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Second-Order SAV Schemes for the Nonlinear Schrödinger Equation and Their Error Analysis

Beichuan Deng[1] · Jie Shen[1] · Qingqu Zhuang[2]

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Abstract
We consider a second-order SAV scheme for the nonlinear Schrödinger equation in the whole space with typical generalized nonlinearities, and carry out a rigorous error analysis. We also develop a fully discretized SAV scheme with Hermite–Galerkin approximation for the space variables, and present numerical experiments to validate our theoretical results.

Keywords Nonlinear Schrödinger equation · SAV approach · Energy conservation · Error analysis · Hermite spectral method

Mathematics Subject Classification 65M12 · 35Q55 · 65M70

1 Introduction

We consider in this paper numerical approximation of the following nonlinear Schrodinger (NLS) equation [20]:

$$\begin{cases} i\,\frac{\partial u}{\partial t} = -\alpha\Delta u - 2\beta f(|u|^2)u, & x \in \mathbb{R}^d,\ t > 0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}^d\ (d = 1, 2, 3), \end{cases} \tag{1.1}$$

with the initial and boundary conditions

$$u(x,0) = u_0(x), \quad \lim_{|x|\to\infty} |u(x,t)| = 0,\ t \geq 0. \tag{1.2}$$

✉ Jie Shen
shen7@purdue.edu

Beichuan Deng
deng192@purdue.edu

Qingqu Zhuang
qqzhuang@hqu.edu.cn

1 Department of Mathematics, Purdue University, West Lafayette 47907, IN, USA

2 Fujian Province University Key Laboratory of Computation Science, School of Mathematical Sciences, Huaqiao University, Quanzhou 362021, China

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In the above, $\alpha > 0$ and $\beta \in \mathbb{R}$ are two dimensionless constants with $\beta < 0$ for the repulsive or defocusing interaction and $\beta > 0$ for the attractive or focusing interaction, i is the imaginary unit, $u(\cdot, t) : \mathbb{R}^d \to \mathbb{C}$ for any $t > 0$, and $f(\cdot)$ is a real-valued smooth function. In this work, we will consider the following typical cases:

(1) $f(\rho) = \rho^\sigma$, where σ is a positive integer, referred to as polynomial nonlinearity with $f(\rho) = \rho$ to be the usual cubic nonlinearity [20].
(2) $f(\rho) = \frac{\rho}{1+\gamma\rho}$ with $\gamma > 0$, referred to as the saturation of the intensity nonlinearity [1].

The NLS equation arises in many areas of sciences and engineering, in particular, it is a mean-field approximation of many-body problems in quantum physics and chemistry [20]. Its analysis, approximation and simulation have attracted enormous attention in past decades, we refer to [12,25] for its mathematical properties and [3,4] for reviews of its numerical approximation.

The NLS equation enjoys many distinctive mathematical properties, including in particular conservations of energy (or Hamiltonian)

$$E_{total}[u](t) := \int_{\mathbb{R}^d} \frac{\alpha}{2}|\nabla u(x,t)|^2 - 2\beta F(|u(x,t)|^2)dx \equiv E_{total}[u](0), \quad \forall t \geq 0, \tag{1.3}$$

where $F(\rho) := \int_0^\rho f(s)ds$, and conservation of mass

$$N[u](t) := \int_{\mathbb{R}^d} |u(x,t)|^2 dx \equiv N[u](0), \quad \forall t \geq 0. \tag{1.4}$$

Thus, it is important for a numerical scheme to conserve (or accurately approximate) the discrete energy and mass. Among the many existing schemes for the NLS equation (1.1), the implicit Crank–Nicolson scheme [2] is perhaps the only scheme which can conserve both energy and mass for general f, and the relaxation finite-difference scheme [5,6,10] conserves both energy and mass for the special case of cubic nonlinearity. The implicit Crank–Nicolson scheme leads to a nonlinear system at each time step while the relaxation finite-difference scheme leads to a linear system with variable coefficients at each time step. Both are second-order accurate in time. We refer to [4,8,9,17,26] for more detail on the various numerical schemes for the NLS equation.

Recently, a powerful approach, the so called scalar auxiliary variable (SAV) approach [22,23], was introduced for gradient flows. The SAV approach leads to numerical schemes with some remarkable properties: (i) unconditionally energy stable; (ii) only requiring solving decoupled linear systems with constant coefficients at each time step. Since the NLS equation also has a variational structure with respect to the free energy (1.3), we can apply the SAV approach to the NLS equation to construct an efficient and accurate discretization in time scheme with the following properties: (i) it is second-order, unconditionally stable and conserve a modified energy; (ii) it only requires solving two Poisson-type equations at each time step. The semi-discrete scheme can be combined with any consistent Galerkin type spatial discretization such as finite-elements [28–30] or spectral methods [11,14,18] to construct fully discrete schemes with the same properties as the semi-discrete scheme. In this paper, we treat the unbounded domain directly using a Hermite-spectral method so as to eliminate the domain truncation error.

While the construction of the SAV scheme for the NLS equation using the SAV approach is quite straightforward since the NLS equation can be reformulated as a gradient flow system, its error analysis can not follow from the analysis in [21] which used essentially the dissipative property of gradient flows to derive a uniform H^2 bound for the numerical solution. However, the NLS equation is dispersive and conserves the energy so there is no dissipation. Therefore, more delicate analyses are needed for the error estimates. The main goals of this paper are to derive optimal error estimates for the semi-discrete SAV scheme.

The rest of the paper is organized as follows. In Sect. 2, we describe the second-order Crank–Nicolson scheme with Adams–Bashforth extrapolation based on the SAV approach in the semi-discrete form, and prove its stability and energy conservation. In Sect. 3, we carry out a rigorous error analysis for the semi-discrete SAV scheme. In Sect. 4, we construct the fully discrete Hermite SAV scheme, and perform some numerical results to verify our theoretical results. Some concluding remarks are given in the last section.

We now describe some notations. We denote $\Omega = \mathbb{R}^d$, $d = 1, 2, 3$. For any complex function v, $\bar{v}$ denotes its complex conjugate, and the inner product in $L^2(\Omega)$ is

$$(w, v) := \int_\Omega w\bar{v}dx.$$

We will use the standard notations $L^2(\Omega)$, $H^k(\Omega)$ and $H_0^k(\Omega)$ to denote the usual Sobolev spaces of complex functions over Ω. The norm corresponding to $H^k(\Omega)$ will be denoted simply by $\|\cdot\|_k$. In particular, we use $\|\cdot\|$ to denote the norm in $L^2(\Omega)$. We shall use C to denote a generic positive constant independent of the time step size τ, and occassionaly we use $A \lesssim B$ to denote that $A \le CB$ for some constant C independent of τ.

We recall a regularity result for (1.1) which plays an important role in the subsequent error analysis.

Theorem 1 (see, for instance, [12], Theorem 4.10.1) *Let $s > \frac{d}{2}$ be an integer. For every $u_0 \in H^s(\mathbb{R}^d)$, there exists $T_{max} > 0$, such that*

- *there is a unique, maximal solution $u \in C([0, T_{max}); H^s(R^d))$ for (1.1);*
- *if $\beta < 0$, then $T_{max} = \infty$;*
- *if $T_{max} < \infty$, then $\lim_{t\to T_{max}} \|u(\cdot, t)\|_{H^s} \to \infty$.*

2 A Semi-discrete SAV Scheme

While the SAV approach was originally introduced for dissipative gradient flows, it can be directly applied to dispersive equations such as NLS with variational structures. Indeed, the key in the SAV approach is to introduce a scalar auxiliary variable (SAV) $r(t) := \sqrt{E[u](t)}$ where, for a given $C_0 > 0$ and $F(\rho) := \int_0^\rho f(s)ds$,

$$E[u](t) := \int_\Omega F(|u(x, t)|^2)dx + C_0. \tag{2.1}$$

We choose C_0 such that $E[u] + C_0 \ge \delta > 0$ for any u. Note that it is important not to include "-2β" in the definition of $E[u](t)$ because, for $\beta > 0$, $-2\beta \int_\Omega F(|u(x, t)|^2)dx$ can not be bounded from below for all u.

We reformulate (1.1) as:

$$\begin{cases} i\frac{\partial u}{\partial t} = -\alpha\Delta u - 2\beta\frac{r}{\sqrt{E[u]}} f(|u|^2)u, \\ \frac{dr}{dt} = \frac{1}{\sqrt{E[u]}} \int_\Omega f(|u|^2)Re(u \cdot \bar{u}_t)dx, \end{cases} \tag{2.2}$$

with the initial and boundary conditions. To simplify the presentation, we shall omit the boundary conditions in (1.2) in all subsequent equations.

Let $0 < T < T_{max}$. Given a time step τ, we set $M = \frac{T}{\tau}$. Then a second-order SAV scheme for (2.2) based on Crank–Nicolson with Adams–Bashforth extrapolation is:

Let $U^0 = u_0$, $r^0 = r(0)$, and denote $H[w] = \frac{f(|w|^2)}{\sqrt{E[w]}}$. We compute U^1 and r^1 by a Crank–Nicholson scheme with a first-order extrapolation

$$i\frac{U^1 - U^0}{\tau} = -\alpha\Delta\frac{U^1 + U_0}{2} - 2\beta\frac{r^1 + r^0}{2}H[U_0]U_0, \tag{2.3}$$

$$r^1 - r^0 = \int_\Omega H[U_0]Re(U_0 \cdot \overline{U^1 - U_0})dx. \tag{2.4}$$

Then for $n = 1, 2, \ldots, M-1$,

$$i\frac{U^{n+1} - U^n}{\tau} = -\alpha\Delta\left(\frac{U^{n+1} + U^n}{2}\right) - 2\beta\frac{r^{n+1} + r^n}{2}H\big[\tilde{U}^{n+\frac{1}{2}}\big]\tilde{U}^{n+\frac{1}{2}}, \tag{2.5}$$

$$r^{n+1} - r^n = \int_\Omega H\big[\tilde{U}^{n+\frac{1}{2}}\big]Re\big[\tilde{U}^{n+\frac{1}{2}} \cdot \big(\overline{U^{n+1} - U^n}\big)\big]dx, \tag{2.6}$$

where $\tilde{U}^{n+\frac{1}{2}} = \frac{3}{2}U^n - \frac{1}{2}U^{n-1}$. We note that the first-order extrapolation used in (2.3)–(2.4) has a second-order local truncation error so the overall accuracy is still second-order. In a recent paper [7], a similar scheme is constructed but the first-step is computed by a nonlinear Crank–Nicolson scheme.

It is clear that the scheme (2.5)–(2.6) is linear but coupled. We show below that it can be efficiently solved. Writing

$$U^{n+1} = \phi^{n+1} + r^{n+1}\varphi^{n+1}, \tag{2.7}$$

in (2.5), we find that ϕ^{n+1} and φ^{n+1} satisfy

$$\frac{i}{\tau}\phi^{n+1} + \frac{\alpha}{2}\Delta\phi^{n+1} = Q^n, \tag{2.8}$$

$$\frac{i}{\tau}\varphi^{n+1} + \frac{\alpha}{2}\Delta\varphi^{n+1} = -\beta H\big[\tilde{U}^{n+\frac{1}{2}}\big]\tilde{U}^{n+\frac{1}{2}}, \tag{2.9}$$

with

$$Q^n = \frac{i}{\tau}U^n - \frac{\alpha}{2}\Delta U^n - \beta r^n H\big[\tilde{U}^{n+\frac{1}{2}}\big]\tilde{U}^{n+\frac{1}{2}}.$$

Then, plugging (2.7) in (2.6), we find

$$r^{n+1} = \frac{r^n + \int_\Omega H\big[\tilde{U}^{n+\frac{1}{2}}\big]Re\big(\tilde{U}^{n+\frac{1}{2}} \cdot \overline{\phi^{n+1} - U^n}\big)dx}{1 - \int_\Omega H\big[\tilde{U}^{n+\frac{1}{2}}\big]Re\big(\tilde{U}^{n+\frac{1}{2}} \cdot \overline{\varphi^{n+1}}\big)dx}. \tag{2.10}$$

In summary, the solution of (2.5)–(2.6) can be determined as follows:

1. Determine ϕ and φ from (2.8) and (2.9), respectively;
2. Compute r^{n+1} from (2.10);
3. Obtain U^{n+1} from (2.7).

Hence, the main computational cost of the scheme (2.5)–(2.6) is to solve the two decoupled linear systems with constant coefficients (2.8)–(2.9), which can be efficiently solved by one's favorite method. The first step (2.3)–(2.4) can be solved similarly.

Theorem 2 *The SAV scheme (2.3)–(2.6) preserves a modified Hamiltonian unconditionally in the sense that*

$$\frac{\alpha}{2}\big\|\nabla U^{n+1}\big\|^2 - \beta\big(r^{n+1}\big)^2 = \frac{\alpha}{2}\|\nabla U^n\|^2 - \beta\big(r^n\big)^2, \quad n = 0, 1, \ldots, M-1.$$

Proof Multiplying Eq. (2.5) by $\overline{U^{n+1}-U^n}$, then integrating it over Ω and taking the real part, we obtain

$$0=\frac{\alpha}{2}\Big(\|\nabla U^{n+1}\|^2-\|\nabla U^n\|^2\Big)-2\beta\frac{r^{n+1}+r^n}{2}\int_\Omega H\big[\tilde{U}^{n+\frac{1}{2}}\big]Re\big(\tilde{U}^{n+\frac{1}{2}}\cdot\overline{U^{n+1}-U^n}\big)dx.$$

Then, by plugging (2.6) into the above equation, it yields

$$\frac{\alpha}{2}\big\|\nabla U^{n+1}\big\|^2-\beta\big(r^{n+1}\big)^2=\frac{\alpha}{2}\big\|\nabla U^n\big\|^2-\beta\big(r^n\big)^2,\quad n=1,\ldots,M-1.$$

We can obtain energy conservation of the first step by applying the same process to (2.3)–(2.4). □

Remark 1 By Theorem 2, we have

$$\alpha\big\|\nabla U^n\big\|^2-2\beta\big(r^n\big)^2=\alpha\|\nabla u_0\|^2-2\beta\left(\int_\Omega F\big(|u_0|^2\big)dx+C_0\right),\quad n=0,1,\ldots,M.$$

Hence, when $\beta<0$ (the repulsive case), $\{r^n\}_{n=0}^M$ is uniformly bounded:

$$|r^n|\le E_0:=\left(\alpha\|\nabla u_0\|^2+2|\beta|\int_\Omega F\big(|u_0|^2\big)dx+C_0\right)^{\frac{1}{2}},\quad n=0,1,\ldots,M. \tag{2.11}$$

When $\beta>0$ (the attractive case), we have

$$(r^n)^2=\frac{\alpha}{2|\beta|}\|\nabla U^n\|^2+D_0,\ \text{where } D_0:=-\frac{\alpha}{2|\beta|}\|\nabla u_0\|^2+\int_\Omega F\big(|u_0|^2\big)dx+C_0,$$

which implies

$$|r^n|\le\sqrt{\frac{\alpha}{2\beta}}\|\nabla U^n\|+\sqrt{|D_0|},\quad n=0,1,\ldots,M. \tag{2.12}$$

3 Error Analysis for the Semi-discretized Scheme

The error analysis will be carried out in two main steps. In the first step, we derive a local (in time) H^s bound for the numerical solution. Then, in the second step, we first use the the local H^s bound to derive a local error estimate, followed by a continuation process to extend the H^s bound and the error estimate to the whole interval $[0,T]$.

3.1 Local H^s Bound of the Numerical Solution

We recall a useful result which will be used in the sequel.

Lemma 1 (see [10], Lemma 2.2) *Let use define*

$$A:=\left(1-\frac{i}{2}\alpha\tau\Delta\right)^{-1}\left(1+\frac{i}{2}\alpha\tau\Delta\right),\quad B:=\left(1-\frac{i}{2}\alpha\tau\Delta\right)^{-1}. \tag{3.1}$$

Then for any $s>0$, we have

- *A is a unitary operator on H^s.*
- *B is a bounded operator on H^s: $\|B\|_s\le1$.*

Next, we shall use Lemma 1 to prove that solutions of the scheme (2.3)–(2.6) are uniformly bounded in H^s. To this end, we express solutions of (2.3)–(2.6) using the operators in (3.1) as follows:

$$\begin{aligned} U^1 &= Au_0 + \beta i\tau \cdot (r^1 + r^0)BW^0, \\ U^{n+1} &= AU^n + \beta i\tau BW^{n+\frac{1}{2}}\left(r^n + r^{n+1}\right), \quad n = 1, 2, \dots, M-1, \end{aligned}$$

where

$$W^{n+\frac{1}{2}} = \frac{1}{\sqrt{E[\tilde{U}^{n+\frac{1}{2}}]}} f\left(\left|\tilde{U}^{n+\frac{1}{2}}\right|^2\right)\tilde{U}^{n+\frac{1}{2}}, \quad n = 0, 1, \dots, M-1. \tag{3.2}$$

Summing them up, we obtain

$$\begin{aligned} U^{n+1} &= A^{n+1}u_0 + \beta i\tau \Big[r^0 A^n BW^0 + r^1\left(A^n BW^0 + A^{n-1}BW^{\frac{3}{2}}\right) \\ &\quad + \sum_{k=2}^{n} r^k \left(A^{n+1-k}BW^{k-\frac{1}{2}} + A^{n-k}BW^{k+\frac{1}{2}}\right)\Big] + \beta i\tau BW^{n+\frac{1}{2}} \cdot r^{n+1}. \end{aligned} \tag{3.3}$$

We first establish a result on the local-in-time boundedness of U^n in H^s.

Theorem 3 *Let $u_0 \in H^s(\mathbb{R}^d)$, with $s > \frac{d}{2} + 1$. Then there exist T^* and $C > 0$, independent of τ but dependent on $\|u_0\|_{H^s}$, such that*

$$\max_{1\le n\le M^*=T^*/\tau}\{\|U^n\|_{H^s}\} \le C = C(\|u_0\|_{H^s}),$$

unconditionally when $\beta < 0$; and conditionally for $\tau \le \tau_0$ when $\beta > 0$, where τ_0 depends on $\|u_0\|_{H^s}$ only.

Proof We derive from (3.3) and Lemma 1 that

$$\begin{aligned} \|U^{n+1}\|_{H^s} &\le \|A^n Au_0\|_{H^s} + |\beta|\tau\Big[|r^0|\|A^n BW^0\|_{H^s} + |r^1|\big(\|A^n BW^0\|_{H^s} + \|A^{n-1}BW^{\frac{3}{2}}\|_{H^s}\big) \\ &\quad + \sum_{k=2}^{n-1}|r^k|\big(\|A^{n+1-k}BW^{k-\frac{1}{2}}\|_{H^s} + \|A^{n-k}BW^{k+\frac{1}{2}}\|_{H^s}\big)\Big] + \tau|\beta r^{n+1}|\|BW^{n+\frac{1}{2}}\|_{H^s} \\ &\le \|u_0\|_{H^s} + |\beta|\tau\Big[|r^0|\|W^0\|_{H^s} + |r^1|\big(\|W^0\|_{H^s} + \|W^{\frac{3}{2}}\|_{H^s}\big) \\ &\quad + \left(\sum_{k=2}^{n-1}|r^k|\big(\|W^{k-\frac{1}{2}}\|_{H^s} + \|W^{k+\frac{1}{2}}\|_{H^s}\big)\right) + |r^{n+1}|\|W^{n+\frac{1}{2}}\|_{H^s}\Big]. \end{aligned} \tag{3.4}$$

Given $u_0 \in H^s(\mathbb{R}^d)$, we define R such that $\|u_0\|_{H^s} = \frac{R}{4}$, and we define the set

$$B_R := \left\{\phi \in H^s(\mathbb{R}^d),\ \|\phi\|_{H^s} \le \frac{R}{2}\right\}.$$

It is clear that U^{n+1} is uniquely determined by (3.3). Next, we prove by induction that there exists $T^* > 0$ such that $U^{n+1} \in B_R$, for all $n = 0, 1 \dots, T^*/\tau - 1$.

Obviously $u_0 \in B_R$. assuming that $U^k \in B_R$, $k = 1, 2, \dots, n$, we have

$$\max_{1\le k\le n}\left\{\left\|\frac{3}{2}U^k - \frac{1}{2}U^{k-1}\right\|_{H^s}\right\} \le R.$$

Since both $H^s(\mathbb{R}^d)$ and $H^{s-1}(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)$ by the Sobolev embedding theorem, there exists a constant C_1 depending on l and s only, s.t.

$$\|g^l\|_{H^s} \le C_1 \|g\|_{H^s}^l, \quad \forall g \in H^s.$$

So for $f(u) = (u)^\sigma$, we have

$$\left\| f\Big(\Big|\frac{3}{2}U^n - \frac{1}{2}U^{n-1}\Big|^2\Big)\Big(\frac{3}{2}U^n - \frac{1}{2}U^{n-1}\Big)\right\|_{H^s} \le C_1 R^{2\sigma+1},$$

while for $f(u) = \frac{(u)}{1+\gamma(u)} \le u$, we have

$$\left\| f\Big(\Big|\frac{3}{2}U^n - \frac{1}{2}U^{n-1}\Big|^2\Big)\Big(\frac{3}{2}U^n - \frac{1}{2}U^{n-1}\Big)\right\|_{H^s} \le \left\|\Big|\frac{3}{2}U^n - \frac{1}{2}U^{n-1}\Big|^2\Big(\frac{3}{2}U^n - \frac{1}{2}U^{n-1}\Big)\right\|_{H^s} \le C_1 R^3.$$

Setting

$$p_0 = \begin{cases} 2\sigma + 1, & \text{if } f(u) = (u)^\sigma, \text{ for } \sigma \in \mathcal{Z}_+ \\ 3, & \text{if } f(u) = \frac{(u)}{1+\gamma(u)} \end{cases},$$

we derive from the above and (3.2) that

$$\|\|BW^{n+\frac{1}{2}}\|_{H^s} \le \frac{C_1}{\delta} R^{p_0}, \quad \forall n. \tag{3.5}$$

We now proceed as follows:

Case 1 $\beta < 0$. By using (2.11), there is a uniform constant K which only depends on u_0, such that

$$\frac{|r^k|}{\sqrt{E\big[\frac{3}{2}U^{k-1} - \frac{1}{2}U^{k-2}\big]}} \le K, \qquad \frac{|r^k|}{\sqrt{E\big[\frac{3}{2}U^{k} - \frac{1}{2}U^{k-1}\big]}} \le K, \quad \forall 2 \le k \le n.$$

Then we derive from (3.4) and (3.5) that there is a constant C_2 independent of n and τ, s.t.

$$\|U^{n+1}\|_{H^s} \le \|u_0\|_{H^s} + C_2 T K R^{p_0}.$$

Hence, for $T^* \le \frac{1}{4C_2 K R^{p_0-1}}$, we have

$$\|U^{n+1}\|_{H^s} \le \|u_0\|_{H^s} + C_2 T K R^{p_0} \le \frac{R}{2}. \tag{3.6}$$

Case 2 $\beta > 0$: By using (2.12) and (3.4), we have

$$\begin{aligned} \left\|U^{n+1}\right\|_{H^s} \le \|u_0\|_{H^s} &+ \sqrt{\alpha\beta}\tau\left(\|\nabla U^0\|\|W^0\|_{H^s} + \left\|\nabla U^{n+1}\right\|\left\|W^{n+\frac{1}{2}}\right\|_{H^s}\right) + \sqrt{\alpha\beta}\tau \\ &\times\left[\|\nabla U^1\|\left(\left\|W^{\frac{1}{2}}\right\|_{H^s} + \left\|W^{\frac{3}{2}}\right\|_{H^s}\right) + \sum_{k=2}^{n-1}\|\nabla U^k\|\left(\|W^{k-\frac{1}{2}}\|_{H^s} + \left\|W^{k+\frac{1}{2}}\right\|_{H^s}\right)\right] \\ &+ \beta\tau\sqrt{|D_0|}\left[\left(\left\|W^{\frac{1}{2}}\right\|_{H^s} + \left\|W^{\frac{3}{2}}\right\|_{H^s}\right) + \sum_{k=2}^{n}\left(\left\|W^{k-\frac{1}{2}}\right\|_{H^s} + \left\|W^{k+\frac{1}{2}}\right\|_{H^s}\right)\right]. \end{aligned}$$

Since $s > 1$, $\|\nabla U^k\| \le \|U^k\|_{H^s} \le \frac{R}{2}$, for any $k = 1, 2, \dots, n$, and $\|\nabla U^{n+1}\| \le \|U^{n+1}\|_{H^s}$. We derive from the above and (3.5) that there is a constant C_3 independent to n and τ, s.t.

$$\big(1 - \tau C_1\sqrt{\alpha\beta}R^{p_0}\big)\|U^{n+1}\|_{H^s} \le \|u_0\|_{H^s} + C_3 T\big(R + \sqrt{|D_0|}\big)R^{p_0}. \tag{3.7}$$

Hence, for $\tau \leq \tau_0 := \frac{1}{4C_1\sqrt{\alpha\beta}R^{p_0}}$ and $T^* \leq \frac{1}{8C_3(R+\sqrt{|D_0|})R^{p_0-1}}$, we derive from the above that $\|U^{n+1}\|_{H^s} \leq \frac{R}{2}$. This completes the induction, and consequently, the proof of the Theorem. □

3.2 Error Estimates

We shall make frequent use of the following version of the discrete Gronwall lemma.

Lemma 2 *Let a_i, b_i, c_i, d_i, τ and e_0, for integers $i \geq 0$, be non-negative numbers such that*

$$a_n + \tau \sum_{i=0}^{n} b_i \leq \tau \sum_{i=0}^{n-1} d_i a_i + \tau \sum_{i=0}^{n-1} c_i + e_0, \quad \forall n \geq 0.$$

Then

$$a_n + \tau \sum_{i=0}^{n} b_i \leq \left(e_0 + \tau \sum_{i=0}^{n-1} c_i \right) \exp\left(\tau \sum_{i=0}^{n-1} d_i \right), \quad \forall n \geq 0.$$

We assume that the solution of (1.1) is sufficiently smooth, more precisely,

$$u_0 \in H^s(\mathbb{R}^d), \quad u \in H^3(0, T; H^s(\mathbb{R}^d)) \cap H^2(0, T; H^{s+2}(\mathbb{R}^d)), \tag{3.8}$$

with $s \geq 2$ when $d = 1$ and $s > \frac{d}{2} + 1$ when $d = 2, 3$.

Lemma 3 *Assuming (3.8), then for any $T < T_{max}$, there exists $K_0 > 0$ such that*

$$\|r_t\|_{L^\infty[0,T]} + \|r_{tt}\|_{L^\infty[0,T]} + \|r_{ttt}\|_{L^\infty[0,T]} \leq K_0.$$

Proof By the definition in (2.1), the desired results can be proved immediately by expressing r_{tt} and r_{ttt} in terms of the integrals of u, u_t, u_{tt} and u_{ttt}, respectively. □

We denote $t_n = n\tau$, $u^n(\cdot) = u(\cdot, t_n)$, and

$$e^n = u^n - U^n, \quad \varepsilon^n = r(t_n) - r^n, \quad n = 0, 1, 2 \ldots, M,$$

where $\|e^0\| = \varepsilon^0 = 0$.

Lemma 4 *Let $H[u] = \frac{f(|u|^2)}{\sqrt{E(u)}}$. Then, we have*

$$\|H[w] - H[v]\| \leq C\|w - v\| \quad \forall w, \quad v \in L^2(\Omega) \cap L^\infty(\Omega). \tag{3.9}$$

Furthermore, for any $T < T_{max}$, if $\|u\|_{L^\infty(0,T;H^2)\cap W^{2,\infty}(0,T;L^2)} + \|U\|_{l^\infty(0,T;H^2)} \leq K$, there exists $C > 0$ s.t.

$$\left\| H\left[\tilde{U}^{n+\frac{1}{2}}\right] - H\left[\tilde{u}^{n+\frac{1}{2}}\right] \right\| \leq C \left(\frac{3}{2}\|e^n\| + \frac{1}{2}\|e^{n-1}\| \right), \tag{3.10}$$

$$\left\| H\left[\tilde{u}^{n+\frac{1}{2}}\right] - H\left[u^{n+\frac{1}{2}}\right] \right\| \leq C\tau^2 \max_{t\in[0,T]} \|u_{tt}(\cdot, t)\|, \tag{3.11}$$

$$\left\| H\left[u^{n+\frac{1}{2}}\right]u^{n+\frac{1}{2}} - H\left[u^{n-\frac{1}{2}}\right]u^{n-\frac{1}{2}} \right\| \leq C\tau \max_{t\in[0,T]} \|u_t(\cdot, t)\|, \tag{3.12}$$

for all $1 \leq n \leq M - 1$ with $M = T/\tau$.

Proof By the triangle inequality, we have

$$\|H[w]-H[v]\| \le 2\frac{\Big|E[v]-E[w]\Big|}{\sqrt{E[v]E[w]}\big(\sqrt{E[v]}+\sqrt{E[w]}\big)}\|w\|_{L^4}^4+\frac{2}{\sqrt{E[v]}}\Big\||w|^2-|v|^2\Big\| := B_1+B_2.$$

Since $w(x), v(x) \in L^2(\Omega)\cap L^\infty(\Omega)$, then $w(x), v(x) \in L^4(\Omega)$, and

$$0 < E[w] = \|w\|_{L^4(\Omega)}^4 < \infty, \text{ and, } 0 < E[v] = \|v\|_{L^4(\Omega)}^4 < \infty.$$

Then by Holder's inequality, we have

$$\begin{aligned} B_1 &\le C\Big|E[w]-E[v]\Big| \le C\big(\|w\|_{L^\infty}^2+\|v\|_{L^\infty}^2\big)(\|w\|+\|v\|)\|w-v\|,\\ B_2 &\le C(\|w\|_{L^\infty}+\|v\|_{L^\infty})\|w-v\|. \end{aligned}$$

On the other hand, by the embedding theorem, we have

$$\|u\|_{L^\infty(0,T;L^\infty)},\ \|U\|_{L^\infty(0,T;L^\infty)} \le cK, \quad \text{for any } n=1,\dots,M.$$

By definition, $E[U^n]$, $E[u^{n+\frac{1}{2}}]$ and $E[u^n]$ are uniformly bounded from below, i.e. there exists $K_1>0$, s.t.

$$\frac{1}{E[U^n]}, \frac{1}{E[u^n]}, \frac{1}{E[u^{n-\frac{1}{2}}]} \le K_1 \text{ for any } n=1,\dots,M.$$

Therefore, by setting $C = 4K_1^2c^2K^3+2c\sqrt{K_1}K$, we have

$$\begin{aligned} \big\|H\big[\tilde{U}^{n+\frac{1}{2}}\big]-H\big[\tilde{u}^{n+\frac{1}{2}}\big]\big\| &\le C\big\|\tilde{U}^{n+\frac{1}{2}}-\tilde{u}^{n+\frac{1}{2}}\big\| = C\left\|\frac{3}{2}e^n-\frac{1}{2}e^{n-1}\right\|,\\ \big\|H\big[\tilde{u}^{n+\frac{1}{2}}\big]-H\big[u^{n+\frac{1}{2}}\big]\big\| &\le C\big\|\tilde{u}^{n+\frac{1}{2}}-u^{n+\frac{1}{2}}\big\| = C\Big\|\int_{t_n}^{t_{n+1}} u_{tt}(x,s)(t_{n+1}-s)ds\Big\|\\ &\lesssim \tau^2\big\|u_{tt}(\cdot,\xi^n)\big\|, \end{aligned}$$

and

$$\begin{aligned} &\big\|H\big[u^{n+\frac{1}{2}}\big]u^{n+\frac{1}{2}}-H\big[u^{n-\frac{1}{2}}\big]u^{n-\frac{1}{2}}\big\|\\ &\le \big\|H\big[u^{n+\frac{1}{2}}\big]u^{n+\frac{1}{2}}-H\big[u^{n+\frac{1}{2}}\big]u^{n-\frac{1}{2}}\big\|+\big\|H\big[u^{n+\frac{1}{2}}\big]u^{n-\frac{1}{2}}-H\big[u^{n-\frac{1}{2}}\big]u^{n-\frac{1}{2}}\big\|\\ &\le cK_1K^3\big\|u^{n+\frac{1}{2}}-u^{n-\frac{1}{2}}\big\| \lesssim \tau\big\|u_t(\cdot,\xi^n)\big\| \text{ with } \xi^n\in\big(t_{n-1/2},t_{n+1/2}\big). \end{aligned}$$

The proof is complete. □

We are now in position to prove our main result.

Theorem 4 *Given $s\ge 2$ when $d=1$ and $s>\frac{d}{2}+1$ when $d=2,3$. We assume that the solution to (1.1) satisfies (3.8). Then, for any $T<T_{max}$, there exists a constant C independent of τ and n, such that, for τ sufficiently small, we have*

$$\|U^n-u(\cdot,t_n)\|_{H^s}+|r^n-r(t_n)| \le C\tau^2, \quad \forall n=0,1,\dots,M=T/\tau.$$

Proof First, we subtract the PDE from the scheme to obtain the error equations:

$$i\frac{e^1}{\tau} = -\frac{\alpha}{2}\Delta e^1-2\beta D^1+T^1, \tag{3.13}$$

$$i\left(\frac{e^{n+1}-e^n}{\tau}\right) = -\alpha\Delta\frac{e^{n+1}+e^n}{2} - 2\beta D^{n+1} + T^{n+1}, \quad n \geq 1, \tag{3.14}$$

where

$$D^1 = \Big[f(|u^1|^2)u^1 - f(|u_0|^2)u_0\Big] + \frac{r(t_1)}{\sqrt{E[u_0]}+\sqrt{E[u^1]}} f\big(|u_0|^2\big)u_0 \times\left[\frac{1}{\sqrt{E[u^1]}} - \frac{1}{\sqrt{E[u_0]}}\right] + \varepsilon^1\frac{f(|u_0|^2)u_0}{\sqrt{E[u_0]}}, \tag{3.15}$$

with

$$\varepsilon^1 = \int_\Omega H[u_0]Re\Big[\Big(u_0\overline{\Big(\int_0^\tau u_{tt}(x,s)(\tau-s)ds\Big)}\Big]dx + \int_\Omega Re\Big[H[u_0]u_0\overline{e^1}\Big]dx + \tau\int_0^\tau r_t(s)ds + \tau\int_\Omega Re\left[\big(H[u_0]u_0 - H[u^1]u^1\big)\,\overline{u_t}\right]dx, \tag{3.16}$$

and

$$\begin{aligned} D^{n+1} &= \frac{\varepsilon^n+\varepsilon^{n+1}}{2\sqrt{E\big[\tilde{U}^{n+\frac12}\big]}} f\big(|u^{n+\frac12}|\big)u^{n+\frac12} \\ &\quad - \frac{\Big(r(t_n)+r(t_{n+1})\Big)f\big(|u^{n+\frac12}|\big)u^{n+\frac12}}{2\sqrt{E\big[u^{n+\frac12}\big]}\sqrt{E\big[\tilde{U}^{n+\frac12}\big]}\Big(\sqrt{E\big[u^{n+\frac12}\big]}+\sqrt{E\big[\tilde{U}^{n+\frac12}\big]}\Big)}\Big(E\big[u^{n+\frac12}\big] - E\big[\tilde{U}^{n+\frac12}\big]\Big) \\ &\quad + \frac{r^n+r^{n+1}}{2\sqrt{E\big[\tilde{U}^{n+\frac12}\big]}}\Big[\Big(f\big(|u^{n+\frac12}|\big)u^{n+\frac12} - f\big(|\tilde{u}^{n+\frac12}|\big)\tilde{u}^{n+\frac12}\Big) \\ &\quad + \Big(f\big(|\tilde{u}^{n+\frac12}|\big)\tilde{u}^{n+\frac12} - f\big(|\tilde{U}^{n+\frac12}|\big)\tilde{U}^{n+\frac12}\Big)\Big] \\ &:= D_1 + D_2 + D_3, \end{aligned} \tag{3.17}$$

$$\begin{aligned} T^{n+1} &= \frac{i}{\tau}\int_{t_n}^{t_{n+1}} u_{ttt}(x,s)(t_{n+1}-s)^2ds + \int_{t_n}^{t_{n+1}} \Delta u_{tt}(x,s)(t_{n+1}-s)ds \\ &\quad + \Big(\int_{t_n}^{t_{n+1}} r_{tt}(s)(t_{n+1}-s)ds\Big) f\big(|u^{n+\frac12}|^2\big)u^{n+\frac12}, \quad n \geq 0, \end{aligned} \tag{3.18}$$

with

$$\begin{aligned} \varepsilon^{n+1} - \varepsilon^n &= \int_\Omega H\big[u^{n+\frac12}\big]Re\big[u^{n+\frac12}\,\overline{\big(e^{n+1}-e^n-\tau T_1^u\big)}\big]dx \\ &\quad + \int_\Omega H\big[u^{n+\frac12}\big]Re\big[\big(\tilde{e}^{n+\frac12}+T_3^u\big)\overline{\big(U^{n+1}-U^n\big)}\big]dx \\ &\quad + \int_\Omega \big(H\big[\tilde{U}^{n+\frac12}\big] - H\big[u^{n+\frac12}\big]\big)Re\big[\tilde{U}^{n+\frac12}\,\overline{\big(U^{n+1}-U^n\big)}\big]dx + \tau T_1^r, \end{aligned} \tag{3.19}$$

where for any function f,

$$\begin{aligned} T_1^f &= f_t\big(t_{n+\frac12}\big) - \frac{f(t_{n+1})-f(t_n)}{\tau} = \frac{1}{\tau}\int_{t_n}^{t_{n+1}} f_{ttt}(s)(t_{n+1}-s)^2ds, \\ T_3^f &= f\big(t_{n+\frac12}\big) - \Big(\frac32 f(t_n) - \frac12 f(t_{n-1})\Big) = \int_{t_{n-1}}^{t_n} f_{tt}(s)(t_n-s)ds. \end{aligned}$$

We can also rewrite the error Eqs. (3.13)–(3.14) as

$$\begin{aligned} e^1 &= i\tau B\big(-2\beta D^1 + T^1\big), \\ e^{n+1} &= Ae^n + i\tau B\big(-2\beta D^{n+1} + T^{n+1}\big), \end{aligned} \tag{3.20}$$

so that for $n = 0, \ldots, M-1$,

$$e^{n+1} = i\tau\Big(A^n B\big(-2\beta D^1 + T^1\big) + \sum_{k=2}^{n+1} A^{n+1-k} B\big(-2\beta D^k + T^k\big)\Big). \tag{3.21}$$

Now let $T^* \le T$ be defined in Theorem 3 and set $M^* = T^*/\tau$. Since $s \ge 2$, Theorem 3 implies there exists $K_1 > 0$, s.t.

$$\Big\|\frac{U^{n+1} - U^n}{\tau}\Big\| \le \|U^{n+1} + U^n\|_{H^2} + \big\|f\big(|\tilde{U}^{n+\frac{1}{2}}|\big)\tilde{U}^{n+\frac{1}{2}}\big\| \le K_1, \quad \forall n = 0, 1, \ldots, M^* - 1.$$

By using the Holder's inequality, Lemmas 3 and 4 and Sobolev embedding that $H^3(\mathbb{R}) \hookrightarrow W^{2,\infty}(\mathbb{R})$, we find from (3.16) that

$$\begin{aligned} |\varepsilon^1| \le\ & \|H[u_0]u_0\|\Big(\Big\|\int_0^\tau u_{tt}(x,s)(\tau - s)ds\Big\| + \|e^1\|\Big) + \tau^2\|r_t\|_{L^\infty(0,T)} \\ & + \tau\|H[u_0]u_0 - H[u^1]u^1\| \cdot \|u_t\| \\ \le\ & \|H[u_0]u_0\|\Big(\tau^2\|u_{tt}\|_{L^\infty(0,\tau;L^2)} + \|e^1\|\Big) + \tau^2\|r_t\|_{L^\infty(0,\tau)} \\ & + \tau^2\|u_t\|^2_{L^\infty(0,\tau,L^2)} \le C(\tau^2 + \|e^1\|). \end{aligned}$$

We rewrite (3.19) as

$$\begin{aligned} \varepsilon^{n+1} & - \int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[u^{n+\frac{1}{2}}\overline{e^{n+1}}\big]dx \\ = & \Big(\varepsilon^n - \int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[u^{n+\frac{1}{2}}\overline{e^n}\big]dx\Big) - \tau\int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[u^{n+\frac{1}{2}}\overline{T_1^u}\big]dx \\ & + \int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[\tilde{e}^{n+\frac{1}{2}}\big(\overline{U^{n+1} - U^n}\big)\big]dx + \int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[T_3^u\big(\overline{U^{n+1} - U^n}\big)\big]dx \\ & + \int_\Omega \big(H\big[\tilde{U}^{n+\frac{1}{2}}\big] - H\big[u^{n+\frac{1}{2}}\big]\big)Re\big[\tilde{U}^{n+\frac{1}{2}}\big(\overline{U^{n+1} - U^n}\big)\big]dx + \tau T_1^r. \end{aligned}$$

Denote

$$G^n := \varepsilon^n - \int_\Omega H\big[u^{n-\frac{1}{2}}\big]Re\big[u^{n-\frac{1}{2}}\overline{e^n}\big]dx, \quad n = 1, \ldots, M^*,$$

Then, we have

$$\varepsilon^n - \int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[u^{n+\frac{1}{2}}\overline{e^n}\big]dx = G^n + \int_\Omega Re\Big[\Big(H\big[u^{n+\frac{1}{2}}\big]u^{n+\frac{1}{2}} - H\big[u^{n-\frac{1}{2}}\big]u^{n-\frac{1}{2}}\Big)\overline{e^n}\Big]dx,$$

and

$$\begin{aligned} G^{n+1} = &\ G^n + \int_\Omega Re\Big[\Big(H\big[u^{n+\frac{1}{2}}\big]u^{n+\frac{1}{2}} - H\big[u^{n-\frac{1}{2}}\big]u^{n-\frac{1}{2}}\Big)\overline{e^n}\Big]dx \\ & + \int_\Omega H\big[u^{n+\frac{1}{2}}\big]Re\big[\tilde{e}^{n+\frac{1}{2}}\big(\overline{U^{n+1} - U^n}\big)\big]dx \end{aligned}$$

$$
\begin{aligned}
&+\int_{\Omega}\left(H\left[\tilde{U}^{n+\frac{1}{2}}\right]-H\left[u^{n+\frac{1}{2}}\right]\right)Re\left[\tilde{U}^{n+\frac{1}{2}}\left(\overline{U^{n+1}-U^{n}}\right)\right]dx\\
&+\tau\left(T_1^r-\int_{\Omega}H\left[u^{n+\frac{1}{2}}\right]Re\left[u^{n+\frac{1}{2}}\overline{T_1^u}\right]dx\right)+\int_{\Omega}H\left[u^{n+\frac{1}{2}}\right]Re\left[T_3^u\left(\overline{U^{n+1}-U^{n}}\right)\right]dx\\
:=\ &G^n+G_1+G_2+G_3+G_4+G_5.
\end{aligned}
$$

The terms G_j can be bounded as follows:

$$
\begin{aligned}
|G_1| &\leq \tau C\|u_t\|\cdot\|e^n\|\leq C\tau\|e^n\|,\\
|G_2| &\leq C\|u^{n+\frac{1}{2}}\|_{L^\infty}^3\left(\frac{3}{2}\|e^n\|+\frac{1}{2}\|e^{n-1}\|\right)\left(\|U^{n+1}-U^n\|\right)\leq C\tau\left(\frac{3}{2}\|e^n\|+\frac{1}{2}\|e^{n-1}\|\right),\\
|G_3| &\leq \left(\frac{3}{2}\|U^n\|_{L^\infty}+\frac{1}{2}\|U^{n-1}\|_{L^\infty}\right)\left(\|U^{n+1}-U^n\|\right)\left(\left\|H\left[\tilde{U}^{n+\frac{1}{2}}\right]\right.\right.\\
&\quad\left.\left.-H\left[\tilde{u}^{n+\frac{1}{2}}\right]\right\|+\left\|H\left[\tilde{u}^{n+\frac{1}{2}}\right]-H\left[u^{n+\frac{1}{2}}\right]\right\|\right)\\
&\leq C\tau\left(\frac{3}{2}\|e^n\|+\frac{1}{2}\|e^{n-1}\|\right)+C\tau^2\int_{t_n}^{t_{n+1}}\|u_{tt}\|ds,\\
|G_4| &\leq \tau^2\int_{t_n}^{t_{n+1}}\left(|r_{ttt}|+\|u_{ttt}\|\right)ds,\\
|G_5| &\leq C\|U^{n+1}-U^n\|\|T_3^u\|=C\tau^2\int_{t_n}^{t_{n+1}}\|u_{tt}\|ds.
\end{aligned}
$$

Therefore,

$$
|G^{n+1}|\leq|G^n|+C\tau(\|e^n\|+\|e^{n-1}\|)+C\tau^2\int_{t_n}^{t_{n+1}}|r_{ttt}|+\|u_{tt}\|+\|u_{ttt}\|ds.
$$

Clearly $|G^1|\lesssim\tau^2$. Then, for any $n\leq M$,

$$
\begin{aligned}
|G^n| &\leq |G^1|+C\tau\sum_{k=1}^{n-1}\left(\|e^k\|+\tau^2\int_{t_{k-1}}^{t_k}|r_{ttt}|+\|u_{tt}\|+\|u_{ttt}\|ds\right)\\
&\leq C\left(\tau^2+\tau\sum_{k=1}^{n-1}\|e^k\|+\tau^2\int_0^{t_n}|r_{ttt}|+\|u_{tt}\|+\|u_{ttt}\|ds\right). \qquad (3.22)
\end{aligned}
$$

Therefore, by the Holder's inequality, there is a uniform constant C_r, s.t.

$$
|\varepsilon^n|\leq|G^n|+\left|\int_{\Omega}H\left[u^{n-\frac{1}{2}}\right]Re\left[u^{n-\frac{1}{2}}\overline{e^n}\right]dx\right|\leq C_r\left(\tau^2+\|e^n\|+\tau\sum_{k=1}^{n-1}\|e^k\|\right),\quad\forall n\leq M^*. \qquad (3.23)
$$

Then, we evaluate L^2 norm on both sides of (3.21) and use Lemma 1, we have:

$$
\begin{aligned}
\|e^{n+1}\| &\leq 2|\beta|\tau\|A^nBD^1\|+2|\beta|\tau\|T^1\|+\tau\sum_{k=2}^{n+1}\left(2|\beta|\|A^{n+1-k}BD^k\|+\|A^{n+1-k}BT^k\|\right)\\
&\leq 2|\beta|\left(\tau\|D^1\|+\tau\sum_{k=2}^{n+1}\|D^k\|\right)+\left(\tau\|T^1\|+\tau\sum_{k=2}^{n+1}\|T^k\|\right). \qquad (3.24)
\end{aligned}
$$

It is easy to see that $\|D^1\|, \|T^1\| \lesssim \tau$. For all $k \geq 2$, there is a uniform constant $C \geq \frac{C_r \| f(|u^{k-\frac{1}{2}}|)u^{k-\frac{1}{2}}\|}{2\sqrt{C_0}} > 0$, such that the following expressions can be derived from (3.17) and (3.18):

$$\begin{aligned}
\|D^k\| &\leq \|D_1\| + \|D_2\| + \|D_3\| \\
&\leq \frac{C_r \left\| f\left(|u^{k-\frac{1}{2}}|\right)u^{k-\frac{1}{2}}\right\|}{2\sqrt{C_0}} \left(2\tau^2 + \|e^k\| + \|e^{k-1}\| + 2\tau \sum_{i=1}^{k-1} \|e^i\|\right) \\
&\quad + \frac{\left(\max_{t\in[0,T]} r(t)\right)\left\| f\left(|u^{k-\frac{1}{2}}|\right)u^{k-\frac{1}{2}}\right\|}{\sqrt{C_0}} \left\| u^{k-\frac{1}{2}} \right. \\
&\quad + \tilde{U}^{k-\frac{1}{2}}\|_{L^6}^3 \left(\frac{3}{2}\|e^{k-1}\| + \frac{1}{2}\|e^{k-2}\| + \left\| \int_{t_{k-1}}^{t_k} u_{tt}(\cdot, s)(t_k - s)ds \right\|\right) \\
&\quad + \frac{r^{k-1} + r^k}{2\sqrt{E[\tilde{U}^{k-\frac{1}{2}}]}} \Big[3\Big(\left\| f\left(|u^{k-\frac{1}{2}}|^2\right)\right\|_{L^\infty} \\
&\quad + \left\| f\left(|\tilde{U}^{k-\frac{1}{2}}|^2\right)\right\|_{L^\infty}\Big)\left(\frac{3}{2}\|e^{k-1}\| + \frac{1}{2}\|e^{k-2}\|\right) + \left\| \int_{t_{k-1}}^{t_k} u_{tt}(\cdot, s)(t_k - s)ds \right\| \Big] \\
&\leq \frac{C_r \left\| f\left(|u^{k-\frac{1}{2}}|\right)u^{k-\frac{1}{2}}\right\|}{2\sqrt{C_0}} \|e^k\| + C\left(\|e^{k-1}\| + \|e^{k-2}\| + \tau \sum_{i=1}^{k-1} \|e^i\| + \tau \int_{t_{k-1}}^{t_k} \|u_{tt}\| ds\right),
\end{aligned} \tag{3.25}$$

$$\|T^k\| \leq \tau\left(\int_{t_{k-1}}^{t_k} \|u_{ttt}\| + \|u_{tt}\|_{H^2} + |r_{tt}| + |r_{ttt}| ds\right). \tag{3.26}$$

Then, from (3.24), we have:

$$\begin{aligned}
&\left(1 - \tau \frac{|\beta| C_r \left\| f\left(|u^{n+\frac{1}{2}}|\right)u^{n+\frac{1}{2}}\right\|}{\sqrt{C_0}}\right)\|e^{n+1}\| \leq \tau \sum_{k=1}^{n} C\left(2 + (n+1-k)\tau\right)\|e^k\| \\
&\quad + \left(\tau\left(\|D^1\| + \|T^1\|\right) + \tau^2 \int_0^T \|u_{ttt}\| + \|u_{tt}\|_{H^2} + |r_{tt}| + |r_{ttt}| ds\right) \\
&\leq \tau \sum_{k=1}^{n} (2C + CT)\|e^k\| + C\tau^2\left(1 + \int_0^T \|u_{ttt}\| + \|u_{tt}\|_{H^2} + |r_{tt}| + |r_{ttt}| ds\right)
\end{aligned}$$

Let τ and C_0 be appropriate numbers, s.t $\tau \frac{|\beta| C_r \| f(|u^{n+\frac{1}{2}}|)u^{n+\frac{1}{2}}\|}{\sqrt{C_0}} \leq \frac{1}{2}$. Then, by applying Lemma 2, we arrive at

$$\|e^{n+1}\| \leq \tau^2 2Ce^{4CT+CT^2} \left(1 + \int_0^T \|u_{ttt}\| + \|u_{tt}\|_{H^2} + |r_{tt}| + |r_{ttt}| ds\right), \quad \forall n \leq M^* - 1.$$

We also derive from (3.23) that:

$$|\varepsilon^n| \leq C_r \left(\tau^2 + \|e^n\| + \tau \sum_{k=1}^{n-1} \|e^k\|\right) \lesssim \tau^2, \quad \forall n \leq M^*.$$

Next we shall use a similar procedure to derive the error estimates in H^s-norm. To this end, we evaluate the H^s norm on both sides of (3.21) and apply Lemma 1 again to obtain

$$\|e^{n+1}\|_{H^s} \le 2|\beta| \left(\tau \|D^1\|_{H^s} + \tau \sum_{k=2}^{n+1} \|D^k\|_{H^s} \right) + \left(\tau \|T^1\|_{H^s} + \tau \sum_{k=2}^{n+1} \|T^k\|_{H^s} \right), \quad \forall n \le M^* - 1.$$

For $s > d/2 + 1$, both $H^s(\mathbb{R}^d)$ and $H^{s-1}(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)$ by the Sobolev embedding theorem. Hence, there exists a constant c depending on l and s only, s.t.

$$\left\| f\big(|g_1|^2\big) g_1 - f\big(|g_2|^2\big) g_2 \right\|_{H^s} \le c\big(\|g_1\|_{H^s}^{p_0-1} + \|g_2\|_{H^s}^{p_0-1}\big)\|g_1 - g_2\|_{H^s}, \quad \forall g_1, g_2 \in H^s.$$

Then we can repeat the process of the error estimates in L^2 above to obtain the H^s estimates. More precisely, we can derive

$$\begin{aligned}
\|D^k\|_{H^s} \le\ & \frac{\left\| f\big(|u^{k-\frac{1}{2}}|\big) u^{k-\frac{1}{2}} \right\|_{H^s}}{2\sqrt{C_0}} \frac{|\varepsilon^n| + |\varepsilon^{n+1}|}{2} \\
& + \frac{\max\{r(t)\} \cdot \left\| u^{k-\frac{1}{2}} + \tilde{U}^{k-\frac{1}{2}} \right\|_{L^6}^3 \cdot \left\| f\big(|u^{k-\frac{1}{2}}|\big) u^{k-\frac{1}{2}} \right\|_{H^s}}{\sqrt{C_0}} \\
& \left(\frac{3}{2} \|e^{k-1}\| + \frac{1}{2} \|e^{k-2}\| + \left\| \int_{t_{k-1}}^{t_k} u_{tt}(\cdot, s)(t_k - s) ds \right\| \right) \\
& + \frac{r^{k-1} + r^k}{2\sqrt{E\big[\tilde{U}^{k-\frac{1}{2}}\big]}} \left[c\Big(\left\| u^{k-\frac{1}{2}} \right\|_{H^s}^{p_0-1} + \left\| \tilde{U}^{k-\frac{1}{2}} \right\|_{H^s}^{p_0-1} \Big) \Big(\frac{3}{2} \|e^{k-1}\|_{H^s} \right. \\
& \left. + \frac{1}{2} \|e^{k-2}\|_{H^s} \Big) + \left\| \int_{t_{k-1}}^{t_k} u_{tt}(\cdot, s)(t_k - s) ds \right\|_{H^s} \right] \\
\le\ & C \Big(\tau^2 + \|e^{k-1}\|_{H^s} + \|e^{k-2}\|_{H^s} + \tau \int_{t_{k-1}}^{t_k} \|u_{tt}\|_{H^s} ds \Big), \\
\|T^k\|_{H^s} \le\ & \tau \Big(\int_{t_{k-1}}^{t_k} \|u_{ttt}\|_{H^s} + \|u_{tt}\|_{H^{s+2}} + |r_{tt}| + |r_{ttt}| ds \Big),
\end{aligned}$$

which leads to

$$\begin{aligned}
\|e^{n+1}\|_{H^s} \le\ & 2C\tau \sum_{k=0}^{n} \|e^k\|_{H^s} \\
& + C\tau^2 \Big(1 + \int_0^T \|u_{ttt}\|_{H^s} + \|u_{tt}\|_{H^{s+2}} + |r_{tt}| + |r_{ttt}| ds \Big), \quad \forall n \le M^* - 1.
\end{aligned}$$

Applying the discrete Gronwall's inequality again, we derive

$$\|e^{n+1}\|_{H^s} \le \tau^2 C e^{2CT} \Big(1 + \int_0^T \|u_{ttt}\|_{H^s} + \|u_{tt}\|_{H^{s+2}} + |r_{tt}| + |r_{ttt}| ds \Big), \quad \forall n \le M^* - 1. \tag{3.27}$$

where C is independent to τ.

With the above error estimate, we now show that T^* in Theorem 3 can be extended to T. Indeed, we set the initial condition to be $U^{T^*/\tau}$ and repeat the process in Theorem 3 and the above arguments. The proof is complete if we can repeat enough times to reach time T.

Otherwise, there exists $T_c < T < T_{\max}$, such that

$$\sum_{k=1}^{\infty} T_k^* \le T_c.$$

where T_k^* is the time range for the k-th time of applying the above process. Since the solution $u(x,t)$ to (1.1) is well defined on $[0, T_c]$, so we define:

$$M_c = \sup_{t\in[0,T_c]} \{\|u(\cdot,t)\|_{H^s}\} + 1.$$

Then, for a sufficiently small τ, we have: for any $k = 0, 1 \ldots$,

$$\|U^{T_k^*/\tau}\|_{H^s} \le M_c.$$

Then according to the calculations in Theorem 3, when $\beta < 0$, by (3.6),

$$T_k^* = \left(4C_2K\|U^{T_{k-1}^*/\tau}\|_{H^s}^{p_0-1}\right)^{-1} \ge \left(4C_2KM_c^{p_0-1}\right)^{-1} := T_{\min}^*,$$

and when $\beta > 0$, by (3.7),

$$\begin{aligned} T_k^* &= \left(8C_3K\left(\left\|U\left(T_{k-1}^*\right)\right\|_{H^s} + \sqrt{D_0}\right)\left\|U\left(T_{k-1}^*\right)\right\|_{H^s}^{p_0-1}\right)^{-1} \\ &\ge \left(8C_3K\left(M_c + \sqrt{D_0}\right)M_c^{p_0-1}\right)^{-1} := T_{\min}^*, \end{aligned}$$

for any $k = 1, 2, \ldots$. But this will lead to the contradiction that

$$\infty = \sum_{k=1}^{\infty} T_{\min}^* \le \sum_{k=1}^{\infty} T_k^* \le T_c.$$

The proof is complete. □

4 A Fully-Discrete Scheme and Numerical Results

Since the problem (1.1) is set in the whole space $\mathbb{R}^d$, we shall use the Hermite spectral method [24] to discretize the whole space directly to avoid additional errors by domain truncation.

4.1 Fully Discretized Hermite-SAV Scheme

We first recall some basic properties of Hermite spectral method.

Let $H_n(x)$ be the n-th degree Hermite polynomial and $\hat{H}_n(x) := \frac{1}{d_n}H_n(x)e^{-\frac{x^2}{2}}$ be the corresponding normalized Hermite function with $d_n = (\pi^{1/4}\sqrt{2^n n!})$. We define the one-dimensional approximation space

$$X_N = \text{span}\{\hat{H}_0, \ldots, \hat{H}_N\}.$$

Let $\{x_j\}_{j=0,N}$ be the Gauss–Hermite collocation points, i.e., zeros of $H_{N+1}(x)$, we define the 1-D discrete inner product by

$$(f, g)_N = \sum_{j=0}^{N} f(x_j)\bar{g}(x_j)\omega_j, \quad \forall f, g \in C(\mathbb{R}), \tag{4.1}$$

where $\{\omega_j\}_{j=0,N}$ are the corresponding weights of the Gauss–Hermite quadrature [24]. The multi-dimensional discrete inner product $(\cdot,\cdot)_N$ is defined through the tensor-product of the 1-D formula. Note that we have in particular [24]

$$(f,g)_N = (f,g), \quad \forall f,g \in X_N^d. \tag{4.2}$$

We construct the fully discrete Hermite-SAV scheme as follows:

Let $U_N^0 = \hat{\Pi}_N u_0$ and $r_N^0 = r(0)$. We first compute $U_N^1 \in X_N^d$ and $r_N^1 \in \mathbb{R}$ such that $\forall v_N \in X_N^d$

$$i\left(\frac{U_N^1 - \hat{\Pi}_N u_0}{\tau}, v_N\right) + \frac{\alpha}{2}\big(\Delta\big(U_N^1 + U_N^0\big), v_N\big) = -\beta\big(r_N^1 + r_N^0\big)\big(H\big[\hat{\Pi}_N u_0\big]\hat{\Pi}_N u_0, v_N\big)_N, \tag{4.3}$$

$$r_N^1 - r_N^0 = \mathrm{Re}\big\{\big(H\big[\hat{\Pi}_N u_0\big]\hat{\Pi}_N u_0, U_N^1 - \hat{\Pi}_N u_0\big)_N\big\}. \tag{4.4}$$

Then for $n \ge 1$, we look for $U_N^{n+1} \in X_N^d$ and $r_N^{n+1} \in \mathbb{R}$, such that $\forall v_N \in X_N^d$

$$i\left(\frac{U_N^{n+1} - U_N^n}{\tau}, v_N\right) + \frac{\alpha}{2}\big(\Delta(U_N^{n+1} + U_N^n), v_N\big) = -\beta\big(r_N^{n+1} + r_N^n\big)\big(H\big[\tilde{U}_N^{n+\frac{1}{2}}\big]\tilde{U}_N^{n+\frac{1}{2}}, v_N\big)_N, \tag{4.5}$$

$$r_N^{n+1} - r_N^n = \mathrm{Re}\big\{\big(H\big[\tilde{U}_N^{n+\frac{1}{2}}\big]\tilde{U}_N^{n+\frac{1}{2}}, U_N^{n+1} - U_N^n\big)_N\big\}, \tag{4.6}$$

where $\tilde{U}_N^{n+\frac{1}{2}} := \frac{3}{2}U_N^n - \frac{1}{2}U_N^{n-1}$. Note that the above spatial discretization is a Galerkin discretization with numerical quadrature.

The above fully discrete scheme can be efficiently implemented as in the semi-discrete case. Indeed, writing

$$U_N^{n+1} = \phi_N^{n+1} + r_N^{n+1}\varphi_N^{n+1}, \tag{4.7}$$

in (4.5), we find that ϕ_N^{n+1} and φ_N^{n+1} satisfy

$$\left(\frac{i}{\tau}\phi_N^{n+1} + \frac{\alpha}{2}\Delta\phi_N^{n+1}, v_N\right) = \big(Q_N^n, v_N\big)_N, \quad \forall v_N \in X_N^d, \tag{4.8}$$

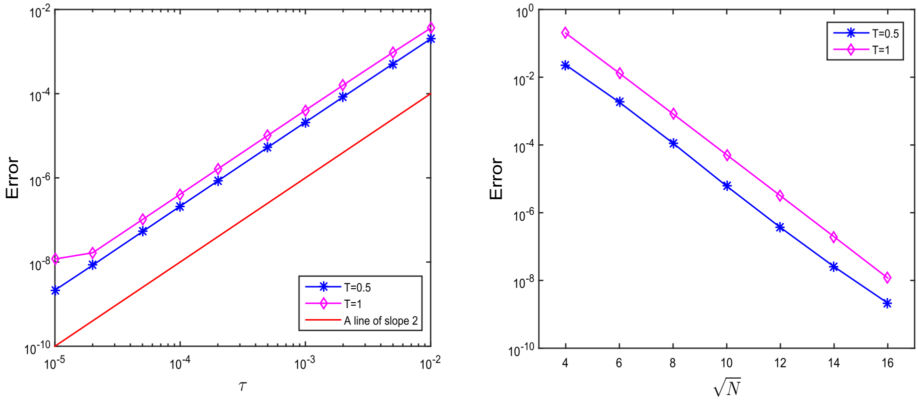
$$\left(\frac{i}{\tau}\varphi_N^{n+1} + \frac{\alpha}{2}\Delta\varphi_N^{n+1}, v_N\right) = -\beta\big(H\big[\tilde{U}_N^{n+\frac{1}{2}}\big]\tilde{U}_N^{n+\frac{1}{2}}, v_N\big)_N, \quad \forall v_N \in X_N^d, \tag{4.9}$$

with

$$Q_N^n = \frac{i}{\tau}U_N^n - \frac{\alpha}{2}\Delta U_N^n - \beta r^n H\big[\tilde{U}_N^{n+\frac{1}{2}}\big]\tilde{U}_N^{n+\frac{1}{2}}.$$

Once ϕ_N^{n+1} and φ_N^{n+1} are known, we can determine r_N^{n+1} explicitly by plugging (4.7) in (4.6). Hence, the main computational cost is to solve (4.8) and (4.9) which can be very efficiently solved using the algorithm presented in [24]. More precisely, in the 1-D case, (4.8) and (4.9) lead to tridiagonal systems, and in the multi-dimensional cases, they lead to sparse linear systems that can be efficiently solved by using the matrix diagonalization technique [24].

By following exactly the same procedure as in the proof of Theorem 2, we can establish the following result:



(a) convergence in time. **(b)** convergence in space.

Fig. 1 Example 4.1: maximum errors of Hermite SAV/CN method

Theorem 5 *The fully discretized SAV scheme (4.3)–(4.6) preserves a modified Hamiltonian unconditionally in the sense that*

$$\frac{\alpha}{2}\left\|\nabla U_N^{n+1}\right\|^2-\beta\left(r_N^{n+1}\right)^2=\frac{\alpha}{2}\left\|\nabla U_N^{n}\right\|^2-\beta\left(r_N^{n}\right)^2,\quad n=0,1,\ldots,M-1.$$

Remark 2 In principle, the error analysis for the above fully discretized scheme can be carried out by combining the analysis in the last section with the approximation properties of the Hermite functions as in [16]. However, this process can be very tedious particularly due to the pseudo-spectral treatment of the nonlinear terms. We leave it for the interested reader.

4.2 Numerical Results

Example 4.1 We consider the one-dimensional nonlinear Schrödinger equation

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial x^2}+2|u|^2u=0, \tag{4.10}$$

with an analytical solution given by [27]

$$u(x,t)=\operatorname{sech}(x-4t)e^{i(2x-3t)}.$$

We first investigate the convergence rate. Fix $N=256$ so that the spatial discretization error is negligible compared with time discretization error. Figure 1a shows clearly that the method has a second convergence rate in time. Next, we take $\tau=0.00001$ so that the time discretization error is negligible compared with the spatial discretization error up to around 10^{-8}. Figure 1b shows clearly that spatial error behaves like $e^{-c\sqrt{N}}$. This exponential convergence is a typical behavior of the Hermite spectral method.

Next, we make a comparison with the results computed by the time-splitting Chebyshev-tau spectral (TSCT) method proposed in [27], where the computational domain is truncated as $[-16, 16]$. To this end, we let $\tau=0.00001$. The maximum errors are listed in Table 1. As we can see from the table, the proposed Hermite-spectral method in the whole space can achieve much higher accuracy than the TSCT method based on domain truncation.

Table 1 Maximum errors at $T = 0.5$ with $\tau = 0.00001$

N	64	128	256
TSCT method [27]	6.9851e−2	1.1099e−4	1.6665e−6
Hermite-SAV scheme (4.3)–(4.6)	1.1268e−4	1.1020e−6	3.9481e-9

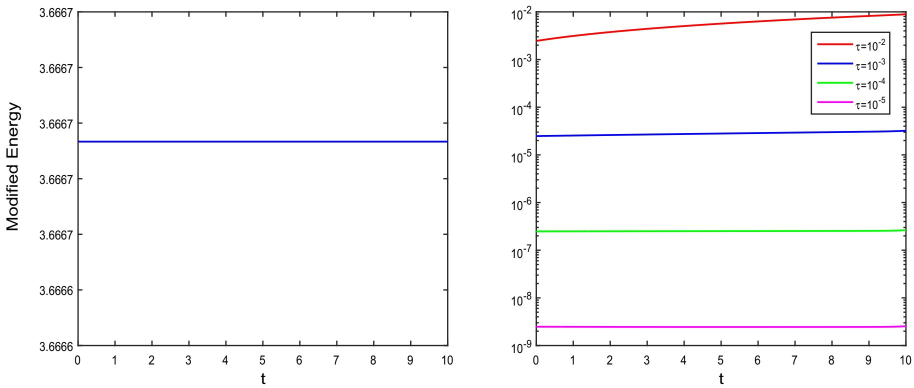


Fig. 2 Example 4.1: Left: Modified energy with $\tau = 0.01$; right: $|E(u_N^n) - \widetilde{E}(u_N^n, r_N^n)|$ with different τ

Next, we examine the conservation of the energy. We plot the discrete modified energy $\widetilde{E}(u^n, r^n)$ computed by the proposed method with $\tau = 0.01$ and $N = 256$ in Fig. 2 (left), and the difference between the original discrete energy $E(u_N^n)$ and the modified energy $\widetilde{E}(u_N^n, r_N^n)$ with different τ in Fig. 2 (right). It is obvious that the proposed scheme indeed conserves modified energy, and the difference between the modified and original discrete energy decays with a second-order rate in time.

Example 4.2 We consider the interaction of two solitons. The initial condition in (4.10) is taken as [15]

$$u_0(x) = \operatorname{sech}(x - 10) \exp(-2i(x - 10)) + \operatorname{sech}(x + 10) \exp(2i(x + 10)).$$

This initial condition represents the interaction of two solitons of equal amplitude 1.

The discretization parameters in the computation are taken as $N = 200$, $\tau = 0.01$. In Fig. 3, we show the interactions of two solitons traveling in opposite directions with velocity 4 at different time. In Fig. 4, we plot the interaction process in space-time. We observe that the two solitons collide, then separate, and return to their original shapes after collision.

Example 4.3 We consider the one-dimensional nonlinear Schrödinger equation (4.10) with the following analytical solution [19]

$$u(x,t) = \left(\frac{9(\sigma+1)}{8}\operatorname{sech}^2\left(\frac{3\sigma}{2}(x - 4t + 5)\right)\right)^{\frac{1}{2\sigma}} \exp\left(2i\left(x - \frac{7}{8}t\right)\right).$$

Figure 5a shows the convergence rate in time with $N = 512$. Figure 5b shows the convergence rate in time with $\tau = 0.00001$. Second order convergence rate in time and exponential convergence in space are observed for $\sigma = 1$ and $\sigma = 2$. Figure 6 (left) shows the conservation property of the discrete modified energy $\widetilde{E}(u^n, r^n)$ using $N = 256$ and $\tau = 0.01$. The

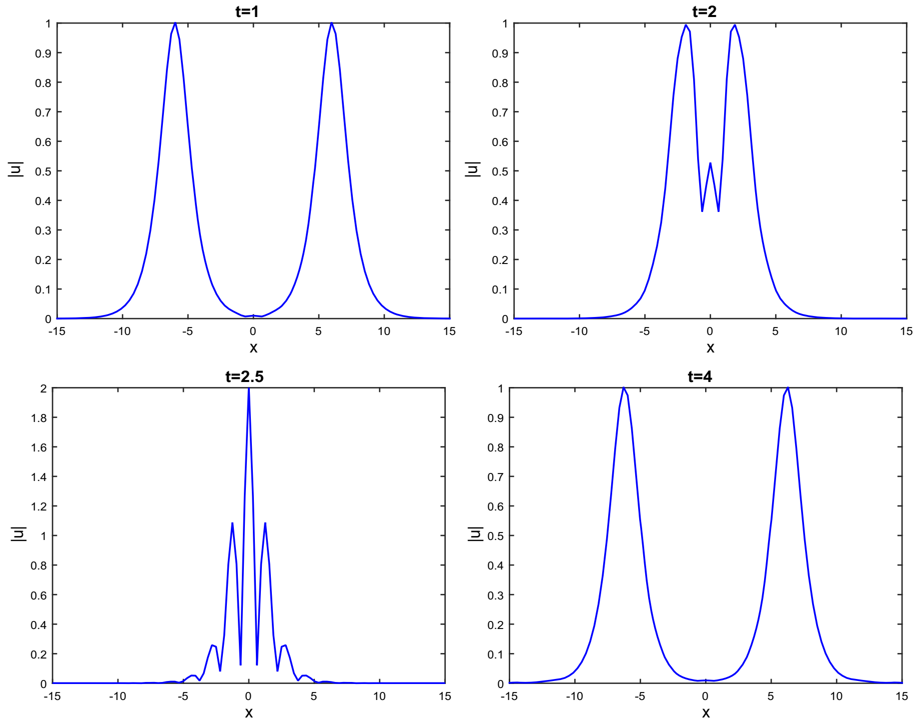
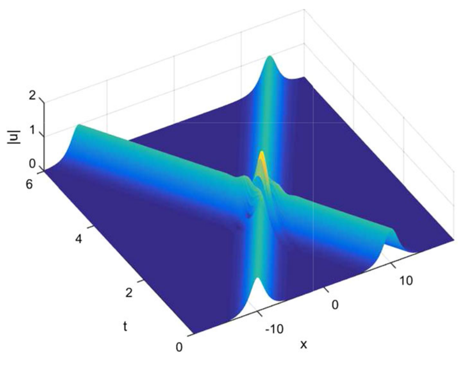


Fig. 3 Example 4.2: The interaction of two solitons of equal amplitude

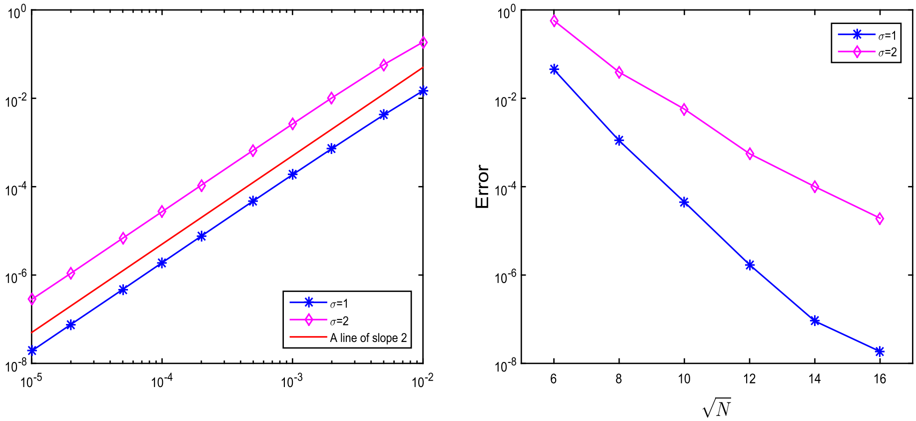
Fig. 4 Example 4.2: Interaction of two solitons



difference between the original discrete energy $E(u_N^n)$ and the modified energy $\widetilde{E}(u_N^n, r_N^n)$ with different τ and $\sigma = 2$ was also showed in Fig. 6 (right). It is obvious that the proposed scheme indeed conserves modified energy, while the convergence rate of the modified energy to the original energy appears to be second-order only.

Example 4.4 In this example, we consider the following Schrödinger equation with saturated nonlinear term

$$i\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2} + 2\beta\frac{|u|^2}{1+|u|^2}u = 0. \tag{4.11}$$



(a) convergence in time. **(b)** convergence in space.

Fig. 5 Example 4.3: Maximum errors of Hermite SAV/CN method with different σ

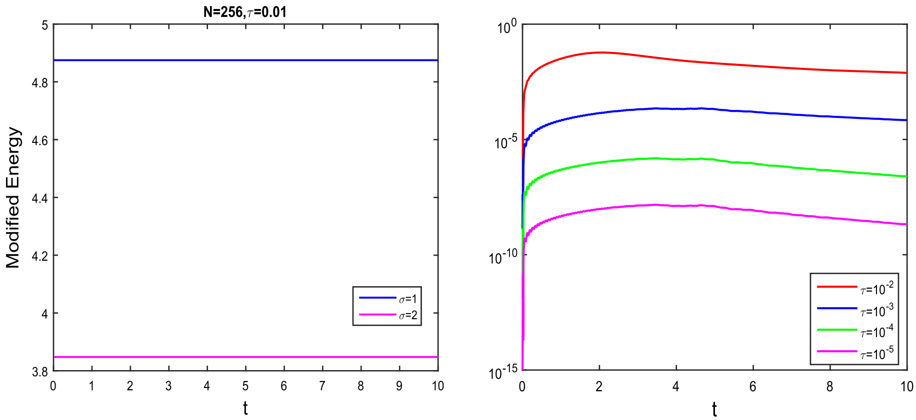


Fig. 6 Example 4.3: Left: Modified energy with $\tau = 0.01$; right: $|E(u_N^n) - \widetilde{E}(u_N^n, r_N^n)|$ with $\sigma = 2$

The initial condition of Eq. (4.11) is taken as the Gaussian-type data

$$u_0(x) = \sqrt{0.1}\exp(-x^2/0.62^2).$$

We fix $\beta = 1$, and take the numerical solution with $N = 256$ and $\tau = 10^{-5}$ as reference solution. We observe from Fig. 7 that the scheme converges with second-order in time.

We also observe from Fig. 8 that the modified energy converges to the original energy with second-order in time.

Example 4.5 We consider the two-dimensional nonlinear Schrödinger equation

$$i\frac{\partial u}{\partial t} + \Delta u + 2|u|^2 u = 0, \tag{4.12}$$

with the initial condition

$$u_0(x) = \text{sech}(x_1)\text{sech}(x_2).$$

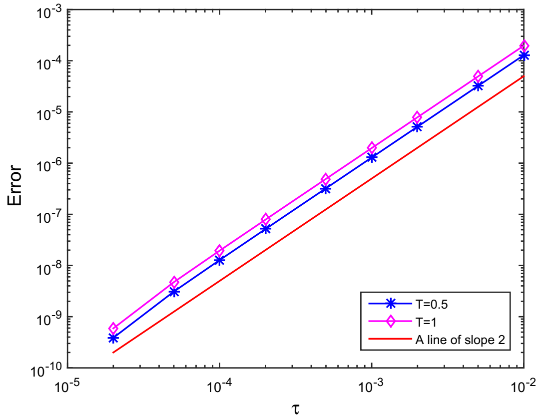


Fig. 7 Example 4.4: Maximum errors of Hermite SAV/CN method

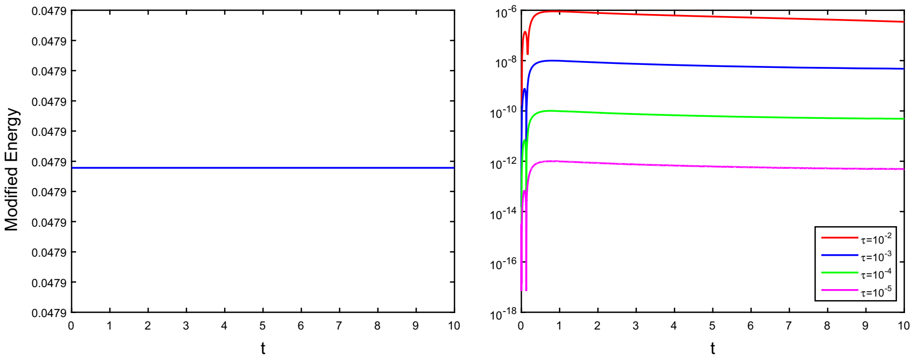


Fig. 8 Example 4.4. Left: Modified energy; Right: $|E(u_N^n) - \widetilde{E}(u_N^n, r_N^n)|$ with different τ

We take the numerical solution obtained with $N = 256$ and $\tau = 10^{-4}$ as reference solution. We observe from Fig. 9 that the scheme convergence rate in time.

Figure 10 (left) shows the modify energy with $\tau = 0.01$. As expected, it is conserved exactly. Figure 10 (right) shows the difference between the modified energy and original energy, and it converges with second-order in time.

5 Concluding Remarks

We considered semi-discrete and fully discrete second-order SAV schemes for the nonlinear Schrödinger equation in the whole space with typical and generalized nonlinearities, and derived rigorous optimal error estimates for the semi-discrete in time scheme. To the best of our knowledge, this is the first rigorous error analysis for a SAV scheme applied to Hamiltonian PDEs.

As with other SAV type schemes, the scheme we consider in this paper unconditionally conserves a modified energy, and only requires solving linear systems with constant coefficients at each time step. Hence, it is very efficient and easy to implement. We also presented numerical experiments which validated the theoretical results and demonstrated the effec-

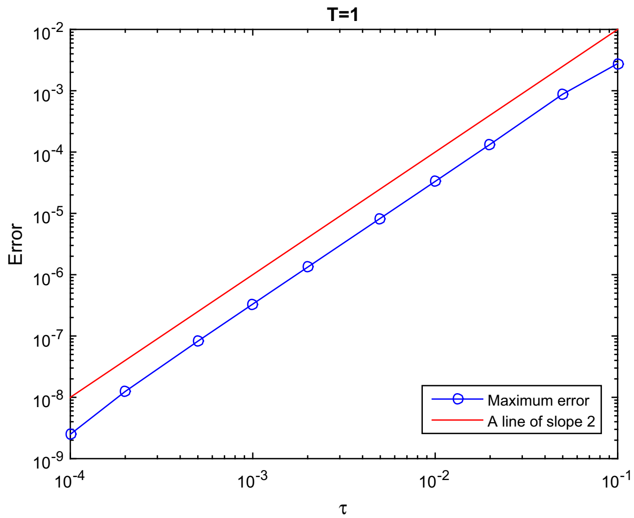


Fig. 9 Example 4.5: Maximum errors of Hermite SAV/CN method

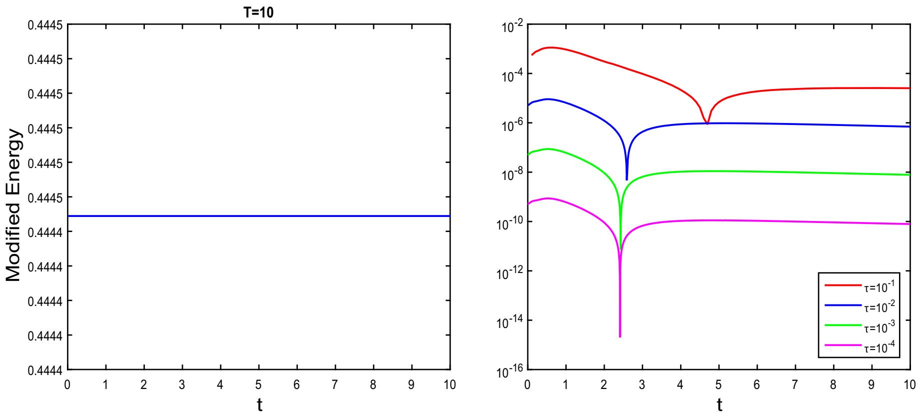


Fig. 10 Example 4.5. Left: Modified energy with $\tau = 0.01$; Right: $|E(u_N^n) - \widetilde{E}(u_N^n, r_N^n)|$ with different τ

tiveness of the scheme. We note that while the SAV scheme presented in this paper does not conserve the original energy, our numerical examples indicate that the modified energy converges to the original energy with second-order accuracy. Note that one can also construct a SAV scheme using a Lagrange multiplier approach [13] to conserve the original energy exactly at the expense of solving a nonlinear algebraic equation at each time step.

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