$
$\tau = 2^{-5}$	6.488E–02	6.506E–02	6.511E–02
$\tau = 2^{-6}$	3.222E–02	3.252E–02	3.260E–02
$\tau = 2^{-7}$	1.570E–02	1.631E–02	1.645E–02
convergence rate	$O(\tau^{1.00})$	$O(\tau^{1.02})$	$O(\tau^{0.99})$

We present the spatial discretization errors $\|u_{\tau,N} - u^{\text{ref}}_{\tau,N_{\text{ref}}}\|_{L^2}$ for both H^2 and H^1 initial data in Tables 3–4 for several sufficiently small stepsize τ with $N_{\text{ref}} = 1024$. From the numerical results we can see that the error from temporal discretization is negligibly small in observing the spatial convergence rates, i.e., αth-order convergence for H^α initial data. This is consistent with the result proved in Theorem 2.1 in the case $\alpha = 1$. The numerical results for $\alpha = 2$ indicate that the convergence order of the spatial discretization increases as the regularity of the initial data increases (though this is not proved in Theorem 2.1).

TABLE 3. Spatial discretization error $\|u_{\tau,N} - u^{\text{ref}}_{\tau,N_{\text{ref}}}\|_{L^2}$ at $T = 1$ with $\alpha = 2$ in (7.1) (for H^2 initial data).

	$\tau = 2^{-14}$	$\tau = 2^{-15}$	$\tau = 2^{-16}$
$N = 8$	7.436E–03	7.436E–03	7.436E–03
$N = 16$	1.893E–03	1.892E–03	1.892E–03
$N = 32$	4.788E–04	4.731E–04	4.712E–04
convergence rate	$O(N^{-1.98})$	$O(N^{-1.99})$	$O(N^{-1.99})$

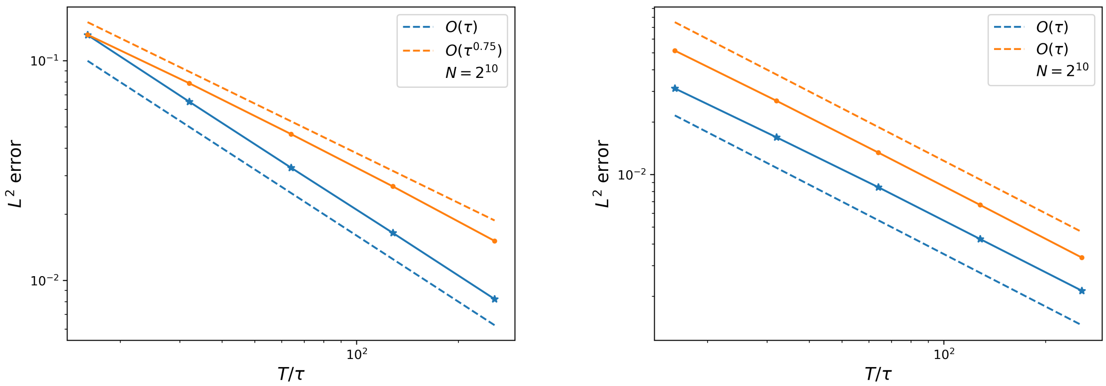
TABLE 4. Spatial discretization error $\|u_{\tau,N} - u^{\text{ref}}_{\tau,N_{\text{ref}}}\|_{L^2}$ at $T = 1$ with $\alpha = 1$ in (7.1) (for H^1 initial data).

	$\tau = 2^{-12}$	$\tau = 2^{-13}$	$\tau = 2^{-14}$
$N = 16$	4.262E–02	4.264E–02	4.266E–02
$N = 32$	2.130E–02	2.127E–02	2.127E–02
$N = 64$	1.068E–02	1.058E–02	1.056E–02
convergence rate	$O(N^{-1.00})$	$O(N^{-1.01})$	$O(N^{-1.00})$

Example 7.2. It is known that the general low-regularity integrator proposed in [23] can weaken the regularity condition for a general nonlinear function $f(u, \bar{u})$, not only for the cubic

nonlinearity $f(u, \bar{u}) = |u|^2 u$. For comparison, we present the numerical solutions given by our proposed method and the general low-regularity integrator proposed in [23] in Figure 1 for both H^1 and H^2 initial data, with $N = 2^{10}$ degrees of freedom in space which is sufficiently large for observing the convergence order in time. The H^1 and H^2 initial values are generated by (7.1) with $\alpha = 1$ and $\alpha = 2$, respectively.

The numerical results show that, for the specific cubic nonlinearity $f(u, \bar{u}) = |u|^2 u$, the method proposed in this article by using the Littlewood–Paley decomposition technique can achieve higher-order convergence for H^1 initial data. Both the methods have first-order convergence for H^2 initial data. For general nonlinearities and general boundary conditions, the method in [23] is the only known low-regularity integrator so far.



(A) H^1 initial data (B) H^2 initial data

FIGURE 1. L^2 errors of the numerical solutions given by different methods where the final time is set to be $T = 1.0$ and the reference timesteps are $\tau_{\text{ref}} = 2^{-16}$, and the reference solutions are computed from (7.2), i.e., the general low-regularity integrator proposed in [23]. The method proposed in this article is in blue, the method of [23] is in yellow.

8. Conclusion

We have constructed a new low-regularity trigonometric cosine integrator for solving the one-dimensional NLS equation in a bounded domain under the Neumann boundary condition. In this case, the frequency analysis in the literature cannot be used for the consistency analysis. The method developed in this article is constructively designed through the consistency analysis by using the Littlewood–Paley decomposition of the solution, in order to have almost first-order convergence for H^1 initial data. We have shown that the proposed method has an error bound of $O(\tau[\ln(1/\tau)]^2 + N^{-1})$ for H^1 initial data, and can be implemented by using FFT with a computational cost of $O(N \ln N)$ at every time level. The approach developed in this article relies on the Littlewood–Paley decomposition of the solution for specific problems and specific boundary conditions. The construction of such low-regularity integrators for other nonlinearities and the Dirichlet boundary condition is still challenging.

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