

A SECOND ORDER LOW-REGULARITY INTEGRATOR FOR THE NONLINEAR SCHRÖDINGER EQUATION

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ABSTRACT. In this paper, we analyse a new exponential-type integrator for the nonlinear cubic Schrödinger equation on the d dimensional torus $\mathbb{T}^d$. The scheme has recently also been derived in a wider context of decorated trees in [3]. It is explicit and efficient to implement. Here, we present an alternative derivation, and we give a rigorous error analysis. In particular, we prove 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 in [17].

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.

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:

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

where $\mathbb{T} = (0, 2\pi)$, $\lambda = \pm 1$, $u = u(t, x) : \mathbb{R}^+ \times \mathbb{T}^d \rightarrow \mathbb{C}$ is the sought-after solution, and $u_0 \in H^\gamma(\mathbb{T}^d)$ for some $\gamma \geq 0$ 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 $H^\gamma(\mathbb{T}^d)$ has been established for $\gamma > \frac{d}{2} - 1$. For details, we refer to [2].

Numerical aspects of the NLS equation have been studied by many authors. A considerable amount of literature has been published on splitting methods and exponential integration methods. For a general introduction to these methods, we refer to [9, 10, 11, 12, 18]. It is well known that schemes of arbitrarily high order can be constructed by assuming that the solution of (1.1) is smooth enough. For instance, second order convergence in H^γ was obtained by requiring four additional derivatives of the solution for the Strang splitting scheme in [16]. Further convergence results for semilinear Schrödinger equations can be found, e.g., in [1, 4, 5, 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

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made in [19], where the authors introduced a new exponential-type numerical scheme and achieved first-order convergence in $H^\gamma(\mathbb{T}^d)$ for $H^{\gamma+1}(\mathbb{T}^d)$ initial data. Later, a first-order integrator was proposed in [22]. It converges in $H^\gamma(\mathbb{T})$ 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 [17]. The integrator is based on the variation-of-constants formula and makes use of certain resonance based approximations in Fourier space. For 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 analyse an improved integrator which 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 non-linearity 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

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

and consider the phase function

$$\phi_3 = |\boldsymbol{\xi}|^2 + |\boldsymbol{\xi}_1|^2 - |\boldsymbol{\xi}_2|^2 - |\boldsymbol{\xi}_3|^2.$$

In [17], letting

$$\alpha = 2|\boldsymbol{\xi}_1|^2, \quad \beta = 2\boldsymbol{\xi}_1 \cdot \boldsymbol{\xi}_2 + 2\boldsymbol{\xi}_1 \cdot \boldsymbol{\xi}_3 + 2\boldsymbol{\xi}_2 \cdot \boldsymbol{\xi}_3,$$

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 present 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 above example) while β has a “bad” structure but still has a low upper-bound, e.g., consisting of mixed derivatives (as in the example above). Then we employ the following approximation

$$e^{is(\alpha+\beta)} \approx e^{is\alpha} + i\beta e^{is\beta} \mathcal{M}_\tau(e^{i\alpha}), \quad (1.3)$$

where the operator $\mathcal{M}_\tau$ is defined by

$$\mathcal{M}_\tau(g) = \frac{1}{\tau} \int_0^\tau \sigma g(\sigma) d\sigma. \quad (1.4)$$

The mean $\mathcal{M}_\tau(e^{i\alpha})$ can be regarded as an approximation to $\tau e^{i\alpha\tau}$ for small τ .

Using the approximation (1.3) has several advantages. First, its integral has a point-wise interpretation in physical space,

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

see Lemma 2.2 below. Here, the functions φ and ψ are defined as

$$\varphi(z) = \begin{cases} \frac{e^z - 1}{z}, & z \neq 0, \\ 1, & z = 0, \end{cases} \quad \psi(z) = \begin{cases} \frac{e^z - 1 - ze^z}{z^2}, & z \neq 0, \\ -\frac{1}{2}, & z = 0. \end{cases} \quad (1.6)$$

Secondly, it is a high-order approximation and requires less regularity. Indeed, we get

$$\int_0^\tau e^{is(\alpha+\beta)} ds = \tau\varphi(i\tau\alpha) - \tau(e^{i\tau\beta} - 1)\psi(i\tau\alpha) + \mathcal{R}_2(\alpha, \beta, \tau), \quad (1.7)$$

where $|\mathcal{R}_2(\alpha, \beta, \tau)| \lesssim \tau^3|\beta|^2$. This 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 $H^\gamma(\mathbb{T}^d)$ for initial data in $H^{\gamma+2}(\mathbb{T}^d)$.

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 integrators with second-order accuracy as

$$\begin{aligned} u^0 &= u_0, \\ u^{n+1} &= e^{i\tau\Delta} u^n + i\tau e^{i\tau\Delta} \left\{ [\varphi(-2i\tau\Delta) + \psi(-2i\tau\Delta)] \bar{u}^n \cdot (u^n)^2 \right\} \\ &\quad - i\tau [e^{i\tau\Delta} \psi(-2i\tau\Delta) \bar{u}^n] \cdot (e^{i\tau\Delta} u^n)^2 - \frac{\tau^2}{2} e^{i\tau\Delta} [|u^n|^4 u^n] \end{aligned} \quad (1.8)$$

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

Theorem 1.1. *Let u^n be the numerical solution (1.8) 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*

$$\|u(t_n, \cdot) - u^n\|_{H^\gamma} \leq C\tau^2, \quad 0 \leq n\tau \leq T. \quad (1.9)$$

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 wider context. In particular, using the formalism of decorated trees, various numerical methods for the nonlinear Schrödinger equation are proposed. The above method (1.8) is stated there in formula (5.17). Nevertheless, we give here 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 Section 2, we introduce some notation and collect some useful lemmas. In Section 3, we discuss the construction of the method and analyse accuracy and regularity requirements of each single approximation step. Collecting all these results, we proof our convergence result (Theorem 1.1) in Section 4. This theoretical result is illustrated with some numerical experiments in Section 5.

2. PRELIMINARIES

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

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

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

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

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

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

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

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

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

We recall the following properties of the Fourier transform:

$$\begin{aligned} \|f\|_{L^2(\mathbb{T}^d)} &= (2\pi)^{\frac{d}{2}} \|\hat{f}\|_{L^2((d\boldsymbol{\xi}))} \quad (\text{Plancherel}); \\ \langle f, g \rangle &= \int_{\mathbb{T}^d} f(\mathbf{x}) \overline{g(\mathbf{x})} d\mathbf{x} = (2\pi)^d \int \hat{f}(\boldsymbol{\xi}) \overline{\hat{g}(\boldsymbol{\xi})} (d\boldsymbol{\xi}) \quad (\text{Parseval}); \\ \widehat{(fg)}(\boldsymbol{\xi}) &= \int \hat{f}(\boldsymbol{\xi} - \boldsymbol{\eta}) \hat{g}(\boldsymbol{\eta}) (d\boldsymbol{\eta}) \quad (\text{convolution}). \end{aligned}$$

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

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

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

2.2. Some estimates. First, we recall the following inequality, which was originally proved in [15].

Lemma 2.1. (*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 $\mathcal{M}_\tau$ be the operator defined in (1.4) and $\alpha, \beta \in \mathbb{R}$. Then, the following properties hold.*

(i) *For φ, ψ defined as in (1.6), we have*

$$\int_0^\tau \left(e^{is\alpha} + i\beta e^{is\beta} \mathcal{M}_\tau(e^{i\alpha\cdot}) \right) ds = \tau\varphi(i\tau\alpha) - \tau(e^{i\tau\beta} - 1)\psi(i\tau\alpha). \quad (2.1)$$

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

$$\int_0^\tau e^{is(\alpha+\beta)} ds = \int_0^\tau \left(e^{is\alpha} + i\beta e^{is\beta} \mathcal{M}_\tau(e^{i\alpha\cdot}) \right) ds + \mathcal{R}_2(\alpha, \beta, \tau), \quad (2.2)$$

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

Proof. (i) The left-hand side of (2.1) is equal to

$$\int_0^\tau e^{is\alpha} ds + \int_0^\tau i\beta e^{is\beta} \mathcal{M}_\tau(e^{i\alpha\cdot}) ds. \quad (2.3)$$

For the first term in (2.3), we have that

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

For the second term in (2.3), using integration-by-parts, we find that

$$\mathcal{M}_\tau(e^{i\alpha\cdot}) = \frac{1}{\tau} \int_0^\tau \sigma e^{i\sigma\alpha} d\sigma = \begin{cases} \frac{e^{i\tau\alpha}}{i\alpha} + \frac{e^{i\tau\alpha} - 1}{\tau\alpha^2}, & \alpha \neq 0, \\ \frac{1}{2}\tau, & \alpha = 0. \end{cases} \quad (2.5)$$

Thus, from the definition of ψ , we infer that

$$\mathcal{M}_\tau(e^{i\alpha\cdot}) = -\tau\psi(i\tau\alpha). \quad (2.6)$$

In addition,

$$\int_0^\tau i\beta e^{is\beta} ds = e^{i\tau\beta} - 1. \quad (2.7)$$

Therefore, combining (2.4) with (2.6) and (2.7) proves the first part of the lemma.

(ii) From (2.2), we obtain

$$\mathcal{R}_2(\alpha, \beta, \tau) = \int_0^\tau \left(e^{is(\alpha+\beta)} - e^{is\alpha} - i\beta e^{is\beta} \mathcal{M}_\tau(e^{i\alpha\cdot}) \right) ds. \quad (2.8)$$

First, we decompose

$$\begin{aligned} \int_0^\tau \left(e^{is(\alpha+\beta)} - e^{is\alpha} \right) ds &= \int_0^\tau \left(e^{is(\alpha+\beta)} - e^{is\alpha} - is\beta e^{is\alpha} \right) ds + i\beta \int_0^\tau s e^{is\alpha} ds \\ &= \int_0^\tau e^{is\alpha} (e^{is\beta} - 1 - is\beta) ds + i\beta \tau \mathcal{M}_\tau(e^{i\alpha\cdot}) \end{aligned}$$

and thus get

$$\mathcal{R}_2(\alpha, \beta, \tau) = \int_0^\tau e^{is\alpha} (e^{is\beta} - 1 - is\beta) ds + i\beta \int_0^\tau (1 - e^{is\beta}) ds \cdot \mathcal{M}_\tau(e^{i\alpha\cdot}). \quad (2.9)$$

Note that

$$\left| e^{is\alpha} (e^{is\beta} - 1 - is\beta) \right| \lesssim s^2 |\beta|^2, \quad \left| 1 - e^{is\beta} \right| \lesssim s |\beta|, \quad |\mathcal{M}_\tau(e^{i\alpha})| \lesssim \tau.$$

Therefore, (2.9) 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 details of the construction. 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

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

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

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

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 Section 3.1.

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

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

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 next lemma. Again, the proof of this lemma is postponed to Section 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

$$\phi_3 = |\boldsymbol{\xi}|^2 + |\boldsymbol{\xi}_1|^2 - |\boldsymbol{\xi}_2|^2 - |\boldsymbol{\xi}_3|^2, \quad \phi_5 = |\boldsymbol{\xi}|^2 + |\boldsymbol{\xi}_1|^2 + |\boldsymbol{\xi}_2|^2 - |\boldsymbol{\xi}_3|^2 - |\boldsymbol{\xi}_4|^2 - |\boldsymbol{\xi}_5|^2,$$

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

Therefore, we consider I_1 first in Fourier space and write

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

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

$$\alpha = 2|\boldsymbol{\xi}_1|^2, \quad \beta = 2\boldsymbol{\xi}_1 \cdot \boldsymbol{\xi}_2 + 2\boldsymbol{\xi}_1 \cdot \boldsymbol{\xi}_3 + 2\boldsymbol{\xi}_2 \cdot \boldsymbol{\xi}_3$$

allows us to write

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

Applying the formulas presented in Lemma 2.2, we get

$$\begin{aligned} \widehat{I}_1(t_n, \boldsymbol{\xi}) &= i\tau \int_{\boldsymbol{\xi}=\boldsymbol{\xi}_1+\boldsymbol{\xi}_2+\boldsymbol{\xi}_3} \varphi(i\tau\alpha) e^{it_n\phi_3} \widehat{v}(t_n, \boldsymbol{\xi}_1) \widehat{v}(t_n, \boldsymbol{\xi}_2) \widehat{v}(t_n, \boldsymbol{\xi}_3) (d\boldsymbol{\xi}_1)(d\boldsymbol{\xi}_2) \\ &\quad - i\tau \int_{\boldsymbol{\xi}=\boldsymbol{\xi}_1+\boldsymbol{\xi}_2+\boldsymbol{\xi}_3} (e^{i\tau\beta} - 1) \psi(i\tau\alpha) e^{it_n\phi_3} \widehat{v}(t_n, \boldsymbol{\xi}_1) \widehat{v}(t_n, \boldsymbol{\xi}_2) \widehat{v}(t_n, \boldsymbol{\xi}_3) (d\boldsymbol{\xi}_1)(d\boldsymbol{\xi}_2) \\ &\quad + \widehat{\mathcal{R}_5^n}(v)(\boldsymbol{\xi}), \end{aligned} \quad (3.6)$$

where the remainder term $\mathcal{R}_5^n(v)$ obeys the bound given in the following lemma. Its proof will be postponed to Section 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 $\beta = \phi_3 - \alpha$, we transform (3.6) back to physical space to get

$$\begin{aligned} I_1 &= i\tau e^{-it_n\Delta} \left\{ [\varphi(-2i\tau\Delta) e^{-it_n\Delta} \bar{v}(t_n)] \cdot \left(e^{it_n\Delta} v(t_n) \right)^2 \right\} \\ &\quad - i\tau e^{-it_{n+1}\Delta} \left\{ [\psi(-2i\tau\Delta) e^{-it_{n+1}\Delta} \bar{v}(t_n)] \cdot \left(e^{it_{n+1}\Delta} v(t_n) \right)^2 \right\} \\ &\quad + i\tau e^{-it_n\Delta} \left\{ [\psi(-2i\tau\Delta) e^{-it_n\Delta} \bar{v}(t_n)] \cdot \left(e^{it_n\Delta} v(t_n) \right)^2 \right\} + \mathcal{R}_5^n(v). \end{aligned} \quad (3.7)$$

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

$$I_2(t_n) = - \int_0^\tau s e^{-it_n\Delta} \left(|e^{it_n\Delta} v(t_n)|^4 e^{it_n\Delta} v(t_n) \right) ds + \mathcal{R}_6^n(v) \quad (3.8)$$

$$= -\frac{1}{2} \tau^2 e^{-it_n\Delta} \left(|e^{it_n\Delta} v(t_n)|^4 e^{it_n\Delta} v(t_n) \right) + \mathcal{R}_6^n(v), \quad (3.9)$$

where the remainder term $\mathcal{R}_6^n(v)$ obeys the bound given in the following lemma. Again, its proof will be postponed to Section 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), (3.7) and (3.9), we have that

$$v(t_{n+1}) = \Phi^n(v(t_n)) + \mathcal{R}_4^n(v) + \mathcal{R}_5^n(v) + \mathcal{R}_6^n(v), \quad (3.10)$$

where the operator Φ^n is defined by

$$\begin{aligned} \Phi^n(f) = & f + i\tau e^{-it_n\Delta} \left\{ \left(\varphi(-2i\tau\Delta) e^{-it_n\Delta} \bar{f} \right) \cdot \left(e^{it_n\Delta} f \right)^2 \right\} \\ & - i\tau e^{-it_{n+1}\Delta} \left\{ \left(\psi(-2i\tau\Delta) e^{-it_{n+1}\Delta} \bar{f} \right) \cdot \left(e^{it_{n+1}\Delta} f \right)^2 \right\} \\ & + i\tau e^{-it_n\Delta} \left\{ \left(\psi(-2i\tau\Delta) e^{-it_n\Delta} \bar{f} \right) \cdot \left(e^{it_n\Delta} f \right)^2 \right\} \\ & - \frac{1}{2} \tau^2 e^{-it_n\Delta} \left(|e^{it_n\Delta} f|^4 e^{it_n\Delta} f \right). \end{aligned} \quad (3.11)$$

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 (3.10). The method for the twisted variable is summarized as follows: let $v^0 = u_0$ and

$$v^{n+1} = \Phi^n(v^n) \quad \text{for } n \geq 0. \quad (3.12)$$

Finally, setting $u^n = e^{it_n\Delta} v^n$, we obtain the announced numerical scheme (1.8) 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

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

Note that from (3.1), Lemma 2.1 (i) and 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 $f \in H^\gamma$,

$$\left\| \left(e^{-i(t_n+\sigma)\Delta} - e^{-i(t_n+s)\Delta} \right) f \right\|_{H^\gamma} \lesssim |\sigma - s| \|f\|_{H^{\gamma+2}}. \quad (3.13)$$

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) shows that the remainder $\mathcal{R}_4^n(v)$ consists of terms of the form

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

where

$$\mathcal{W}_1 = v(t_n), \quad \mathcal{W}_2 = i s e^{-i(t_n+s)\Delta} \left(|e^{i(t_n+s)\Delta} v(t_n)|^2 e^{i(t_n+s)\Delta} v(t_n) \right), \quad \mathcal{W}_3 = \mathcal{R}_3^n(v, s).$$

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

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

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 by their absolute values).

From Lemma 2.2, we have

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

and further

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

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

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

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

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

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

Proof of Lemma 3.4. By (3.5) and (3.8), we have that

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

Then, the claimed result follows directly from (3.13) and Lemma 2.1 (i). $\square$

4. PROOF OF THEOREM 1.1

Taking the difference between the numerical scheme (3.12) 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 (3.10), 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 (3.11), 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

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

$$\Phi_4^n(f) = -\frac{1}{2}\tau^2 e^{-it_n\Delta} \left(|e^{it_n\Delta} f|^4 e^{it_n\Delta} f \right).$$

Note that by the definition of φ and ψ in (1.6), 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),

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

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

Similarly, we get that

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

Combining the above estimates, we finally obtain

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

which is the desired result. $\square$

4.3. Proof of Theorem 1.1. Now, combining the local error estimate with the stability result, we give the proof of 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

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

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. $\square$

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 $\varepsilon = 0$.

We choose $N = 2^7$, i.e. 2^{14} grid points, and measure the temporal discretisation error $w = u(t_n, \cdot) - u_{\tau, N}^n$ in the discrete H^γ -norm

$$\|w\|_{H_N^\gamma} = \left\| (1 + \sqrt{-\Delta})^\gamma w \right\|_{L_N^2},$$

where

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

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 of our scheme (1.8). 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.

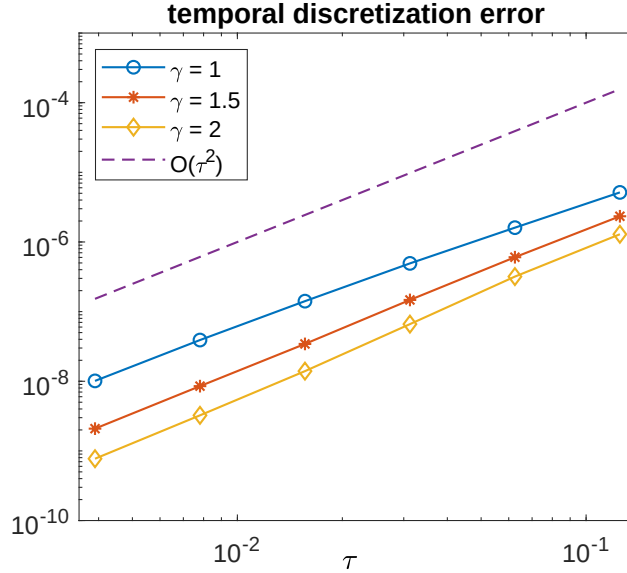


FIGURE 1. Temporal discretisation error in H^γ for initial data in $H^{\gamma+2}$ for various values of γ . The errors are measured at $T = 1$ for various step sizes τ . The dashed line has slope 2.

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Not applicable.

Competing interests

The authors declare that they have no competing interests.

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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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