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A second-order low-regularity integrator for the nonlinear Schrödinger equation

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Abstract

In this paper, we analyze a new exponential-type integrator for the nonlinear cubic Schrödinger equation on the d dimensional torus \mathbb{T}^d . The scheme has also been derived recently in a wider context of decorated trees (Bruned et al. in *Forum Math. Pi* 10:1–76, 2022). It is explicit and efficient to implement. Here, we present an alternative derivation and give a rigorous error analysis. In particular, we prove the second-order convergence in $H^\gamma(\mathbb{T}^d)$ for initial data in $H^{\gamma+2}(\mathbb{T}^d)$ for any $\gamma > d/2$. This improves the previous work (Knöller et al. in *SIAM J. Numer. Anal.* 57:1967–1986, 2019).

The design of the scheme is based on a new method to approximate the nonlinear frequency interaction. This allows us to deal with the complex resonance structure in arbitrary dimensions. Numerical experiments that are in line with the theoretical result complement this work.

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1 Introduction

The nonlinear Schrödinger equation (NLS) arises as a model equation in several areas of physics see, e.g., Sulem and Sulem [20]. In this paper, we are concerned with the numerical integration of the NLS equation on a d dimensional torus:

$$\begin{cases} i\partial_t u(t, \mathbf{x}) + \Delta u(t, \mathbf{x}) + \lambda |u(t, \mathbf{x})|^2 u(t, \mathbf{x}) = 0, & t > 0, \mathbf{x} \in \mathbb{T}^d, \\ u(0, \mathbf{x}) = u_0(\mathbf{x}), & \mathbf{x} \in \mathbb{T}^d, \end{cases} \quad (1.1)$$

where $\mathbb{T} = (0, 2\pi)$, $\lambda = \pm 1$, $u = u(t, \mathbf{x}) : \mathbb{R}^+ \times \mathbb{T}^d \rightarrow \mathbb{C}$ is the sought-after solution, and $u_0 \in H^\vartheta(\mathbb{T}^d)$ for some $\vartheta \geq 0$ is the given initial data. Here we only consider the case $\lambda = 1$; the case $\lambda = -1$ can be treated in exactly the same way. Note that the well-posedness of the nonlinear Schrödinger equation in $H^\vartheta(\mathbb{T}^d)$ has been established for $\vartheta > \frac{d}{2} - 1$. For details, we refer to [2].

Many authors studied numerical aspects of the NLS equation. A considerable amount of literature has been published on splitting and exponential integration methods. For a general introduction to these methods, we refer to [9–12, 18]. It is well known that

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schemes of an arbitrarily high order can be constructed assuming that the solution of (1.1) is smooth enough. For instance, the second-order convergence in H^ϑ was obtained by requiring four additional derivatives of the solution for the Strang splitting scheme [17]. Further convergence results for the semilinear Schrödinger equation can be found, e.g., in [1, 4–6, 8, 13, 14, 21].

For classical methods and their analysis, strong regularity assumptions are unavoidable. Recently, however, so-called low-regularity integrators have emerged as a powerful tool for reducing the regularity requirements. The first breakthrough was made in [19], where the authors introduced a new exponential-type numerical scheme and achieved first-order convergence in $H^\vartheta(\mathbb{T}^d)$ for $H^{\vartheta+1}(\mathbb{T}^d)$ initial data with $\vartheta > \frac{d}{2}$. Later, a first-order integrator was proposed in [22]. It converges in $H^\vartheta(\mathbb{T})$ without any loss of regularity and conserves mass up to order five. A second-order Fourier-type integrator was given by Knöller, Ostermann, and Schratz [16]. The integrator is based on the variation-of-constants formula and uses certain resonance-based approximations in Fourier space. For the second-order convergence, the scheme requires two additional derivatives of the solution in one space dimension and three derivatives in higher space dimensions. In this paper, we present and analyze an improved integrator that enables us to get the desired second-order accuracy with only two additional bounded spatial derivatives in dimensions $d \geq 1$.

There are two main difficulties in designing low-regularity integrators. The first one is to control the spatial derivatives in the approximation while keeping the nonlinearity point-wise defined in physical space rather than in Fourier space. The second one is to overcome the difficulties caused by the complicated structure of resonances in higher dimensions. To explain this, let

$$\xi = (\xi^1, \dots, \xi^d) \in \mathbb{Z}^d, \quad \xi \cdot \eta = \xi^1 \eta^1 + \dots + \xi^d \eta^d, \quad |\xi|^2 = \xi \cdot \xi.$$

and consider the phase function

$$\phi_3 = |\xi|^2 + |\xi_1|^2 - |\xi_2|^2 - |\xi_3|^2.$$

In [16], letting

$$\alpha = 2|\xi_1|^2, \quad \beta = 2\xi_1 \cdot \xi_2 + 2\xi_1 \cdot \xi_3 + 2\xi_2 \cdot \xi_3,$$

the authors approximated the phase function by

$$e^{is\phi_3} = e^{is\alpha + is\beta} = e^{is\alpha} + e^{is\beta} - 1 + \mathcal{R}_1(\alpha, \beta, s), \quad (1.2)$$

where $|\mathcal{R}_1(\alpha, \beta, s)| \lesssim s^2 |\alpha| |\beta|$. This choice requires three additional derivatives in higher space dimensions for second-order convergence.

Now we explain our current approach, for which we consider a slightly more general situation. Assume that α has a “good” structure, which means $\int_0^\tau e^{is\alpha} ds$ is point-wise defined (as in the example above) while β has a “bad” structure but still has a low upper bound, e.g., consisting of mixed derivatives (as in the example above). In order to approximate

$$\int_0^\tau e^{is(\alpha + \beta)} ds = \tau \varphi(i\tau(\alpha + \beta)),$$

where

$$\varphi(z) = \begin{cases} \frac{e^z - 1}{z}, & z \neq 0, \\ 1, & z = 0, \end{cases} \quad (1.3)$$

we employ the Taylor series expansion

$$\varphi(i\tau(\alpha + \beta)) \approx \varphi(i\tau\alpha) + i\tau\beta\varphi'(i\tau\alpha).$$

Next, we use that

$$\varphi'(z) = -\psi(z),$$

where

$$\psi(z) = \begin{cases} \frac{e^z - 1 - ze^z}{z^2}, & z \neq 0, \\ -\frac{1}{2}, & z = 0, \end{cases} \quad (1.4)$$

and replace $i\beta\pi$ by $e^{i\beta\tau} - 1$. Then, we obtain

$$\int_0^\tau e^{is(\alpha+\beta)} ds = \tau\varphi(i\tau\alpha) - \tau(e^{i\tau\beta} - 1)\psi(i\tau\alpha) + \mathcal{R}_2(\alpha, \beta, \tau), \quad (1.5)$$

where $|\mathcal{R}_2(\alpha, \beta, \tau)| \lesssim \tau^3|\beta|^2$. This bound will be proved in Lemma 2.2 below. Relying on this structure, the scheme requires only two additional derivatives for τ^2 , which gives convergence in $H^\vartheta(\mathbb{T}^d)$ for initial data in $H^{\vartheta+2}(\mathbb{T}^d)$.

Finally, it does not require any specific structure of β . In particular, β^{-1} is not contained in the expression (1.5). This is another advantage compared to (1.2), for which the integration (or a further approximation) of $\int_0^\tau e^{is\beta} ds$ is needed.

Now we state the main result of this paper. We define the new low-regularity integrator with second-order accuracy as

$$\begin{aligned} u^0 &= u_0, \\ u^{n+1} &= e^{i\tau\Delta} u^n + i\tau e^{i\tau\Delta} \left\{ \left[\varphi(-2i\tau\Delta) + \psi(-2i\tau\Delta) \right] \bar{u}^n \cdot (u^n)^2 \right\} \\ &\quad - i\tau \left[e^{i\tau\Delta} \psi(-2i\tau\Delta) \bar{u}^n \right] \cdot (e^{i\tau\Delta} u^n)^2 - \frac{\tau^2}{2} e^{i\tau\Delta} [|u^n|^4 u^n] \end{aligned} \quad (1.6)$$

for $n \geq 0$. For this method, we have the following convergence result.

Theorem 1.1 *Let u^n be the numerical solution (1.6) of the Schrödinger equation (1.1) up to some fixed time $T > 0$. Under the assumption that $u_0 \in H^{\gamma+2}(\mathbb{T}^d)$ for some $\gamma > \frac{d}{2}$, there exist constants $\tau_0, C > 0$ such that for any $0 < \tau \leq \tau_0$, it holds*

$$\|u(t_n, \cdot) - u^n\|_{H^\gamma} \leq C\tau^2, \quad 0 \leq n\tau \leq T. \quad (1.7)$$

The constants τ_0 and C only depend on T and $\|u\|_{L^\infty((0,T);H^{\gamma+2}(\mathbb{T}^d))}$.

Having finished the analysis of this paper, we became aware of the recent work [3] by Bruned and Schratz, in which low-regularity integrators for dispersive equations are discussed in a broader context. In particular, using the formalism of decorated trees, various numerical methods for the nonlinear Schrödinger equation are proposed. The above method (1.6) is stated in formula (5.17). Nevertheless, we give here an alternative (and brief) derivation of the method because the employed approximations form the basis of our rigorous error analysis.

The paper is organized as follows: In Sect. 2, we introduce some notations and collect some useful lemmas. In Sect. 3, we discuss the construction of the method and analyze the accuracy and regularity requirements of each single approximation step. Collecting all these results, we prove our convergence result (Theorem 1.1) in Sect. 4. This theoretical result is illustrated with some numerical experiments in Sect. 5.

2 Preliminaries

In this section, we introduce some notations, recall a result from harmonic analysis, and give some elementary estimates. All of these will be used frequently in the following sections.

2.1 Some notations

We start with notations, some of which are borrowed from [7]. We write $A \lesssim B$ or $B \gtrsim A$ to denote the statement that $A \leq CB$ for some constant $C > 0$. This constant may vary from line to line, but it is independent of τ or n . Further, we write $A \sim B$ for $A \lesssim B \lesssim A$, we denote

$$\langle \xi \rangle = \sqrt{1 + \xi \cdot \xi}, \quad \xi = (\xi^1, \dots, \xi^d) \in \mathbb{Z}^d$$

and define $(d\xi)$ to be the normalized counting measure on \mathbb{Z}^d such that

$$\int a(\xi)(d\xi) = \sum_{\xi \in \mathbb{Z}^d} a(\xi).$$

The Fourier transform of a function f on \mathbb{T}^d is defined by

$$\hat{f}(\xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} e^{-i\mathbf{x} \cdot \xi} f(\mathbf{x}) d\mathbf{x}.$$

Instead of \hat{f} , we sometimes also write $\mathcal{F}f$ or $\mathcal{F}(f)$. The Fourier inversion formula takes the form

$$f(\mathbf{x}) = \int e^{i\mathbf{x} \cdot \xi} \hat{f}(\xi)(d\xi).$$

We recall the following properties of the Fourier transform:

$$\|f\|_{L^2(\mathbb{T}^d)} = (2\pi)^{\frac{d}{2}} \|\hat{f}\|_{L^2(\mathbb{Z}^d)} \quad (\text{Plancherel});$$

$$\langle f, g \rangle = \int_{\mathbb{T}^d} f(\mathbf{x}) \overline{g(\mathbf{x})} d\mathbf{x} = (2\pi)^d \int \hat{f}(\xi) \overline{\hat{g}(\xi)}(d\xi) \quad (\text{Parseval});$$

$$\widehat{fg}(\xi) = \int \hat{f}(\xi - \eta) \hat{g}(\eta)(d\eta) \quad (\text{convolution}).$$

For the Sobolev space $H^s(\mathbb{T}^d)$, $s \geq 0$, we consider the equivalent norm

$$\|f\|_{H^s(\mathbb{T}^d)} = \|J^s f\|_{L^2(\mathbb{T}^d)} = (2\pi)^{\frac{d}{2}} \left\| (1 + |\xi|^2)^{\frac{s}{2}} \hat{f}(\xi) \right\|_{L^2(\mathbb{Z}^d)},$$

where $J^s = (1 - \Delta)^{\frac{s}{2}}$.

2.2 Some estimates

First, we recall the following inequalities, which were originally proved in [15].

Lemma 2.1 (The Kato-Ponce inequality, [15]) *The following inequalities hold:*

(i) *For any $\gamma > \frac{d}{2}$ and $f, g \in H^\gamma$, we have*

$$\|J^\gamma(fg)\|_{L^2} \lesssim \|f\|_{H^\gamma} \|g\|_{H^\gamma}.$$

(ii) *For any $\delta \geq 0$, $\gamma > \frac{d}{2}$ and $f \in H^{\delta+\gamma}$, $g \in H^\delta$, we have*

$$\|J^\delta(fg)\|_{L^2} \lesssim \|f\|_{H^{\delta+\gamma}} \|g\|_{H^\delta}.$$

The next lemma plays a crucial role in the analysis of this paper.

Lemma 2.2 *Let $\alpha, \beta \in \mathbb{R}$. Then, the following properties hold:*

(i) *For ψ defined as in (1.4), we have*

$$\frac{1}{\tau} \int_0^\tau s e^{is\alpha} ds = -\tau \psi(i\tau\alpha). \quad (2.1)$$

(ii) *There exists a function $\mathcal{R}_2(\alpha, \beta, \tau)$ such that*

$$\int_0^\tau e^{is(\alpha+\beta)} ds = \tau \varphi(i\tau\alpha) - \tau(e^{i\tau\beta} - 1)\psi(i\tau\alpha) + \mathcal{R}_2(\alpha, \beta, \tau) \quad (2.2)$$

$$\text{with } |\mathcal{R}_2(\alpha, \beta, \tau)| \lesssim \tau^3 |\beta|^2.$$

Proof (i) We first note that

$$\int_0^\tau e^{is\alpha} ds = \begin{cases} \frac{e^{i\tau\alpha} - 1}{i\alpha}, & \alpha \neq 0 \\ \tau, & \alpha = 0 \end{cases} = \tau \varphi(i\tau\alpha). \quad (2.3)$$

Using integration by parts, we then find that

$$\frac{1}{\tau} \int_0^\tau s e^{is\alpha} ds = \begin{cases} \frac{e^{i\tau\alpha}}{i\alpha} + \frac{e^{i\tau\alpha} - 1}{\tau\alpha^2}, & \alpha \neq 0, \\ \frac{1}{2}\tau, & \alpha = 0, \end{cases} \quad (2.4)$$

which proves (i).

(ii) From (2.2), we obtain that the remainder \mathcal{R}_2 satisfies

$$\mathcal{R}_2(\alpha, \beta, \tau) = \int_0^\tau e^{is(\alpha+\beta)} ds - \tau \varphi(i\tau\alpha) + \tau(e^{i\tau\beta} - 1)\psi(i\tau\alpha). \quad (2.5)$$

Using (2.1) and (2.3), we rewrite (2.5) in the following way

$$\mathcal{R}_2(\alpha, \beta, \tau) = \int_0^\tau \left(e^{is(\alpha+\beta)} - e^{is\alpha} - i\beta e^{is\beta} \cdot \frac{1}{\tau} \int_0^\tau \sigma e^{i\sigma\alpha} d\sigma \right) ds.$$

First, we decompose

$$\int_0^\tau (e^{is(\alpha+\beta)} - e^{is\alpha}) ds = \int_0^\tau (e^{is(\alpha+\beta)} - e^{is\alpha} - is\beta e^{is\alpha}) ds + i\beta \int_0^\tau s e^{is\alpha} ds,$$

and thus get

$$\mathcal{R}_2(\alpha, \beta, \tau) = \int_0^\tau e^{is\alpha} (e^{is\beta} - 1 - is\beta) ds + i\beta \int_0^\tau (1 - e^{is\beta}) ds \cdot \frac{1}{\tau} \int_0^\tau s e^{is\alpha} ds. \quad (2.6)$$

Finally, note that

$$|e^{is\alpha} (e^{is\beta} - 1 - is\beta)| \lesssim s^2 |\beta|^2, \quad |1 - e^{is\beta}| \lesssim s |\beta|, \quad \left| \frac{1}{\tau} \int_0^\tau s e^{is\alpha} ds \right| \lesssim \tau.$$

Therefore, (2.6) can be controlled by $C\tau^3 |\beta|^2$. \square

3 Construction of the method

Now we derive a second-order numerical method for (1.1). Since the employed approximations form the basis of our error analysis, we present some construction details. For an alternative derivation of this method, we refer to [3].

Let $\tau > 0$ be the time step size and $t_n = n\tau$, $n \geq 0$ the temporal grid points. First, by employing the twisted variable $v = e^{-it\Delta} u$ and Duhamel's formula, we get

$$v(t_n + \sigma) = v(t_n) + i \int_0^\sigma e^{-i(t_n+\rho)\Delta} (|e^{i(t_n+\rho)\Delta} v(t_n + \rho)|^2 e^{i(t_n+\rho)\Delta} v(t_n + \rho)) d\rho. \quad (3.1)$$

Then, freezing the nonlinear interaction by approximating $e^{i(t_n+\rho)\Delta} \approx e^{i(t_n+\sigma)\Delta}$ and $v(t_n + \rho) \approx v(t_n)$, we get

$$v(t_n + \sigma) = v(t_n) + i\sigma e^{-i(t_n+\sigma)\Delta} (|e^{i(t_n+\sigma)\Delta} v(t_n)|^2 e^{i(t_n+\sigma)\Delta} v(t_n)) + \mathcal{R}_3^n(v, \sigma). \quad (3.2)$$

The remainder term $\mathcal{R}_3^n(v, \sigma)$ satisfies the following estimate.

Lemma 3.1 *Let $\gamma > \frac{d}{2}$, $\sigma \in [0, \tau]$ and $v \in L^\infty((0, T); H^{\gamma+2})$. Then,*

$$\|\mathcal{R}_3^n(v, \sigma)\|_{H^\gamma} \lesssim \tau^2 (\|v\|_{L^\infty((0, T); H^{\gamma+2})} + \|v\|_{L^\infty((0, T); H^{\gamma+2})}^3).$$

We postpone the proof of the lemma to Sect. 3.1.

Next, we derive a second-order expansion of Duhamel's formula

$$v(t_n + \tau) = v(t_n) + i \int_0^\tau e^{-i(t_n+\sigma)\Delta} (|e^{i(t_n+\sigma)\Delta} v(t_n + \sigma)|^2 e^{i(t_n+\sigma)\Delta} v(t_n + \sigma)) d\sigma. \quad (3.3)$$

Replacing $v(t_n + \sigma)$ by (3.2), we infer that

$$v(t_{n+1}) = v(t_n) + I_1(t_n) + I_2(t_n) + \mathcal{R}_4^n(v), \quad (3.4)$$

where

$$\begin{aligned} I_1(t_n) &= i \int_0^\tau e^{-i(t_n+s)\Delta} \left(|e^{i(t_n+s)\Delta} v(t_n)|^2 e^{i(t_n+s)\Delta} v(t_n) \right) ds, \\ I_2(t_n) &= - \int_0^\tau s e^{-i(t_n+s)\Delta} \left(|e^{i(t_n+s)\Delta} v(t_n)|^4 e^{i(t_n+s)\Delta} v(t_n) \right) ds. \end{aligned} \quad (3.5)$$

The remainder term $\mathcal{R}_4^n(v)$ can be bounded as stated in the following lemma. Again, the proof of this lemma is postponed to Sect. 3.1.

Lemma 3.2 *Let $\gamma > \frac{d}{2}$ and $0 < \tau \leq 1$. Then, for $v \in L^\infty((0, T); H^{\gamma+2})$,*

$$\|\mathcal{R}_4^n(v)\|_{H^\gamma} \leq C\tau^3,$$

where the constant C only depends on $\|v\|_{L^\infty((0, T); H^{\gamma+2})}$.

Due to the complexity of the phase functions

$$\phi_3 = |\xi|^2 + |\xi_1|^2 - |\xi_2|^2 - |\xi_3|^2, \quad \phi_5 = |\xi|^2 + |\xi_1|^2 + |\xi_2|^2 - |\xi_3|^2 - |\xi_4|^2 - |\xi_5|^2,$$

we note that the terms in I_1 and I_2 cannot be easily expressed in physical space.

Therefore, we consider I_1 first in Fourier space. Using

$$e^{is\Delta} w(\mathbf{x}) = \int e^{is\mathbf{x} \cdot \boldsymbol{\eta}} e^{-is|\boldsymbol{\eta}|^2} \hat{w}(\boldsymbol{\eta}) (d\boldsymbol{\eta}), \quad (3.6)$$

we get

$$\widehat{I_1}(t_n, \boldsymbol{\xi}) = i \int_0^\tau \int_{\boldsymbol{\xi} = \boldsymbol{\xi}_1 + \boldsymbol{\xi}_2 + \boldsymbol{\xi}_3} e^{i(t_n+s)\phi_3} \widehat{v}(t_n, \boldsymbol{\xi}_1) \widehat{v}(t_n, \boldsymbol{\xi}_2) \widehat{v}(t_n, \boldsymbol{\xi}_3) (d\boldsymbol{\xi}_1) (d\boldsymbol{\xi}_2) ds.$$

The main problem concerns the handling of the phase $e^{is\phi_3}$. Defining

$$\alpha = 2|\xi_1|^2, \quad \beta = 2\xi_1 \cdot \xi_2 + 2\xi_1 \cdot \xi_3 + 2\xi_2 \cdot \xi_3$$

allows us to write

$$e^{is\phi_3} = e^{is\alpha + is\beta}.$$

Applying the formulas presented in Lemma 2.2, we get

$$\begin{aligned} \widehat{I_1}(t_n, \boldsymbol{\xi}) &= i\tau \int_{\boldsymbol{\xi} = \boldsymbol{\xi}_1 + \boldsymbol{\xi}_2 + \boldsymbol{\xi}_3} \varphi(i\tau\alpha) e^{it_n\phi_3} \widehat{v}(t_n, \boldsymbol{\xi}_1) \widehat{v}(t_n, \boldsymbol{\xi}_2) \widehat{v}(t_n, \boldsymbol{\xi}_3) (d\boldsymbol{\xi}_1) (d\boldsymbol{\xi}_2) \\ &\quad - i\tau \int_{\boldsymbol{\xi} = \boldsymbol{\xi}_1 + \boldsymbol{\xi}_2 + \boldsymbol{\xi}_3} (e^{i\tau\beta} - 1) \psi(i\tau\alpha) e^{it_n\phi_3} \widehat{v}(t_n, \boldsymbol{\xi}_1) \widehat{v}(t_n, \boldsymbol{\xi}_2) \widehat{v}(t_n, \boldsymbol{\xi}_3) (d\boldsymbol{\xi}_1) (d\boldsymbol{\xi}_2) \end{aligned}$$

$$+ \widehat{\mathcal{R}}_5^n(v)(\xi), \quad (3.7)$$

where the remainder term $\mathcal{R}_5^n(v)$ obeys the bound given in the following lemma. Its proof will be postponed to Sect. 3.1.

Lemma 3.3 *Let $\gamma > \frac{d}{2}$ and $v \in L^\infty((0, T); H^{\gamma+2})$. Then,*

$$\|\mathcal{R}_5^n(v)\|_{H^\gamma} \lesssim \tau^3 \|v\|_{L^\infty((0, T); H^{\gamma+2})}^3.$$

Using $\beta = \phi_3 - \alpha$ and (3.6), we transform (3.7) back to physical space to get

$$\begin{aligned} I_1(t_n) &= i\tau e^{-it_n\Delta} \left\{ [\varphi(-2i\tau\Delta) e^{-it_n\Delta} \bar{v}(t_n)] \cdot (e^{it_n\Delta} v(t_n))^2 \right\} \\ &\quad - i\tau e^{-it_{n+1}\Delta} \left\{ [\psi(-2i\tau\Delta) e^{-it_{n+1}\Delta} \bar{v}(t_n)] \cdot (e^{it_{n+1}\Delta} v(t_n))^2 \right\} \\ &\quad + i\tau e^{-it_n\Delta} \left\{ [\psi(-2i\tau\Delta) e^{-it_n\Delta} \bar{v}(t_n)] \cdot (e^{it_n\Delta} v(t_n))^2 \right\} + \mathcal{R}_5^n(v). \end{aligned} \quad (3.8)$$

The term I_2 is of higher order in τ . Therefore, it is sufficient to freeze the linear flow and approximate the term as

$$I_2(t_n) = - \int_0^\tau s e^{-it_n\Delta} (|e^{it_n\Delta} v(t_n)|^4 e^{it_n\Delta} v(t_n)) ds + \mathcal{R}_6^n(v) \quad (3.9)$$

$$= -\frac{1}{2} \tau^2 e^{-it_n\Delta} (|e^{it_n\Delta} v(t_n)|^4 e^{it_n\Delta} v(t_n)) + \mathcal{R}_6^n(v), \quad (3.10)$$

where the remainder term $\mathcal{R}_6^n(v)$ obeys the bound given in the following lemma. Again, its proof will be postponed to Sect. 3.1.

Lemma 3.4 *Let $\gamma > \frac{d}{2}$ and $v \in L^\infty((0, T); H^{\gamma+2})$. Then*

$$\|\mathcal{R}_6^n(v)\|_{H^\gamma} \lesssim \tau^3 \|v\|_{L^\infty((0, T); H^{\gamma+2})}^5.$$

Now combining (3.4), (3.8), and (3.10), we have that

$$v(t_{n+1}) = \Phi^n(v(t_n)) + \mathcal{R}_4^n(v) + \mathcal{R}_5^n(v) + \mathcal{R}_6^n(v), \quad (3.11)$$

where the operator Φ^n is defined by

$$\begin{aligned} \Phi^n(f) &= f + i\tau e^{-it_n\Delta} \left\{ (\varphi(-2i\tau\Delta) e^{-it_n\Delta} \bar{f}) \cdot (e^{it_n\Delta} f)^2 \right\} \\ &\quad - i\tau e^{-it_{n+1}\Delta} \left\{ (\psi(-2i\tau\Delta) e^{-it_{n+1}\Delta} \bar{f}) \cdot (e^{it_{n+1}\Delta} f)^2 \right\} \\ &\quad + i\tau e^{-it_n\Delta} \left\{ (\psi(-2i\tau\Delta) e^{-it_n\Delta} \bar{f}) \cdot (e^{it_n\Delta} f)^2 \right\} \\ &\quad - \frac{1}{2} \tau^2 e^{-it_n\Delta} (|e^{it_n\Delta} f|^4 e^{it_n\Delta} f). \end{aligned} \quad (3.12)$$

Our second-order low-regularity integrator is obtained by dropping the remainder terms \mathcal{R}_4^n , \mathcal{R}_5^n , \mathcal{R}_6^n in (3.11). The method for the twisted variable is summarized as follows: let $v^0 = u_0$ and

$$v^{n+1} = \Phi^n(v^n) \quad \text{for } n \geq 0. \quad (3.13)$$

Finally, setting $u^n = e^{it_n \Delta} v^n$, we obtain the announced numerical scheme (1.6) for the NLS equation (1.1).

3.1 Estimates of the remainder terms

Now we prove Lemmas 3.1 to 3.4.

Proof of Lemma 3.1 By (3.2), we have that

$$\begin{aligned} \mathcal{R}_3^n(v, s) &= i \int_0^s (e^{-i(t_n+\sigma)\Delta} - e^{-i(t_n+s)\Delta}) (|e^{i(t_n+\sigma)\Delta} v(t_n+\sigma)|^2 e^{i(t_n+\sigma)\Delta} v(t_n+\sigma)) d\sigma \\ &\quad + i \int_0^s e^{-i(t_n+s)\Delta} (|e^{i(t_n+\sigma)\Delta} v(t_n+\sigma)|^2 - |e^{i(t_n+s)\Delta} v(t_n+s)|^2) e^{i(t_n+\sigma)\Delta} v(t_n+\sigma) d\sigma \\ &\quad + i \int_0^s e^{-i(t_n+s)\Delta} (|e^{i(t_n+s)\Delta} v(t_n+s)|^2 (e^{i(t_n+\sigma)\Delta} v(t_n+\sigma) - e^{i(t_n+s)\Delta} v(t_n))) d\sigma. \end{aligned}$$

Note that from (3.1), Lemma 2.1(i), and the Sobolev embedding, we get

$$\sup_{0 \leq \sigma \leq \tau} \|v(t_n+\sigma) - v(t_n)\|_{H^\gamma} \lesssim \tau \|v\|_{L^\infty((0,T);H^\gamma)}^3.$$

Moreover, for any $f \in H^\gamma$,

$$\|(e^{-i(t_n+\sigma)\Delta} - e^{-i(t_n+s)\Delta})f\|_{H^\gamma} \lesssim |\sigma - s| \|f\|_{H^{\gamma+2}}. \quad (3.14)$$

Applying these two estimates, we obtain

$$\|e^{i(t_n+\sigma)\Delta} v(t_n+\sigma) - e^{i(t_n+s)\Delta} v(t_n)\|_{H^\gamma} \lesssim \tau (\|v\|_{L^\infty((0,T);H^{\gamma+2})} + \|v\|_{L^\infty((0,T);H^{\gamma+2})}^3)$$

and thus

$$\|\mathcal{R}_3^n(v, s)\|_{H^\gamma} \lesssim \tau^2 (\|v\|_{L^\infty((0,T);H^{\gamma+2})} + \|v\|_{L^\infty((0,T);H^{\gamma+2})}^3).$$

This is the desired result. \square

Proof of Lemma 3.2 Inserting (3.2) with $\sigma = \rho$ in (3.1) and using (3.4), we find that the remainder $\mathcal{R}_4^n(v)$ consists of terms of the form

$$i \int_0^\tau e^{-i(t_n+s)\Delta} (e^{i(t_n+s)\Delta} \mathcal{W}_j \cdot e^{-i(t_n+s)\Delta} \overline{\mathcal{W}_k} \cdot e^{i(t_n+s)\Delta} \mathcal{W}_\ell) ds, \quad j+k+\ell \geq 5,$$

where

$$\begin{aligned} \mathcal{W}_1 &= v(t_n), \\ \mathcal{W}_2 &= i s e^{-i(t_n+s)\Delta} (|e^{i(t_n+s)\Delta} v(t_n)|^2 e^{i(t_n+s)\Delta} v(t_n)), \\ \mathcal{W}_3 &= \mathcal{R}_3^n(v, s). \end{aligned}$$

By Lemma 3.1 and Lemma 2.1(i), we thus get

$$\|\mathcal{R}_4^n(v)\|_{H^\gamma} \lesssim C(\|v(t_n)\|_{L^\infty((0,t);H^{\gamma+2})})\tau^3.$$

This finishes the proof of the lemma. \square

Proof of Lemma 3.3 Without loss of generality, we may assume that $\hat{v}(t_n)$ and $\hat{\hat{v}}(t_n)$ are positive (otherwise, one may replace them with their absolute values).

From Lemma 2.2, we have

$$\widehat{\mathcal{R}_5^n(v)}(\xi) = \int_{\xi=\xi_1+\xi_2+\xi_3} \mathcal{R}_2(\alpha, \beta, \tau) e^{it_n\phi_3} \hat{v}(t_n, \xi_1) \hat{v}(t_n, \xi_2) \hat{v}(t_n, \xi_3) (d\xi_1)(d\xi_2)$$

and further

$$|\widehat{\mathcal{R}_5^n(v)}(\xi)| \lesssim \tau^3 \int_{\xi=\xi_1+\xi_2+\xi_3} \beta^2 \hat{v}(t_n, \xi_1) \hat{v}(t_n, \xi_2) \hat{v}(t_n, \xi_3) (d\xi_1)(d\xi_2).$$

By symmetry, we may assume that $|\xi_1| \geq |\xi_2| \geq |\xi_3|$. This yields

$$\begin{aligned} \langle \xi \rangle^\gamma \beta^2 &\lesssim \langle \xi \rangle^\gamma (|\xi_1|^2 |\xi_2|^2 + |\xi_1|^2 |\xi_3|^2 + |\xi_2|^2 |\xi_3|^2) \\ &\lesssim |\xi_1|^{2+\gamma} |\xi_2|^2. \end{aligned}$$

Using this estimate, we get

$$\begin{aligned} \langle \xi \rangle^\gamma |\widehat{\mathcal{R}_5^n(v)}(\xi)| &\lesssim \tau^3 \int_{\xi=\xi_1+\xi_2+\xi_3, |\xi_1| \geq |\xi_2| \geq |\xi_3|} |\xi_1|^{2+\gamma} |\xi_2|^2 \hat{v}(t_n, \xi_1) \hat{v}(t_n, \xi_2) \hat{v}(t_n, \xi_3) (d\xi_1)(d\xi_2) \\ &\lesssim \tau^3 \mathcal{F}((-\Delta)^{1+\gamma/2} \tilde{v} \cdot (-\Delta)v \cdot v)(t_n, \xi). \end{aligned}$$

Therefore, by Plancherel's identity and Lemma 2.1(ii) with $\delta = 0$, we obtain that for any $\gamma_1 > \frac{d}{2}$,

$$\begin{aligned} \|\mathcal{R}_5^n(v)\|_{H^\gamma} &\lesssim \tau^3 \|(-\Delta)^{1+\gamma/2} \tilde{v} \cdot (-\Delta)v \cdot v\|_{L^\infty((0,T);L^2)} \\ &\lesssim \tau^3 \|v\|_{L^\infty((0,T);H^{\gamma+2})} \|v\|_{L^\infty((0,T);H^{\gamma_1+2})} \|v\|_{L^\infty((0,T);H^{\gamma_1})}. \end{aligned}$$

Since $\gamma > \frac{d}{2}$, choosing $\gamma_1 = \gamma$, we get the desired result. \square

Proof of Lemma 3.4 By (3.5) and (3.9), we have that

$$\begin{aligned} \mathcal{R}_6^n &= - \int_0^\tau s(e^{-i(t_n+s)\Delta} - e^{-it_n\Delta})(|e^{i(t_n+s)\Delta} v(t_n)|^4 e^{i(t_n+s)\Delta} v(t_n)) ds \\ &\quad - \int_0^\tau s e^{-it_n\Delta} (|e^{i(t_n+s)\Delta} v(t_n)|^4 - |e^{it_n\Delta} v(t_n)|^4) e^{i(t_n+s)\Delta} v(t_n) ds \\ &\quad - \int_0^\tau s e^{-it_n\Delta} (|e^{it_n\Delta} v(t_n)|^4 \cdot (e^{-i(t_n+s)\Delta} - e^{-it_n\Delta}) v(t_n)) ds. \end{aligned}$$

Then, the claimed result follows directly from (3.14) and Lemma 2.1(i). \square

4 Proof of Theorem 1.1

Taking the difference between the numerical scheme (3.13) and the exact solution gives

$$\begin{aligned} v^{n+1} - v(t_{n+1}) &= \Phi^n(v(t_n)) - v(t_{n+1}) + \Phi^n(v^n) - \Phi^n(v(t_n)) \\ &= \mathcal{L}^n + \Phi^n(v^n) - \Phi^n(v(t_n)), \end{aligned}$$

where $\mathcal{L}^n = \Phi^n(v(t_n)) - v(t_{n+1})$ is the local error.

4.1 Local error

The following bound on the local error holds.

Lemma 4.1 *Let $\gamma > \frac{d}{2}$ and $0 < \tau \leq 1$. Then,*

$$\|\mathcal{L}^n\|_{H^\gamma} \leq C\tau^3,$$

where the constant C only depends on $\|v\|_{L^\infty((0,T);H^{\gamma+2})}$.

Proof By (3.11), we get that

$$\mathcal{L}^n = -\mathcal{R}_4^n(v) - \mathcal{R}_5^n(v) - \mathcal{R}_6^n(v).$$

Thus, the desired estimate follows from Lemmas 3.2, 3.3, and 3.4. \square

4.2 Stability

The main result in this subsection is the following stability estimate.

Lemma 4.2 *Let $\gamma > \frac{d}{2}$. Then,*

$$\|\Phi^n(v^n) - \Phi^n(v(t_n))\|_{H^\gamma} \leq (1 + C\tau)\|v^n - v(t_n)\|_{H^\gamma} + C\tau\|v^n - v(t_n)\|_{H^\gamma}^5,$$

where the constant C only depends on $\|v\|_{L^\infty((0,T);H^\gamma)}$.

Proof For short, we denote $g_n = v^n - v(t_n)$. Then, using (3.12), we have

$$\Phi^n(v^n) - \Phi^n(v(t_n)) = g_n + \sum_{j=1}^4 (\Phi_j^n(v^n) - \Phi_j^n(v(t_n))),$$

where

$$\begin{aligned} \Phi_1^n(f) &= i\tau e^{-it_n\Delta} \{ (\varphi(-2i\tau\Delta) e^{-it_n\Delta} \bar{f}) \cdot (e^{it_n\Delta} f)^2 \} \\ \Phi_2^n(f) &= -i\tau e^{-it_{n+1}\Delta} \{ (\psi(-2i\tau\Delta) e^{-it_{n+1}\Delta} \bar{f}) \cdot (e^{it_{n+1}\Delta} f)^2 \} \\ \Phi_3^n(f) &= i\tau e^{-it_n\Delta} \{ (\psi(-2i\tau\Delta) e^{-it_n\Delta} \bar{f}) \cdot (e^{it_n\Delta} f)^2 \} \\ \Phi_4^n(f) &= -\frac{1}{2} \tau^2 e^{-it_n\Delta} (|e^{it_n\Delta} f|^4 e^{it_n\Delta} f). \end{aligned}$$

Note that by the definition of φ and ψ in (1.4), we have that

$$\|\varphi(-2i\tau\Delta)f\|_{H^\gamma} \lesssim \|f\|_{H^\gamma}, \quad \|\psi(-2i\tau\Delta)f\|_{H^\gamma} \lesssim \|f\|_{H^\gamma}.$$

Hence, by Lemma 2.1(i),

$$\|\Phi_1''(v^n) - \Phi_1''(v(t_n))\|_{H^\gamma} \leq C\tau(\|g_n\|_{H^\gamma} + \|g_n\|_{H^\gamma}^3),$$

where C only depends on $\|v\|_{L^\infty((0,T);H^\gamma)}$.

Similarly, we get that

$$\sum_{j=2}^4 \|\Phi_j''(v^n) - \Phi_j''(v(t_n))\|_{H^\gamma} \leq C\tau(\|g_n\|_{H^\gamma} + \|g_n\|_{H^\gamma}^5). \quad (4.1)$$

Combining the above estimates, we finally obtain

$$\|\Phi''(v(t_n)) - \Phi''(v^n)\|_{H^\gamma} \leq \|g_n\|_{H^\gamma} + C\tau(\|g_n\|_{H^\gamma} + \|g_n\|_{H^\gamma}^5),$$

which is the desired result. \square

4.3 Proof of Theorem 1.1

Now, combining the local error estimate with the stability result, we prove Theorem 1.1. From Lemma 4.1 and Lemma 4.2, we infer that there exists a constant C depending only on $\|v\|_{L^\infty((0,T);H^{\gamma+2})}$ such that for $0 < \tau \leq 1$, we have

$$\|v(t_{n+1}) - v^{n+1}\|_{H^\gamma} \leq C\tau^3 + (1 + C\tau)\|v(t_n) - v^n\|_{H^\gamma} + C\tau\|v(t_n) - v^n\|_{H^\gamma}^5, \quad n \geq 0.$$

By recursion, we get from this the bound

$$\|v(t_{n+1}) - v^{n+1}\|_{H^\gamma} \leq C\tau \sum_{j=0}^n (1 + C\tau)^j [\|v(t_{n-j}) - v^{n-j}\|_{H^\gamma}^5 + C\tau^2].$$

From this estimate, we infer that there exist positive constants τ_0 and C such that for any $\tau \in [0, \tau_0]$,

$$\|v(t_{n+1}) - v^{n+1}\|_{H^\gamma} \leq C\tau^3 \sum_{j=0}^n (1 + C\tau)^j \leq C\tau^2, \quad n \geq 0.$$

Note that the constants τ_0 and C only depend on T and $\|u\|_{L^\infty((0,T);H^{\gamma+2})}$. This proves Theorem 1.1.

5 Numerical experiments

In this section, we carry out some numerical experiments to illustrate our convergence result in two space dimensions. For this purpose, we consider the nonlinear Schrödinger equation (1.1) with initial data

$$u_0(x_1, x_2) = \sum_{(k,\ell) \in \mathbb{Z}^2} (1 + \sqrt{k^2 + \ell^2})^{-\frac{1}{2} - \gamma - \varepsilon} (1 + i) e^{i(kx_1 + \ell x_2)}, \quad \varepsilon > 0, \quad (5.1)$$

where γ is used to set the regularity of the data. This choice guarantees that $u^0 \in H^\gamma(\mathbb{T}^2)$. In the experiment, we set $\varepsilon = 0$.

In order to be able to use FFT techniques, we discretize space by equidistant grid points

$$x_1^j = \frac{2\pi j}{N}, \quad x_2^m = \frac{2\pi m}{N}, \quad 0 \leq j, m \leq N-1.$$

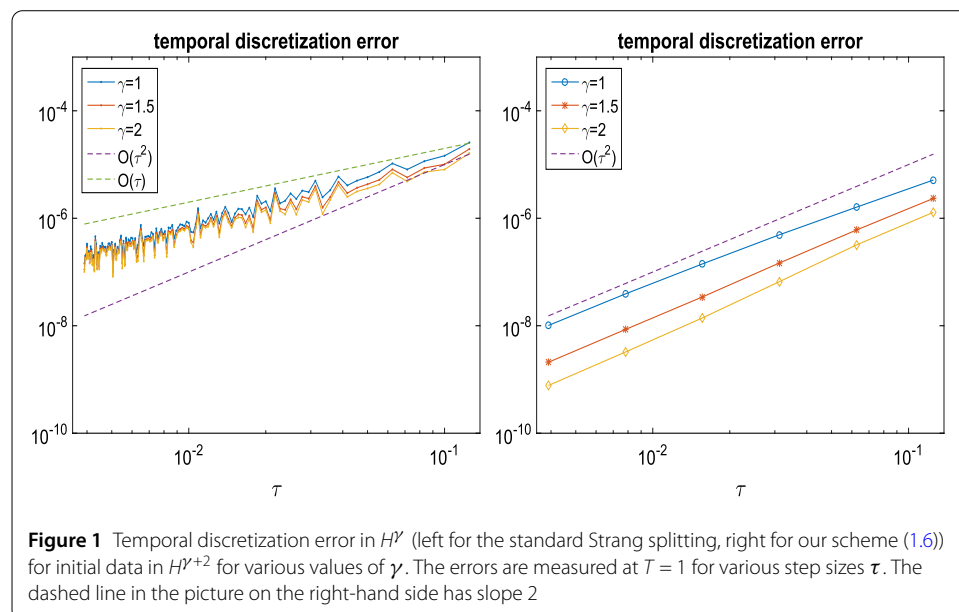
The numerical approximation, obtained with step size τ at $t = t_n = n\tau$ on this grid will be denoted by $u_{\tau,N}^n$. We choose $N = 2^7$, i.e., 2^{14} grid points, and measure the temporal discretization error $w = u(t_n, \cdot) - u_{\tau,N}^n$, defined on the grid by $w(t_n, x_1^j, x_2^m) = u(t_n, x_1^j, x_2^m) - u_{\tau,N}^n(j, m)$. We consider this matrix as an element of the linear space L_N^2 with norm $\|\cdot\|_{L_N^2}$ defined by

$$\|w\|_{L_N^2}^2 = \frac{4\pi^2}{N^2} \sum_{j,m=0}^{N-1} |w(x_1^j, x_2^m)|^2.$$

The discrete H_N^γ spaces are then defined in the usual way with the help of the discrete Fourier transform, i.e.,

$$\|w\|_{H_N^\gamma} = 2\pi \left\| \sum_{j,m=0}^{N-1} \left(1 + \sqrt{j^2 + m^2}\right)^\gamma \widehat{w}_{j,m} \right\|_{L_N^2}.$$

Our results for initial data $u_0 \in H^{\gamma+2}(\mathbb{T}^2)$ are presented in Fig. 1. We choose the three different values $\gamma = 1, 1.5, 2$ to illustrate the convergence rate. In the left panel, we present the results for the standard Strang splitting. As expected, the Strang splitting shows a strong order reduction and irregular error behavior. For our scheme (1.6), the results are given in the right panel. As expected, the slopes of the error curves are 2 whenever γ is bigger than 1. The slope of the curve for $\gamma = 1$ is slightly less regular. This is also expected because the value $\gamma = 1$ is the limit case in two space dimensions. Thus, the results agree well with the corresponding results of the theoretical analysis given in Theorem 1.1.



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Competing interests

The authors declare that they have no competing interests.

Authors' contributions

The authors declare that the study was realized in collaboration with equal responsibility. All authors read and approved the final manuscript.

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