



HAL
open science

Convergence, error analysis and longtime behavior of the Scalar Auxiliary Variable method for the nonlinear Schrödinger equation

Alexandre Poulain, Katharina Schratz

► **To cite this version:**

Alexandre Poulain, Katharina Schratz. Convergence, error analysis and longtime behavior of the Scalar Auxiliary Variable method for the nonlinear Schrödinger equation. 2020. hal-03088926v1

HAL Id: hal-03088926

<https://hal.science/hal-03088926v1>

Preprint submitted on 27 Dec 2020 (v1), last revised 6 Jul 2021 (v2)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Convergence, error analysis and longtime behavior of the Scalar Auxiliary Variable method for the nonlinear Schrödinger equation

Alexandre Poulain ^{*†} Katharina Schratz ^{‡§}

December 27, 2020

Abstract

We carry out the convergence analysis of the Scalar Auxiliary Variable (SAV) method applied to the nonlinear Schrödinger equation which preserves a modified Hamiltonian on the discrete level. We derive a weak and strong convergence result, establish second-order global error bounds and present long time error estimates on the modified Hamiltonian. In addition, we illustrate the favorable energy conservation of the SAV method compared to classical splitting schemes in certain applications.

2010 *Mathematics Subject Classification.* 35Q55, 65M70, 65M12, 65M15

Keywords and phrases. Nonlinear Schrödinger equation; Scalar Auxiliary Variable; Pseudospectral method, Error bounds.

1 Introduction

We consider the Gross-Pitaevskii [13] equation (NLS) set on the d -dimensional torus $\Omega = \mathbb{T}^d = (\mathbb{R}/2\pi\mathbb{Z})^d$ (where $d \leq 3$)

$$i\partial_t u(t, x) = -\Delta u(t, x) + V(x)u(t, x) + f(|u(t, x)|^2)u(t, x), \quad t \in (0, T] \quad (1.1)$$

with initial conditions $u(0, x) = u^0(x)$, a real-valued interaction potential $V(x)$ and nonlinearity $f(|u|^2)$.

The Hamiltonian energy associated to equation (1.1) takes the form

$$H(u, \bar{u}) = \frac{1}{2} \int_{\Omega} \left(|\nabla u|^2 + V(x)|u|^2 + F(|u|^2) \right) dx,$$

^{*}Sorbonne Université, Inria, Laboratoire Jacques-Louis Lions, F-75005 Paris, France. email: poulain@ljl.math.upmc.fr

[†]The author has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 740623)

[‡]Sorbonne Université, Laboratoire Jacques-Louis Lions, F-75005 Paris, France. email: katharina.schratz@ljl.math.upmc.fr

[§]The author has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 850941)

where $F(|u|^2)$ is defined by $F'(|u|^2) = f(|u|^2)$. Note that the Hamiltonian $H(u(t), \bar{u}(t))$ as well as the probability density $\|u(t, \cdot)\|_{L^2(\Omega)}^2$ is preserved by the system (1.1).

In the following we will denote by \mathcal{E}_1 the sum of the nonlinear and potential part of the Hamiltonian

$$\mathcal{E}_1 = \frac{1}{2} \int_{\Omega} V(x) |u|^2 + F(|u|^2) dx.$$

Using the decomposition $u(t, x) = p(t, x) + iq(t, x)$, equation (1.1) can be furthermore rewritten as the Hamiltonian system

$$\begin{cases} \partial_t p &= -\Delta q + \frac{\delta \mathcal{E}_1[t]}{\delta q}, \\ \partial_t q &= \Delta p - \frac{\delta \mathcal{E}_1[t]}{\delta p}, \end{cases} \quad (1.2)$$

with the associated Hamiltonian

$$H(p, q) = \frac{1}{2} \int_{\Omega} |\nabla p|^2 + |\nabla q|^2 + V(x) (|p|^2 + |q|^2) + F(|p|^2, |q|^2) dx.$$

In this notation, \mathcal{E}_1 takes the form

$$\mathcal{E}_1 = \frac{1}{2} \int_{\Omega} V(x) (|p|^2 + |q|^2) + F(|p|^2, |q|^2) dx.$$

Due to their importance in numerous applications, reaching from Bose-Einstein condensation over nonlinear optics up to plasma physics, nonlinear Schrödinger equations are nowadays very well studied numerically. In the last decades a large variety of different numerical schemes has been proposed. Thanks to their simplicity and accuracy, a popular choice thereby lies in so-called splitting methods, where the right hand side of (1.1) is split into the linear and nonlinear part, respectively, see, e.g., [4, 6, 3] and the references therein. The popularity of splitting methods also stems from their structure preservation. They conserve exactly the L^2 norm of the solution and allow for near energy conservation over long times, see, e.g., [10]. However, in [14] the authors show that in certain applications splitting methods suffer from severe order reduction such as in case of non-linearities with non-integer exponents. The latter arises for instance in context of optical dark and power law solitons with surface plasmonic interactions [9]. As a solution to that issue, the authors proposed in [14] a new class of low regularity exponential-type integrators for NLS. In this article we use a different approach based on the so-called Scalar Auxiliary Variable (SAV) method which was originally proposed to design structure-preserving numerical schemes for gradient flows [16, 17]. Very recently it also became popular in context of Hamiltonian systems [2, 11, 7]. The main advantage of the SAV method lies in the fact that it preserves a modified Hamiltonian on the discrete level. Due to its generality, it can be applied to a large class of equations involving any kind of nonlinearity. The resulting numerical schemes are linearly implicit and allow for efficient calculations.

The main idea behind the SAV method is to introduce a scalar variable $r(t) = \sqrt{\mathcal{E}_1}$ (that will become an unknown at the discrete level) together with the corresponding equation describing its time evolution $\partial_t r(t)$. In case of the nonlinear Schrödinger equation (1.1) the continuous SAV model takes the form

$$\begin{cases} \partial_t p &= -\Delta q + r(t)g_1(p, q), \\ \partial_t q &= \Delta p - r(t)g_2(p, q), \\ \partial_t r(t) &= \frac{1}{2} [(g_1(p, q), \partial_t q) + (g_2(p, q), \partial_t p)], \end{cases} \quad (1.3)$$

where (\cdot, \cdot) denotes the standard L^2 scalar product and

$$g_1(p, q) = \frac{1}{\sqrt{\mathcal{E}_1[t]}} \frac{\delta \mathcal{E}_1[t]}{\delta q}, \quad g_2(p, q) = \frac{1}{\sqrt{\mathcal{E}_1[t]}} \frac{\delta \mathcal{E}_1[t]}{\delta p}.$$

Associated to this SAV model we find the Hamiltonian

$$\tilde{H}(p, q) = \frac{1}{2} \int_{\Omega} |\nabla p|^2 + |\nabla q|^2 dx + |r|^2$$

which is conserved by the SAV model (1.3). In the following we assume that for $i = 1, 2$

$$|g'_i(p, q)| \leq C \left((|p| + |q|)^\beta + 1 \right), \quad |g''_i(p, q)| \leq C \left((|p| + |q|)^{\beta'} + 1 \right) \quad (1.4)$$

for some $\beta, \beta' > 0$.

Following the works of Antoine *et al.* [2] and Fu *et al.* [11], we analyze a fully discrete SAV scheme for the nonlinear Schrödinger equation (1.1) based on a Crank-Nicholson time discretization of the NLS SAV model (1.3) coupled with a pseudo-spectral discretization for the spatial discretization. Energy conservation properties of the SAV method for nonlinear Schrödinger equations were recently derived in [2, 11] and their convergence was extensively tested numerically. The main contribution of this article lies in establishing global error estimates on the fully discrete NLS SAV scheme. More precisely, we derive weak and strong convergence and prove second order error estimates for the fully discrete scheme. Our theoretical convergence analysis is inspired by the analysis of the SAV method in the context of gradient flows [15]. We underline our convergence results with numerical experiments and compare the SAV scheme with classical splitting methods. Our numerical findings suggest that in certain cases, such as in case of non-linearities involving a non-integer exponent, the SAV scheme preserves its second order energy conservation property while classical splitting methods suffer from sever order reduction.

Outline of the paper. In the first part of the paper we carry out a fully discrete error analysis of the SAV scheme and establish second order convergence estimates, see Theorem 11. Our theoretical convergence results are then numerically underlined in the second part of the paper, see Section 6.

Notations. Let $L^p(\Omega)$, $W^{m,p}(\Omega)$ with $H^m(\Omega) = W^{m,2}(\Omega)$, where $1 \leq p \leq +\infty$ and $m \in \mathbb{N}$, denote the standard Lebesgue and Sobolev spaces equipped with the corresponding norms $\|\cdot\|_{m,p}$, $\|\cdot\|_m$ and semi-norms $|\cdot|_{m,p}$, $|\cdot|_m$. We also denote by $H_p^m(\Omega)$ the subset of $H^m(\Omega)$ that consists of 2π -periodic functions that are in $H^m(\Omega)$. We denote by $L^p(0, T; V)$ the Bochner spaces i.e. the spaces with values in Sobolev spaces [1]. The norm in these spaces is defined for all Bochner measurable functions η by

$$\|\eta\|_{L^p(0,T;V)} = \left(\int_0^T \|\eta\|_V^p dt \right)^{1/p}, \quad \|\eta\|_{L^\infty(0,T;V)} = \operatorname{ess\,sup}_{t \in (0,T)} \|\eta\|_V.$$

The standard L^2 inner product is denoted by $(\cdot, \cdot)_\Omega$ and the duality pairing between $(H^1(\Omega))' = H^{-1}(\Omega)$ and $H^1(\Omega)$ by $\langle \cdot, \cdot \rangle_\Omega$. The dual space $H^{-1}(\Omega)$ is endowed with the norm

$$\|\phi\|_{H^{-1}(\Omega)} = \sup_{\eta \in H^1(\Omega)} \{ \langle \phi, \eta \rangle_\Omega, \quad \|\eta\|_1^2 \leq 1 \}.$$

2 Numerical scheme

2.1 Time and space discretisation of the SAV model

We use a standard Fourier pseudospectral method for the spatial discretization of the SAV model (1.3). Thereby, we denote by X_N the space spanned by the trigonometric functions up to degree $N/2$

$$X_N := \text{span}\{e^{ikx/L} : -N/2 \leq k \leq N/2 - 1\}.$$

For the time discretisation of the SAV system (1.3) we apply a Crank-Nicholson discretisation with time step τ such that $t^k = k\tau$ for $k \in \mathbb{N}$. At each grid point we thereby approximate the time derivative by

$$\partial_t u(t^{k+1}, x) \approx \frac{u(t^{k+1}, x) - u(t^k, x)}{\tau}.$$

Let us give the details of the approximation in dimension $d = 1$, where the domain is defined by $\Omega = [-\pi, \pi]$ with a mesh size h . In this case the collocation points are $x_a = \frac{2\pi a}{N}$ where $a \in \mathcal{B}$ with

$$\mathcal{B} := \begin{cases} \{-P, \dots, P-1\} & \text{if } N = 2P \text{ is even,} \\ \{-P, \dots, P\} & \text{if } N = 2P + 1 \text{ is odd.} \end{cases}$$

We denote by $U^k(x_a)$ the approximation of $u(t^k, x_a)$. The Fourier pseudo-spectral discretization is given by

$$U^k(x_a) = \sum_{p \in \mathcal{B}} \hat{u}_p^k \exp(2i\pi ap/N)$$

with the Fourier coefficients defined by

$$\hat{u}_p^k = \frac{1}{N} \sum_{b \in \mathcal{B}} U^k(x_b) \exp(-2i\pi bp/N).$$

We approximate the Laplacian by the Fourier differentiation matrix $D^{(2)}$ which for $j, l = 0, \dots, N-1$ takes the form

$$\left(D^{(2)}\right)_{jl} = \begin{cases} \frac{1}{4}(-1)^{j+l}N + \frac{(-1)^{j+l+1}}{2\sin^2\left(\frac{(j-l)\pi}{N}\right)}, & \text{if } j \neq l \\ -\frac{(N-1)(N-2)}{12}, & \text{otherwise.} \end{cases}$$

For the N collocation points x_a , we define the interpolation operation I_N by

$$(I_N u)(x) = \sum_{p \in \mathcal{B}} \tilde{u}_p e^{2i\pi xp/N}.$$

We have the following interpolation error [8]:

Lemma 1 (Interpolation error) *For any $u \in C(0, T; H_p^m)$ with $m > 1/2$,*

$$\begin{cases} \left\| \partial_x^{(l)} (I_N u - u) \right\|_0 \leq N^{l-m} |u|_m, & 0 \leq l \leq m, \\ \left\| \partial_x^{(l)} (I_N \partial_t u - \partial_t u) \right\|_0 \leq N^{l-m} |\partial_t u|_m, & 0 \leq l \leq m. \end{cases}$$

2.2 The fully discrete SAV scheme

Applying the time discretization described in the previous section, for $k = 0 \rightarrow N_T$, the semi-discrete model of (1.3) reads

$$\begin{cases} \frac{p^{k+1}-p^k}{\tau} &= -\Delta q^{k+1/2} + r^{k+1/2} \tilde{g}_1^{k+1/2}, \\ \frac{q^{k+1}-q^k}{\tau} &= \Delta p^{k+1/2} - r^{k+1/2} \tilde{g}_2^{k+1/2}, \\ r^{k+1} - r^k &= \frac{1}{2} \left[\left(\tilde{g}_1^{k+1/2}, q^{k+1} - q^k \right) + \left(\tilde{g}_2^{k+1/2}, p^{k+1} - p^k \right) \right], \end{cases} \quad (2.1)$$

where $\phi^{k+1/2} = (\phi^{k+1} + \phi^k) / 2$ and $\tilde{g}_i^{k+1/2}$ is a second order extrapolation of g_i at time $t = t^{k+1/2}$.

Denoting by capital letters the vectors of unknowns P^k, Q^k that are approximations at each collocation nodes of the continuous (in space) unknowns p^k, q^k , the fully discrete space-time scheme then takes the form

$$\begin{cases} \frac{P^{k+1}-P^k}{\tau} &= -D^{(2)} Q^{k+1/2} + R^{k+1/2} \tilde{G}_1^{k+1/2}, \\ \frac{Q^{k+1}-Q^k}{\tau} &= D^{(2)} P^{k+1/2} - R^{k+1/2} \tilde{G}_2^{k+1/2}, \\ r^{k+1} - r^k &= \frac{1}{2} \left[\left(\tilde{G}_1^{k+1/2}, Q^{k+1} - Q^k \right) + \left(\tilde{G}_2^{k+1/2}, P^{k+1} - P^k \right) \right], \end{cases} \quad (2.2)$$

where \tilde{G}_1, \tilde{G}_2 are the vectors associated to the functions \tilde{g}_1 and \tilde{g}_2 .

Let us now present two algorithms for the efficient solution of the fully discrete SAV system (2.2). The two methods are equivalent and reduce the problem to two linear systems involving the invert of a constant matrix that can be calculated at the beginning of the simulation.

Algorithm 1

The algorithm below was originally proposed for solving the fully discrete SAV system arising in gradient flows [16].

Let us give the procedure on how to solve the system (2.2). First, we need to replace r^{k+1} in the first two equations using the third equation. This yields that

$$\begin{cases} (P^{k+1} - P^k) &= -\tau D^{(2)} \frac{(Q^{k+1} + Q^k)}{2} + \tau \left(r^k + \frac{1}{4} \left[\left(\tilde{G}_1^{k+1/2}, Q^{k+1} - Q^k \right) + \left(\tilde{G}_2^{k+1/2}, P^{k+1} - P^k \right) \right] \right) \tilde{G}_1^{k+1/2}, \\ (Q^{k+1} - Q^k) &= \tau D^{(2)} \frac{(P^{k+1} - P^k)}{2} - \tau \left(r^k + \frac{1}{4} \left[\left(\tilde{G}_1^{k+1/2}, Q^{k+1} - Q^k \right) + \left(\tilde{G}_2^{k+1/2}, P^{k+1} - P^k \right) \right] \right) \tilde{G}_2^{k+1/2}. \end{cases}$$

Next we set

$$Z^k = \begin{pmatrix} P^k \\ Q^k \end{pmatrix}, \tilde{G}^{k+1/2} = \begin{pmatrix} \tilde{G}_2^{k+1/2} \\ \tilde{G}_1^{k+1/2} \end{pmatrix}, \tilde{B}^{k+1/2} = \begin{pmatrix} -\tilde{G}_1^{k+1/2} \\ \tilde{G}_2^{k+1/2} \end{pmatrix}.$$

This allows us to rewrite the system into a matrix form

$$AZ^{k+1} + \frac{\tau}{4} \left(\tilde{G}^{k+1/2}, Z^{k+1} \right) \tilde{B}^{k+1/2} = C^k, \quad (2.3)$$

where

$$A = \begin{bmatrix} I & \frac{\tau}{2} D^{(2)} \\ -\frac{\tau}{2} D^{(2)} & I \end{bmatrix}, \quad \text{and} \quad C^k = \begin{pmatrix} I & -\frac{\tau}{2} D^{(2)} \\ \frac{\tau}{2} D^{(2)} & I \end{pmatrix} Z^k - \tau r^k \tilde{B}^{k+1/2} + \frac{\tau}{4} \left(\tilde{G}^{k+1/2}, Z^k \right) \tilde{B}^{k+1/2}.$$

Multiplying (2.3) by A^{-1} and taking the discrete inner product with $\tilde{G}^{k+1/2}$, we finally obtain

$$\left(\tilde{G}^{k+1/2}, Z^{k+1}\right) = \frac{\left(\tilde{G}^{k+1/2}, A^{-1}C^k\right)}{1 + \frac{\tau}{4}\left(\tilde{G}^{k+1/2}, A^{-1}\tilde{B}^{k+1/2}\right)}. \quad (2.4)$$

Then, knowing $\left(\tilde{G}^{k+1/2}, Z^{k+1}\right)$, Z^{k+1} is computed using (2.3) and r^{k+1} is calculated from the third equation of (2.2). Therefore, solving the fully discrete SAV model (2.2) reduces to solving the linear system constituted by the equations (2.4) and (2.3). One advantage of this algorithm is that the matrix A is constant and needs to be inverted only once.

Algorithm 2

Below we describe a second algorithm recently proposed in [2] for the numerical solution of the fully discrete NLS SAV scheme (2.2). Rewriting the scheme in its matrix form we have

$$\begin{cases} \frac{Z^{k+1} - Z^k}{\tau} &= -JZ^{k+1/2} - r^{k+1/2}\tilde{B}^{k+1/2}, \\ r^{k+1} - r^k &= \frac{1}{2}\left[\left(\tilde{G}_1^{k+1/2}, Q^{k+1} - Q^k\right) + \left(\tilde{G}_2^{k+1/2}, P^{k+1} - P^k\right)\right], \end{cases} \quad (2.5)$$

where

$$J = \begin{bmatrix} 0 & D^{(2)} \\ -D^{(2)} & 0 \end{bmatrix}.$$

Using the decomposition

$$Z^{k+1/2} = Z_1^{k+1/2} + r^{k+1/2}Z_2^{k+1/2}, \quad (2.6)$$

and adding $\frac{2}{\tau}Z^k$ on both sides of the first equation of (2.5), we furthermore obtain that

$$\frac{2}{\tau}\left[Z^{k+1/2} + r^{k+1/2}Z_2^{k+1/2}\right] = \frac{2}{\tau}Z^k - J\left[Z_1^{k+1/2} + r^{k+1/2}Z_2^{k+1/2}\right] - r^{k+1/2}\tilde{B}^{k+1/2}. \quad (2.7)$$

Applying the same decomposition to the second equation of (2.5) and adding $2r^k$ on both sides, we get

$$2r^{k+1/2} = 2r^k + \left(\tilde{G}^{k+1/2}, \left[Z_1^{k+1/2} + r^{k+1/2}Z_2^{k+1/2}\right] - Z^k\right). \quad (2.8)$$

Hence we first solve the equation (2.7) using the system

$$\begin{cases} \left[\frac{2}{\tau} + J\right] Z_1^{k+1/2} = \frac{2}{\tau}Z^k \\ \left[\frac{2}{\tau} + J\right] Z_2^{k+1/2} = -\tilde{B}^{k+1/2}. \end{cases}$$

Then we compute $r^{k+1/2}$ by solving equation (2.8) which yields that

$$r^{k+1/2} = \frac{2r^k + \left(\tilde{G}^{k+1/2}, Z_1^{k+1/2} - Z^k\right)}{2 - \left(\tilde{G}^{k+1/2}, Z_2^{k+1/2}\right)}.$$

From the decomposition (2.6) we get $Z^{k+1/2}$ from which we compute Z^{k+1} and r^{k+1} . As in algorithm 1 the solution of the fully discrete SAV system (2.2) reduces to solving a linear problem only requiring the inversion of a constant matrix $\left[\frac{2}{\tau} + J\right]$ at the beginning of the computation. However, this algorithm seems more efficient since it involves less matrix-vector multiplications.

Remark 2 Referring to [16], we remark that the inversion of the matrix A of the first algorithm and $[\frac{2}{\tau} + J]$ of the second can be computed efficiently using the Sherman-Morrison-Woodbury formula [12]

$$(A + UV^T)^{-1} = A^{-1} - A^{-1}U(I + V^T A^{-1}U)^{-1}V^T A^{-1},$$

where A is a $n \times n$ and U, V are $n \times k$ matrices, and I is the $k \times k$ identity matrix.

3 Conservation properties and inequalities

In this section we outline the conserved quantities of the SAV method. We briefly recall the proofs of the conservation properties and refer to [11, 2], where they have been first set in context of nonlinear Schrödinger equations.

Theorem 3 (Conservation of the modified discrete energy) *The scheme (2.1) is associated to the discrete modified Hamiltonian*

$$\tilde{H}^{k+1} = \frac{1}{2} \left(|Q^{k+1}|_1^2 + |P^{k+1}|_1^2 \right) + |r^{k+1}|^2, \quad (3.1)$$

and conserves the modified Hamiltonian energy through time i.e.

$$\tilde{H}^{k+1} = \tilde{H}^k. \quad (3.2)$$

Proof. Taking the inner product with $Q^{k+1} - Q^k$ for the first equation of (2.2) and for the second with $-(P^{k+1} - P^k)$, then summing the results we get

$$0 = \frac{1}{2} \left(|Q^{k+1}|_1^2 - |Q^k|_1^2 + |P^{k+1}|_1^2 - |P^k|_1^2 \right) + r^{k+1/2} \left[\left(\tilde{G}_1^{k+1/2}, Q^{k+1} - Q^k \right) + \left(\tilde{G}_2^{k+1/2}, P^{k+1} - P^k \right) \right],$$

where $|\cdot|_1 = \|\nabla \cdot\|_0$ is the H^1 -seminorm. Then, multiplying the third equation of (2.2) by $2R^{k+1/2}$ and using the result in the previous equation, we obtain

$$0 = \frac{1}{2} \left(|Q^{k+1}|_1^2 - |Q^k|_1^2 + |P^{k+1}|_1^2 - |P^k|_1^2 \right) + \left(|r^{k+1}|^2 - |r^k|^2 \right),$$

from which we can conclude both (3.1) and (3.2). \square

The SAV scheme also preserves the mass up to an error of order $\mathcal{O}(\tau^3)$, where the latter error is introduced by the second-order extrapolation.

Theorem 4 (Conservation of the L^2 norm) *The scheme (1.3) conserves the L^2 norm of the solution up to an order $\mathcal{O}(\tau^3)$ i.e.*

$$\|U^{k+1}\|_0^2 = \|U^k\|_0^2 + \mathcal{O}(\tau^3). \quad (3.3)$$

Proof. Taking the inner product of first equation of (2.2) with $2P^{k+1/2}$, the second equation with $2Q^{k+1/2}$, and summing the two we get

$$\frac{1}{\tau} \left(\|P^{k+1}\|_0^2 - \|P^k\|_0^2 + \|Q^{k+1}\|_0^2 - \|Q^k\|_0^2 \right) = 2r^{k+1/2} \left(- \left(\tilde{G}_2^{k+1/2}, Q^{k+1/2} \right) + \left(\tilde{G}_1^{k+1/2}, P^{k+1/2} \right) \right).$$

Since $\tilde{G}_i^{k+1/2}$ is a second-order approximation of $G_i^{k+1/2}$, we can write

$$\frac{1}{\tau} \left(\|U^{k+1}\|_0^2 - \|U^k\|_0^2 \right) = 2r^{k+1/2} \left(- \left(G_2^{k+1/2}, Q^{k+1/2} \right) + \left(G_1^{k+1/2}, P^{k+1/2} \right) \right) + \mathcal{O}(\tau^2),$$

from which we obtain (3.3) since

$$- \left(G_2^{k+1/2}, Q^{k+1/2} \right) + \left(G_1^{k+1/2}, P^{k+1/2} \right) = 0.$$

□

Next we present two inequalities that are later useful in the convergence analysis.

Proposition 5 (Stability inequality) *The solution of (2.1) satisfies the stability inequality*

$$\max_{k=0, \dots, N_T-1} \left[\|P^{k+1}\|_0^2 + \|Q^{k+1}\|_0^2 \right] + \tau^2 \sum_{k=0}^{N_T-1} \left[\left\| \frac{P^{k+1} - P^k}{\tau} \right\|_0^2 + \tau^2 \left\| \frac{Q^{k+1} - Q^k}{\tau} \right\|_0^2 \right] \leq C(\tau, H^0, N_T). \quad (3.4)$$

Proof. Multiplying the first equation with $2\tau P^{k+1}$, integrating over Ω and using $2(a-b)a = a^2 - b^2 + (a-b)^2$, we obtain

$$\|P^{k+1}\|_0^2 + \tau^2 \left\| \frac{P^{k+1} - P^k}{\tau} \right\|_0^2 - \|P^k\|_0^2 = -2\tau \left(\nabla Q^{k+1/2}, \nabla P^{k+1} \right) + 2\tau r^{k+1/2} \left(\tilde{G}_1^{k+1/2}, P^{k+1} \right).$$

From which, using the Cauchy-Schwartz inequality, assuming that the initial energy is finite, and knowing that the scheme preserves the L^2 norm of U , we have

$$\|P^{k+1}\|_0^2 + \tau^2 \left\| \frac{P^{k+1} - P^k}{\tau} \right\|_0^2 \leq C.$$

The same can be found for the second equation by repeating the same calculations. Summing for $k = 0 \rightarrow N_T - 1$, we find (3.4). □

Proposition 6 (H^2 bound on the numerical solution) *The solution $\{P^{k+1}, Q^{k+1}\}$ of (2.1) satisfies*

$$\max_{k=1, \dots, N_T-1} \left[\|\Delta P^{k+1}\|_0^2 + \|\Delta Q^{k+1}\|_0^2 \right] \leq C + \|\Delta P^0\|_0^2 + \|\Delta Q^0\|_0^2. \quad (3.5)$$

Proof. Multiplying the first equation of (2.1) by $-\Delta(Q^{k+1} - Q^k)$, the second equation by $\Delta(P^{k+1} - P^k)$, integrating over Ω and summing the two, we obtain

$$0 = \left\| \Delta Q^{k+1} \right\|_0^2 - \left\| \Delta Q^k \right\|_0^2 + \left\| \Delta P^{k+1} \right\|_0^2 - \left\| \Delta P^k \right\|_0^2 \\ - r^{k+\frac{1}{2}} \left(\nabla \tilde{G}_1^{k+\frac{1}{2}}, \nabla(Q^{k+1} - Q^k) \right) - R^{k+\frac{1}{2}} \left(\nabla \tilde{G}_2^{k+\frac{1}{2}}, \nabla(P^{k+1} - P^k) \right).$$

The previous equation is found using integration per parts and the periodic boundary conditions. Then, from the Cauchy-Schwartz inequality, we have

$$\left(\nabla \tilde{G}_1^{k+\frac{1}{2}}, \nabla(Q^{k+1} - Q^k) \right) \leq \left\| \nabla \tilde{G}_1^{k+\frac{1}{2}} \right\|_0 \left\| \nabla(Q^{k+1} - Q^k) \right\|_0.$$

However, since

$$\nabla \tilde{G}_1^{k+\frac{1}{2}} \leq G'_1(P^{k+\frac{1}{2}}, Q^{k+\frac{1}{2}}) \left(\nabla P^{k+\frac{1}{2}} + \nabla Q^{k+\frac{1}{2}} \right) + C(\tau),$$

and from (1.4), together with the conservation of the Hamiltonian, it exists a constant $C > 0$ such that

$$-C \leq \left(\nabla \tilde{G}_1^{k+\frac{1}{2}}, \nabla(Q^{k+1} - Q^k) \right) \leq C.$$

The same can be found for $\left(\nabla \tilde{G}_2^{k+\frac{1}{2}}, \nabla(P^{k+1} - P^k) \right)$ using similar arguments. Altogether, we find

$$\left\| \Delta P^{k+1} \right\|_0^2 - \left\| \Delta P^k \right\|_0^2 + \left\| \Delta Q^{k+1} \right\|_0^2 - \left\| \Delta Q^k \right\|_0^2 \leq C,$$

and summing from $k = 0 \rightarrow N_T$, we obtain (3.5). \square

4 Convergence analysis

4.1 Notations

To study the convergence of the scheme, we introduce the following notation: For $k = 0, \dots, N_T - 1$ we set

$$U(t, x) := \frac{t - t^k}{\tau} U^{k+1} + \frac{t^{k+1} - t}{\tau} U^k, \quad t \in (t^k, t^{k+1}],$$

and

$$\frac{\partial U}{\partial t} := \frac{U^{k+1} - U^k}{\tau} \quad t \in (t^k, t^{k+1}].$$

We also define

$$U^+ := U^{k+1}, \quad U^- := U^k,$$

and

$$U - U^+ = (t - t^{k+1}) \frac{\partial U}{\partial t}, \quad U - U^- = (t - t^k) \frac{\partial U}{\partial t} \quad t \in (t^k, t^{k+1}], \quad k \geq 0.$$

In addition, we take analogous definitions for P and Q : For $k = 0, \dots, K_T - 1$ we set

$$\begin{aligned} P(t, x) &:= \frac{t - t^k}{\tau} P^{k+1} + \frac{t^{k+1} - t}{\tau} P^k, \quad t \in (t^k, t^{k+1}], \\ \frac{\partial P}{\partial t} &:= \frac{P^{k+1} - P^k}{\tau} \quad t \in (t^k, t^{k+1}], \\ P^+ &:= P^{k+1}, \quad P^- := P^k, \end{aligned}$$

and

$$P - P^+ = (t - t^{k+1}) \frac{\partial P}{\partial t}, \quad \text{and} \quad P - P^- = (t - t^k) \frac{\partial P}{\partial t} \quad t \in (t^k, t^{k+1}], \quad k \geq 0.$$

4.2 Convergence theorem

Now we are in the position to establish time convergence for the semi discrete SAV scheme (2.1).

Theorem 7 (Convergence) *Let $\{p, q\}$ be a pair of functions such that*

$$\begin{cases} p(t, x) \in L^2([0, T]; H^1(\Omega)) \cap H^1([0, T]; (H^1(\Omega))') \\ q(t, x) \in L^2([0, T]; H^1(\Omega)) \cap H^1([0, T]; (H^1(\Omega))'). \end{cases}$$

Then for $\tau \rightarrow 0$ we can extract a subsequence of solutions of (2.1), such that

$$P, P^\pm \rightarrow p \quad \text{strongly in } L^2([0, T]; L^2(\Omega)), \quad (4.1)$$

$$Q, Q^\pm \rightarrow q \quad \text{strongly in } L^2([0, T]; L^2(\Omega)), \quad (4.2)$$

$$P, P^\pm \rightharpoonup p \quad \text{weakly in } L^2([0, T]; H^1(\Omega)), \quad (4.3)$$

$$Q, Q^\pm \rightharpoonup q \quad \text{weakly in } L^2([0, T]; H^1(\Omega)), \quad (4.4)$$

$$\frac{\partial P}{\partial t} \rightharpoonup \frac{\partial p}{\partial t} \quad \text{weakly in } L^2([0, T]; (H^1(\Omega))'), \quad (4.5)$$

$$\frac{\partial Q}{\partial t} \rightharpoonup \frac{\partial q}{\partial t} \quad \text{weakly in } L^2([0, T]; (H^1(\Omega))'), \quad (4.6)$$

$$r^{k+1} \rightharpoonup r(t) = \sqrt{\mathcal{E}_1[t]} \quad \text{weak-star in } L^\infty(0, T). \quad (4.7)$$

The limit $\{p, q\}$ satisfies the nonlinear Schrödinger model (1.2) in the following weak sense

$$\begin{cases} \int_0^T \left\langle \frac{\partial p}{\partial t}, \eta \right\rangle dt = \int_0^T \int_\Omega \nabla q \nabla \eta + \left(V(x)q + \frac{\partial F(|p|^2, |q|^2)}{\partial q} \right) \eta \, dx \, dt \\ \int_0^T \left\langle \frac{\partial q}{\partial t}, \eta \right\rangle dt = \int_0^T \int_\Omega -\nabla p \nabla \eta - \left(V(x)p + \frac{\partial F(|p|^2, |q|^2)}{\partial p} \right) \eta \, dx \, dt, \end{cases} \quad (4.8)$$

for all $\eta \in L^2([0, T]; H^1(\Omega))$.

Proof.

Step 1: Weak and strong convergences. First, the weak convergences (4.3), (4.4), (4.5) and (4.6) follow from the assumption that the initial Hamiltonian energy is bounded and the stability inequality (3.4).

Then, the weak-star convergence (4.7) also holds true by the conservation of the modified Hamiltonian and the boundedness of the initial state.

From the compact embedding $H^1(\Omega) \subset L^2(\Omega) \equiv (L^2(\Omega))'$, we can apply the Lions-Aubin Lemma to find both convergences (4.1) and (4.2).

Step 2: Limit system. Let us work on the first equation of the discrete system. We use a test function $\eta \in L^2([0, T]; H^1(\Omega))$ and analyze the convergence of the terms separately. First, from the weak convergence (4.4), we have

$$\int_0^T \int_{\Omega} \nabla \left(\frac{Q^+ + Q^-}{2} \right) \nabla \eta \, dx \, dt \rightarrow \int_0^T \int_{\Omega} \nabla q \nabla \eta \, dx \, dt.$$

Secondly, from the fact that $\tilde{G}_1^{k+1/2}$ is a second-order approximation of $G_1^{k+1/2}$, we have

$$\int_0^T \int_{\Omega} r^{k+1/2} \tilde{G}_1^{k+1/2} \eta \, dx \, dt = \int_0^T \int_{\Omega} r^{k+1/2} G_1^{k+1/2} \eta \, dx \, dt + \int_0^T \int_{\Omega} r^{k+1/2} \mathcal{O}(\tau^2) \eta \, dx \, dt.$$

From the inequality

$$\left| \mathcal{E}_1(U^{k+1/2}) - \mathcal{E}_1(u) \right| \leq C \left\| U^{k+1/2} \right\|_{L^1(\Omega)}^2,$$

and the fact that

$$P^{\pm}, Q^{\pm} \rightharpoonup p, q \quad \text{weak-star in } L^{\infty}(0, T; H^1(\Omega)),$$

which follows from the conservation of both the Hamiltonian energy and the L^2 norm, we have

$$\mathcal{E}_1(U^{k+1/2}) \rightharpoonup \mathcal{E}_1(u) \quad \text{weak-star in } L^{\infty}(0, T).$$

The same holds true for $\frac{\delta \mathcal{E}_1^{k+1/2}}{\delta q}$ and $\frac{\delta \mathcal{E}_1^{k+1/2}}{\delta p}$ using similar arguments. Then, using also the strong convergences (4.1) and (4.2), together with the weak-star convergence (4.7), we obtain

$$\int_0^T \int_{\Omega} r^{k+1/2} G_1^{k+1/2} \eta \, dx \, dt + \int_0^T \int_{\Omega} r^{k+1/2} \mathcal{O}(\tau^2) \eta \, dx \, dt \rightarrow \int_0^T \int_{\Omega} r(t) g_1(t) \eta \, dx \, dt.$$

Finally, for any $\eta \in H^1([0, T]; H^1(\Omega))$, by integration by parts we have

$$\int_0^T \left(\frac{\partial P}{\partial t}, \eta \right) \, dt = - \int_0^T \left(P, \frac{\partial \eta}{\partial t} \right) \, dt + (P(T), \eta(T)) - (P(0), \eta(0)).$$

Hence, from the regularity of η and the convergence (4.1), we obtain

$$\int_0^T \left(P, \frac{\partial \eta}{\partial t} \right) \, dt \rightarrow \int_0^T \left(p, \frac{\partial \eta}{\partial t} \right) \, dt \quad \text{as } \tau \rightarrow 0 \quad \text{and} \quad \forall \eta \in H^1([0, T]; H^1(\Omega)).$$

Gathering the previous convergences, we have

$$(p(T), \eta(T)) - (p(0), \eta(0)) - \int_0^T \left(p, \frac{\partial \eta}{\partial t} \right) \, dt = \int_0^T \int_{\Omega} \nabla q \nabla \eta + \left(V(x)q + \frac{\partial F(|p|^2, |q|^2)}{\partial q} \right) \eta \, dx \, dt.$$

Since $\nabla q + \left(V(x)q + \frac{\partial F(|p|^2, |q|^2)}{\partial q} \right) \in L^2(\Omega)$ which follow from the conservation of the Hamiltonian energy, we know that $p \in H^1([0, T]; H^{-1}(\Omega))$. Finally, we find the first equation of the limit system (4.8) and the same arguments can be applied to the second equation. This yields the result. \square

5 Error analysis

In this section we analyse the difference between the exact and modified Hamiltonian, and establish a bound on

$$\left| H[p(t^k), q(t^k)] - \tilde{H}[P^k, Q^k] \right|.$$

In addition we prove second-order convergence of the fully discrete SAV scheme (2.2) approximating the solution of the nonlinear Schrödinger equation (1.1). We introduce the following notation to study the error

$$e_u^k = \theta_u^k + \rho_u^k, \quad (5.1)$$

where

$$\theta_u^k = U^k - (I_N u)(t^k, x), \quad \rho_u^k = (I_N u)(t^k, x) - u(t^k, x).$$

For our convergence result we assume that the solution u of (1.1) is sufficiently smooth satisfying

$$\|\partial_{ttt} u\|_{L^\infty(0,T;H^1(\Omega))} + \|u\|_{L^\infty(0,T;H^2(\Omega))} \leq C. \quad (5.2)$$

We define the different truncation errors by

$$\begin{aligned} T_u^{k+\frac{1}{2}} &= \frac{u^{k+1} - u^k}{\Delta t} - \partial_t u(t^{k+\frac{1}{2}}), \\ \bar{T}_u^{k+\frac{1}{2}} &= u^{k+\frac{1}{2}} - u(t^{k+\frac{1}{2}}) = \frac{u^{k+1} + u^k}{2} - u(t^{k+\frac{1}{2}}). \end{aligned}$$

We commence with two important lemma that will be useful in the global error analysis.

Lemma 8 (Boundedness of nonlinear functions) *If (p, q) is a solution of (1.3) satisfying (5.2), we have for $i = 1, 2$*

$$|g_i(p, q)|, \left| \frac{\partial g_i}{\partial p} \right|, \left| \frac{\partial g_i}{\partial q} \right|, \left| \frac{\partial^2 g_i}{\partial p \partial q} \right|, \left| \frac{\partial^2 g_i}{\partial p^2} \right|, \left| \frac{\partial^2 g_i}{\partial q^2} \right| \leq C.$$

Remark 9 *From Lemma 8, and the hypothesis (5.2), we know that*

$$|\partial_{ttt} r| \leq C \left(\|\partial_{ttt} p\|_0^2 + \|\partial_{ttt} q\|_0^2 \right).$$

Lemma 10 (Truncation errors) *For $\alpha = -1, 0, 1, 2$, we have*

$$\begin{aligned} \left\| T_\psi^{k+\frac{1}{2}} \right\|_{H^\alpha(\Omega)}^2 &\leq \tau^3 \int_{t^k}^{t^{k+1}} \|\partial_{ttt} \psi(s)\|_{H^\alpha(\Omega)}^2 \, ds, \\ \left\| \bar{T}_\psi^{k+\frac{1}{2}} \right\|_{H^\alpha(\Omega)}^2 &\leq \tau^3 \int_{t^k}^{t^{k+1}} \|\partial_{ttt} \psi(s)\|_{H^\alpha(\Omega)}^2 \, ds, \end{aligned}$$

Theorem 11 (Error analysis) Assume that the solution of (1.2) satisfies (5.2) with initial condition $u^0 \in H^3(\Omega)$. Then the discrete solution $\{P^{k+1}, Q^{k+1}\}$ of the fully discrete SAV scheme (2.2) satisfies the error estimate

$$\frac{1}{2} \left\| \nabla e_q^{k+1} \right\|_0^2 + \frac{1}{2} \left\| \nabla e_p^{k+1} \right\|_0^2 + \left| e_r^{k+1} \right|^2 \leq C \exp \left([1 - C\tau]^{-1} t^{k+1} \right) (\tau^4 + N^{-4}),$$

where the constant C depends on the smoothness of the solution (5.2).

Proof.

Step 1: Error equations. We begin by evaluating the model (1.3) at time $t^{k+1/2}$

$$\begin{cases} \partial_t p(t^{k+1/2}) &= -\Delta q(t^{k+1/2}) + r(t^{k+1/2})g_1(t^{k+1/2}), \\ \partial_t q(t^{k+1/2}) &= \Delta p(t^{k+1/2}) - r(t^{k+1/2})g_2(t^{k+1/2}), \\ \frac{dr}{dt}(t^{k+1/2}) &= \frac{1}{2} \left[(g_1(t^{k+1/2}), \partial_t q(t^{k+1/2})) + (g_2(t^{k+1/2}), \partial_t p(t^{k+1/2})) \right]. \end{cases}$$

Subtracting the above equations from (2.2) yields

$$\begin{cases} \frac{e_p^{k+1} - e_p^k}{\tau} + T_p^{k+1/2} &= -\Delta \left(e_q^{k+1/2} + \bar{T}_q^{k+1/2} \right) + R^{k+1/2} \tilde{G}_1^{k+1/2} - r(t^{k+1/2})g_1(t^{k+1/2}), \\ \frac{e_q^{k+1} - e_q^k}{\tau} + T_q^{k+1/2} &= \Delta \left(e_p^{k+1/2} + \bar{T}_p^{k+1/2} \right) - R^{k+1/2} \tilde{G}_2^{k+1/2} + r(t^{k+1/2})g_2(t^{k+1/2}), \\ \frac{e_r^{k+1} - e_r^k}{\tau} + T_r^{k+1/2} &= \frac{1}{2} \left[\left(\tilde{G}_1^{k+1/2}, \frac{Q^{k+1} - Q^k}{\tau} \right) + \left(\tilde{G}_2^{k+1/2}, \frac{P^{k+1} - P^k}{\tau} \right) \right. \\ &\quad \left. - (g_1(t^{k+1/2}), \partial_t q(t^{k+1/2})) - (g_2(t^{k+1/2}), \partial_t p(t^{k+1/2})) \right]. \end{cases} \quad (5.3)$$

We introduce the error

$$e_{g,1}^{k+1/2} = \tilde{G}_1^{k+1/2} - g_1(t^{k+1/2}).$$

The rightmost terms of the two first equations of (5.3) can be replaced by

$$R^{k+1/2} \tilde{G}_1^{k+1/2} - r(t^{k+1/2})g_1(t^{k+1/2}) = \tilde{G}_1^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right) + r(t^{k+1/2})e_{g,1}^{k+1/2}, \quad (5.4)$$

and

$$R^{k+1/2} \tilde{G}_2^{k+1/2} - r(t^{k+1/2})g_2(t^{k+1/2}) = \tilde{G}_2^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right) + r(t^{k+1/2})e_{g,2}^{k+1/2}. \quad (5.5)$$

Similarly, we have

$$\begin{aligned} & \frac{1}{2} \left[\left(\tilde{G}_1^{k+1/2}, \frac{Q^{k+1} - Q^k}{\tau} \right) - (g_1(t^{k+1/2}), \partial_t q(t^{k+1/2})) \right] \\ &= \frac{1}{2} \left[\left(\tilde{G}_1^{k+1/2}, \frac{e_q^{k+1} - e_q^k}{\tau} + T_q^{k+1/2} \right) + \left(e_{g,1}^{k+1/2}, \partial_t q(t^{k+1/2}) \right) \right], \end{aligned} \quad (5.6)$$

and

$$\begin{aligned} & \frac{1}{2} \left[\left(\tilde{G}_2^{k+1/2}, \frac{P^{k+1} - P^k}{\tau} \right) - (g_2(t^{k+1/2}), \partial_t p(t^{k+1/2})) \right] \\ &= \frac{1}{2} \left[\left(\tilde{G}_2^{k+1/2}, \frac{e_p^{k+1} - e_p^k}{\tau} + T_p^{k+1/2} \right) + \left(e_{g,2}^{k+1/2}, \partial_t p(t^{k+1/2}) \right) \right]. \end{aligned} \quad (5.7)$$

Plugging (5.4), (5.5), (5.6), and (5.7) into (5.3), we thus obtain

$$\begin{cases} \frac{e_p^{k+1} - e_p^k}{\tau} + T_p^{k+1/2} &= -\Delta \left(e_q^{k+1/2} + \bar{T}_q^{k+1/2} \right) + \tilde{G}_1^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right) + r(t^{k+1/2}) e_{g,1}^{k+1/2}, \\ \frac{e_q^{k+1} - e_q^k}{\tau} + T_q^{k+1/2} &= \Delta \left(e_p^{k+1/2} + \bar{T}_p^{k+1/2} \right) - \tilde{G}_2^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right) - r(t^{k+1/2}) e_{g,2}^{k+1/2}, \\ \frac{e_r^{k+1} - e_r^k}{\tau} + T_r^{k+1/2} &= \frac{1}{2} \left[\left(\tilde{G}_1^{k+1/2}, \frac{e_q^{k+1} - e_q^k}{\tau} + T_q^{k+1/2} \right) + \left(e_{g,1}^{k+1/2}, \partial_t q(t^{k+1/2}) \right) \right. \\ &\quad \left. + \left(\tilde{G}_2^{k+1/2}, \frac{e_p^{k+1} - e_p^k}{\tau} + T_p^{k+1/2} \right) + \left(e_{g,2}^{k+1/2}, \partial_t p(t^{k+1/2}) \right) \right]. \end{cases}$$

Using the decomposition of the error (5.1), we furthermore obtain

$$\begin{cases} \frac{\theta_p^{k+1} - \theta_p^k}{\tau} + \Delta \left(\frac{\theta_q^{k+1} + \theta_q^k}{2} \right) &= -\frac{\rho_p^{k+1} - \rho_p^k}{\tau} - \Delta \left(\rho_q^{k+1/2} + \bar{T}_q^{k+1/2} \right) + \tilde{G}_1^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right) \\ &\quad + r(t^{k+1/2}) e_{g,1}^{k+1/2} - T_p^{k+1/2}, \\ \frac{\theta_q^{k+1} - \theta_q^k}{\tau} - \Delta \left(\frac{\theta_p^{k+1} + \theta_p^k}{2} \right) &= -\frac{\rho_q^{k+1} - \rho_q^k}{\tau} + \Delta \left(\rho_p^{k+1/2} + \bar{T}_p^{k+1/2} \right) - \tilde{G}_2^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right) \\ &\quad - r(t^{k+1/2}) e_{g,2}^{k+1/2} - T_q^{k+1/2}, \\ \frac{e_r^{k+1} - e_r^k}{\tau} + T_r^{k+1/2} &= \frac{1}{2} \left[\left(\tilde{G}_1^{k+1/2}, \frac{e_q^{k+1} - e_q^k}{\tau} + T_q^{k+1/2} \right) + \left(e_{g,1}^{k+1/2}, \partial_t q(t^{k+1/2}) \right) \right. \\ &\quad \left. + \left(\tilde{G}_2^{k+1/2}, \frac{e_p^{k+1} - e_p^k}{\tau} + T_p^{k+1/2} \right) + \left(e_{g,2}^{k+1/2}, \partial_t p(t^{k+1/2}) \right) \right]. \end{cases} \quad (5.8)$$

Step 2. Error estimate formula. We use the following notations to make the results more compact

$$D_\tau^1 \theta_p^{k+1} = \frac{\theta_p^{k+1} - \theta_p^k}{\tau}, \quad D^1 \theta_p^{k+1} = \theta_p^{k+1} - \theta_p^k.$$

Taking the inner product of the first equation of the system (5.8) with $-D^1 \theta_q^{k+1}$ and the second with $D^1 \theta_p^{k+1}$, and summing the results, we also have,

$$\begin{aligned} \frac{1}{2} D^1 \left\| \nabla \theta_q^{k+1} \right\|_0^2 + \frac{1}{2} D^1 \left\| \nabla \theta_p^{k+1} \right\|_0^2 &= \left(D_\tau^1 \rho_p^{k+1}, D^1 \theta_q^{k+1} \right) - \left(D_\tau^1 \rho_q^{k+1}, D^1 \theta_p^{k+1} \right) \\ &\quad - \left(\nabla \rho_q^{k+1/2}, \nabla D^1 \theta_q^{k+1} \right) - \left(\nabla \rho_p^{k+1/2}, \nabla D^1 \theta_p^{k+1} \right) \\ &\quad - \left(\nabla \bar{T}_q^{k+1/2}, \nabla D^1 \theta_q^{k+1} \right) - \left(\nabla \bar{T}_p^{k+1/2}, \nabla D^1 \theta_p^{k+1} \right) \\ &\quad - \left(\tilde{G}_1^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right), D^1 \theta_q^{k+1} \right) \\ &\quad - \left(\tilde{G}_2^{k+1/2} \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2} \right), D^1 \theta_p^{k+1} \right) \\ &\quad - \left(r(t^{k+1/2}) e_{g,1}^{k+1/2} - T_p^{k+1/2}, D^1 \theta_q^{k+1} \right) \\ &\quad - \left(r(t^{k+1/2}) e_{g,2}^{k+1/2} + T_p^{k+1/2}, D^1 \theta_p^{k+1} \right). \end{aligned} \quad (5.9)$$

Multiplying the third equation of (5.8) by $2\tau e_r^{k+1/2}$, we have

$$\begin{aligned}
D^1 \left| e_r^{k+1} \right|^2 + 2\tau T_r^{k+1/2} e_r^{k+1/2} - \tau e_r^{k+1/2} & \left[\left(\tilde{G}_1^{k+1/2}, D_\tau^1 \rho_q^{k+1} + T_q^{k+1/2} \right) \right. \\
& + \left(\tilde{G}_2^{k+1/2}, D_\tau^1 \rho_p^{k+1} + T_p^{k+1/2} \right) + \left(e_{g,1}^{k+1/2}, \partial_t q(t^{k+1/2}) \right) + \left(e_{g,2}^{k+1/2}, \partial_t p(t^{k+1/2}) \right) \left. \right] \\
& = e_r^{k+1/2} \left[\left(\tilde{G}_1^{k+1/2}, D^1 \theta_q^{k+1} \right) + \left(\tilde{G}_2^{k+1/2}, D^1 \theta_p^{k+1} \right) \right]. \tag{5.10}
\end{aligned}$$

Using (5.10) in (5.9), we have

$$\begin{aligned}
& \frac{1}{2} D^1 \left\| \nabla \theta_q^{k+1} \right\|_0^2 + \frac{1}{2} D^1 \left\| \nabla \theta_p^{k+1} \right\|_0^2 + D^1 \left| e_r^{k+1} \right|^2 \\
& = \left(D_\tau^1 \rho_p^{k+1}, D^1 \theta_q^{k+1} \right) - \left(D_\tau^1 \rho_q^{k+1}, D^1 \theta_p^{k+1} \right) \\
& - \left(\nabla \left(\rho_q^{k+1/2} + \bar{T}_q^{k+1/2} \right), \nabla D^1 \theta_q^{k+1} \right) - \left(\nabla \left(\rho_p^{k+1/2} + \bar{T}_p^{k+1/2} \right), \nabla D^1 \theta_p^{k+1} \right) \\
& - \bar{T}_r^{k+1/2} \left[\left(\tilde{G}_1^{k+1/2}, D^1 \theta_q^{k+1} \right) + \left(\tilde{G}_2^{k+1/2}, D^1 \theta_p^{k+1} \right) \right] \\
& - 2\tau T_r^{k+1/2} e_r^{k+1/2} + \tau e_r^{k+1/2} \left[\left(\tilde{G}_1^{k+1/2}, D_\tau^1 \rho_q^{k+1} + T_q^{k+1/2} \right) \right. \\
& + \left(\tilde{G}_2^{k+1/2}, D_\tau^1 \rho_p^{k+1} + T_p^{k+1/2} \right) + \left(e_{g,1}^{k+1/2}, \partial_t q(t^{k+1/2}) \right) + \left(e_{g,2}^{k+1/2}, \partial_t p(t^{k+1/2}) \right) \left. \right] \\
& - \left(r(t^{k+1/2}) e_{g,1}^{k+1/2} - T_p^{k+1/2}, D^1 \theta_q^{k+1} \right) \\
& - \left(r(t^{k+1/2}) e_{g,2}^{k+1/2} + T_p^{k+1/2}, D^1 \theta_p^{k+1} \right). \tag{5.11}
\end{aligned}$$

Step 3. Inequalities for the terms on the right-hand side of (5.11).

Now, we bound the right-hand side of (5.11). Using Lemma 1, Lemma 10 and Young's inequality we have

$$\begin{aligned}
\left(D_\tau^1 \rho_p^{k+1}, D^1 \theta_q^{k+1} \right) & \leq 4 \left\| D_\tau^1 \rho_p^{k+1} \right\|_0^2 + \frac{1}{16} \left\| D^1 \theta_q^{k+1} \right\|_0^2 \leq CN^{-6} + \frac{1}{16} \left\| D^1 \theta_q^{k+1} \right\|_0^2, \\
- \left(D_\tau^1 \rho_q^{k+1}, D^1 \theta_p^{k+1} \right) & \leq 4 \left\| D_\tau^1 \rho_q^{k+1} \right\|_0^2 + \frac{1}{16} \left\| D^1 \theta_p^{k+1} \right\|_0^2 \leq CN^{-6} + \frac{1}{16} \left\| D^1 \theta_p^{k+1} \right\|_0^2.
\end{aligned}$$

Then, from Theorem (3), we have

$$\begin{aligned}
& - \left(\nabla \rho_q^{k+1/2}, \nabla D^1 \theta_q^{k+1} \right) - \left(\nabla \rho_p^{k+1/2}, \nabla D^1 \theta_p^{k+1} \right) \\
& \leq \left(\left\| \nabla \rho_q^{k+1/2} \right\|_0^2 \left\| \nabla D^1 \theta_q^{k+1} \right\|_0^2 + \left\| \nabla \rho_p^{k+1/2} \right\|_0^2 \left\| \nabla D^1 \theta_p^{k+1} \right\|_0^2 \right) \\
& \leq CN^{-4},
\end{aligned}$$

and

$$\begin{aligned}
& - \left(\nabla \bar{T}_q^{k+1/2}, \nabla D^1 \theta_q^{k+1} \right) - \left(\nabla \bar{T}_p^{k+1/2}, \nabla D^1 \theta_p^{k+1} \right) \\
& \leq \left(\left\| \nabla \bar{T}_q^{k+1/2} \right\|_0^2 \left\| \nabla D^1 \theta_q^{k+1} \right\|_0^2 + \left\| \nabla \bar{T}_p^{k+1/2} \right\|_0^2 \left\| \nabla D^1 \theta_p^{k+1} \right\|_0^2 \right) \\
& \leq C\tau^4,
\end{aligned}$$

For the rest of the terms on the right-hand side of (5.11), we use Lemma 10, and Proposition 5 together with Lemma 8, and Remark 9, to obtain

$$\begin{aligned}
& -\overline{T}_r^{k+1/2} \left[\left(\tilde{G}_1^{k+1/2}, D^1 \theta_q^{k+1} \right) + \left(\tilde{G}_2^{k+1/2}, D^1 \theta_p^{k+1} \right) \right] \\
& \leq 4 \left| \overline{T}_r^{k+1/2} \right|^2 \left(\left\| \tilde{G}_1^{k+1/2} \right\|_0^2 + \left\| \tilde{G}_1^{k+1/2} \right\|_0^2 \right) + \frac{1}{16} \left(\left\| D^1 \theta_q^{k+1} \right\|_0^2 + \left\| D^1 \theta_p^{k+1} \right\|_0^2 \right) \\
& \leq C\tau^4 + \frac{1}{16} \left(\left\| D^1 \theta_q^{k+1} \right\|_0^2 + \left\| D^1 \theta_p^{k+1} \right\|_0^2 \right),
\end{aligned} \tag{5.12}$$

$$-2\tau T_r^{k+1/2} e_r^{k+1/2} \leq C\tau \left(\left\| T_r^{k+1/2} \right\|_0^2 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right) \leq C\tau^5 + \tau \left| e_r^{k+1} \right|^2 + \tau \left| e_r^k \right|^2,$$

$$\begin{aligned}
& \tau e_r^{k+1/2} \left(\tilde{G}_1^{k+1/2}, D_\tau^1 \rho_q^{k+1} + T_q^{k+1/2} \right) \\
& \leq \frac{\tau}{2} \left\| \tilde{G}_1^{k+1/2} \right\|_0^2 \left(\left\| D_\tau^1 \rho_q^{k+1} \right\|_0^2 + \left\| T_q^{k+1/2} \right\|_0^2 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right) \\
& \leq C\tau \left(N^{-6} + \tau^4 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right),
\end{aligned}$$

$$\begin{aligned}
& \tau e_r^{k+1/2} \left(\tilde{G}_2^{k+1/2}, D_\tau^1 \rho_p^{k+1} + T_p^{k+1/2} \right) \\
& \leq \frac{\tau}{2} \left\| \tilde{G}_2^{k+1/2} \right\|_0^2 \left(\left\| D_\tau^1 \rho_p^{k+1} \right\|_0^2 + \left\| T_p^{k+1/2} \right\|_0^2 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right) \\
& \leq C\tau \left(N^{-6} + \tau^4 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right),
\end{aligned}$$

$$\begin{aligned}
& \tau e_r^{k+1/2} \left[\left(e_{g,1}^{k+1/2}, \partial_t q(t^{k+1/2}) \right) + \left(e_{g,2}^{k+1/2}, \partial_t p(t^{k+1/2}) \right) \right] \\
& \leq \frac{\tau}{2} \left\| \partial_t q(t^{k+1/2}) \right\|_0^2 \left(\left\| e_{g,1}^{k+1/2} \right\|_0^2 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right) \\
& \quad + \frac{\tau}{2} \left\| \partial_t p(t^{k+1/2}) \right\|_0^2 \left(\left\| e_{g,2}^{k+1/2} \right\|_0^2 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right) \\
& \leq C\tau \left(\left\| e_{g,1}^{k+1/2} \right\|_0^2 + \left\| e_{g,2}^{k+1/2} \right\|_0^2 + \left| e_r^{k+1} \right|^2 + \left| e_r^k \right|^2 \right),
\end{aligned}$$

and

$$\begin{aligned}
& - \left(r(t^{k+1/2}) e_{g,1}^{k+1/2} - T_p^{k+1/2}, D^1 \theta_q^{k+1} \right) - \left(r(t^{k+1/2}) e_{g,2}^{k+1/2} + T_p^{k+1/2}, D^1 \theta_p^{k+1} \right) \\
& \leq 4 \left| r(t^{k+1/2}) \right|^2 \left(\left\| e_{g,1}^{k+1/2} \right\|_0^2 + \left\| e_{g,2}^{k+1/2} \right\|_0^2 + \left\| T_p^{k+1/2} \right\|_0^2 + \left\| T_q^{k+1/2} \right\|_0^2 \right) \\
& \quad + \frac{1}{16} \left(\left\| D^1 \theta_q^{k+1} \right\|_0^2 + \left\| D^1 \theta_p^{k+1} \right\|_0^2 \right) \\
& \leq C \left(\left\| e_{g,1}^{k+1/2} \right\|_0^2 + \left\| e_{g,2}^{k+1/2} \right\|_0^2 + 2\tau^4 \right) + \frac{1}{16} \left(\left\| D^1 \theta_q^{k+1} \right\|_0^2 + \left\| D^1 \theta_p^{k+1} \right\|_0^2 \right).
\end{aligned} \tag{5.13}$$

Step 4. Estimating the terms in the inequalities (5.12)–(5.13). First, we aim to eliminate the terms $\|D^1\theta_p^{k+1}\|_0^2$ and $\|D^1\theta_q^{k+1}\|_0^2$ in the above inequalities. Taking the inner product of the first equation of (5.8) with $2\tau\theta_p^{k+1}$, we obtain

$$\begin{aligned} \left(D_\tau^1\theta_p^{k+1}, 2\tau\theta_p^{k+1}\right) &= 2\tau \left(\nabla\theta_q^{k+1/2}, \nabla\theta_p^{k+1}\right) - 2\tau \left(D_\tau^1\rho_p^{k+1}, \theta_p^{k+1}\right) + 2\tau \left(\nabla\left(\rho_q^{k+1/2} + \bar{T}_q^{k+1/2}\right), \nabla\theta_p^{k+1}\right) \\ &\quad + 2\tau \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2}\right) \left(\tilde{G}_1^{k+1/2}, \theta_p^{k+1}\right) + 2\tau \left(r(t^{k+1/2})e_{g,1}^{k+1/2} - T_p^{k+1/2}, \theta_p^{k+1}\right). \end{aligned}$$

Knowing that

$$\left(D_\tau^1\theta_p^{k+1}, 2\tau\theta_p^{k+1}\right) \geq \|D^1\theta_p^{k+1}\|_0^2,$$

we have

$$\begin{aligned} \|D^1\theta_p^{k+1}\|_0^2 &\leq 2\tau \left(\nabla\theta_q^{k+1/2}, \nabla\theta_p^{k+1}\right) - 2\tau \left(D_\tau^1\rho_p^{k+1}, \theta_p^{k+1}\right) + 2\tau \left(\nabla\left(\rho_q^{k+1/2} + \bar{T}_q^{k+1/2}\right), \nabla\theta_p^{k+1}\right) \\ &\quad + 2\tau \left(e_r^{k+1/2} + \bar{T}_r^{k+1/2}\right) \left(\tilde{G}_1^{k+1/2}, \theta_p^{k+1}\right) + 2\tau \left(r(t^{k+1/2})e_{g,1}^{k+1/2} - T_p^{k+1/2}, \theta_p^{k+1}\right). \end{aligned} \quad (5.14)$$

Let us bound the terms on the right-hand side of (5.14). Using Lemma 1 we find that

$$\begin{aligned} 2\tau \left(\nabla\theta_q^{k+1/2}, \nabla\theta_p^{k+1}\right) &\leq \tau \left(\|\nabla\theta_q^{k+1}\|_0^2 + \|\nabla\theta_q^k\|_0^2 + \|\nabla\theta_p^{k+1}\|_0^2\right), \\ -2\tau \left(D_\tau^1\rho_p^{k+1}, \theta_p^{k+1}\right) &\leq \tau \left(\|D_\tau^1\rho_p^{k+1}\|_{H^{-1}(\Omega)}^2 + \|\nabla\theta_p^{k+1}\|_0^2\right) \leq \tau \left(N^{-6} + \|\nabla\theta_p^{k+1}\|_0^2\right), \\ 2\tau \left(\nabla\left(\rho_q^{k+1/2} + \bar{T}_q^{k+1/2}\right), \nabla\theta_p^{k+1}\right) &\leq \tau \left(CN^{-4} + C\tau^4 + \|\nabla\theta_p^{k+1}\|_0^2\right), \\ 2\tau \left(r(t^{k+1/2})e_{g,1}^{k+1/2} - T_p^{k+1/2}, \theta_p^{k+1}\right) &\leq \tau \left(C\|e_{g,1}^{k+1/2}\|_0^2 + \tau^4 + C\|\nabla\theta_p^{k+1}\|_0^2\right), \end{aligned}$$

where we have used the Poincaré inequality to obtain the last inequality. Plugging the previous inequalities into (5.14), we obtain

$$\|D^1\theta_p^{k+1}\|_0^2 \leq \tau \left(\|\nabla\theta_q^{k+1}\|_0^2 + \|\nabla\theta_q^k\|_0^2 + CN^{-4} + C\tau^4 + C\|e_{g,1}^{k+1/2}\|_0^2 + C\|\nabla\theta_p^{k+1}\|_0^2\right). \quad (5.15)$$

Similarly, taking the inner product of the second equation of (5.8) with $2\tau\theta_q^{k+1}$ and repeating the same steps as before, we obtain

$$\|D^1\theta_q^{k+1}\|_0^2 \leq \tau \left(\|\nabla\theta_p^{k+1}\|_0^2 + \|\nabla\theta_p^k\|_0^2 + CN^{-4} + C\tau^4 + C\|e_{g,2}^{k+1/2}\|_0^2 + C\|\nabla\theta_q^{k+1}\|_0^2\right). \quad (5.16)$$

Step 5. Estimating $\|e_{g,1}^{k+1/2}\|_0^2$ and $\|e_{g,2}^{k+1/2}\|_0^2$. Using the notations

$$S(p, q) = \sqrt{\mathcal{E}_1(p, q) + C},$$

and

$$N_1(p, q) = \frac{\delta}{\delta q}\mathcal{E}_1(p, q), \quad N_2(p, q) = \frac{\delta}{\delta p}\mathcal{E}_1(p, q)$$

we have that

$$\begin{aligned}
e_{g,1}^{k+1/2} &= G_1(P^{k+1/2}, Q^{k+1/2}) - g_1(p(t^{k+1/2}), q(t^{k+1/2})) \\
&= \frac{N_1(P^{k+1/2}, Q^{k+1/2})}{S(P^{k+1/2}, Q^{k+1/2})} - \frac{N_1(p(t^{k+1/2}), q(t^{k+1/2}))}{S(p(t^{k+1/2}), q(t^{k+1/2}))} \\
&= \frac{N_1(P^{k+1/2}, Q^{k+1/2})}{S(P^{k+1/2}, Q^{k+1/2})} - \frac{N_1(P^{k+1/2}, Q^{k+1/2})}{S(p(t^{k+1/2}), q(t^{k+1/2}))} + \frac{N_1(P^{k+1/2}, Q^{k+1/2})}{S(p(t^{k+1/2}), q(t^{k+1/2}))} \\
&\quad - \frac{N_1(p(t^{k+1/2}), q(t^{k+1/2}))}{S(p(t^{k+1/2}), q(t^{k+1/2}))} \\
&= \frac{N_1(P^{k+1/2}, Q^{k+1/2}) [\mathcal{E}_1(p(t^{k+1/2}), q(t^{k+1/2})) - \mathcal{E}_1(P^{k+1/2}, Q^{k+1/2})]}{S(P^{k+1/2}, Q^{k+1/2})S(p(t^{k+1/2}), q(t^{k+1/2})) [S(P^{k+1/2}, Q^{k+1/2}) + S(p(t^{k+1/2}), q(t^{k+1/2}))]} \\
&\quad + \frac{N_1(P^{k+1/2}, Q^{k+1/2}) - N_1(p(t^{k+1/2}), q(t^{k+1/2}))}{S(p(t^{k+1/2}), q(t^{k+1/2}))}.
\end{aligned}$$

From the smoothness assumption (5.2) and Lemma 8, we have

$$\|e_{g,1}^{k+1/2}\|_0^2 \leq C \left[\|P^{k+1/2} - p(t^{k+1/2})\|_0^2 + \|Q^{k+1/2} - q(t^{k+1/2})\|_0^2 \right].$$

Then, using the notation (5.1) and Lemma 10, we obtain

$$\begin{aligned}
\|e_{g,1}^{k+1/2}\|_0^2 &\leq C \left[\|\theta_p^{k+1}\|_0^2 + \|\theta_p^k\|_0^2 + \|\theta_q^{k+1}\|_0^2 + \|\theta_q^k\|_0^2 + \tau^3 + N^{-4} \right] \\
&\leq C \left[\|\nabla\theta_p^{k+1}\|_0^2 + \|\nabla\theta_p^k\|_0^2 + \|\nabla\theta_q^{k+1}\|_0^2 + \|\nabla\theta_q^k\|_0^2 + \tau^3 + N^{-4} \right].
\end{aligned}$$

Similarly, we have

$$\|e_{g,2}^{k+1/2}\|_0^2 \leq C \left[\|\nabla\theta_q^{k+1}\|_0^2 + \|\nabla\theta_q^k\|_0^2 + \|\nabla\theta_p^{k+1}\|_0^2 + \|\nabla\theta_p^k\|_0^2 + \tau^3 + N^{-4} \right].$$

Step 6. Discrete Gronwall Lemma. The above two estimates together with (5.15) and (5.16) imply

$$\begin{aligned}
&\frac{1}{2}D^1 \|\nabla\theta_q^{k+1}\|_0^2 + \frac{1}{2}D^1 \|\nabla\theta_p^{k+1}\|_0^2 + D^1 |e_r^{k+1}|^2 \\
&\leq \tau C \left[\|\nabla\theta_p^{k+1}\|_0^2 + \|\nabla\theta_p^k\|_0^2 + \|\nabla\theta_q^{k+1}\|_0^2 + \|\nabla\theta_q^k\|_0^2 + |e_r^{k+1}|^2 + |e_r^k|^2 \right] + C [\tau^4 + N^{-4}].
\end{aligned}$$

Therefore, by the use of Gronwall's Lemma, we can conclude that

$$\frac{1}{2} \|\nabla\theta_q^{k+1}\|_0^2 + \frac{1}{2} \|\nabla\theta_p^{k+1}\|_0^2 + |e_r^{k+1}|^2 \leq C \exp \left([1 - C\tau]^{-1} t^{k+1} \right) (\tau^4 + N^{-4}).$$

□

6 Numerical experiments

In this section we numerically confirm our theoretical convergence result given in Theorem 11 and illustrate the long time energy conservation of the SAV method. Our numerical findings suggest the favorable energy preservation of the SAV method compared to classical splitting methods in certain applications such as for non-linearities with non-integer exponents which arise for instance in context of optical dark and power law solitons with surface plasmonic interactions [9]. For the comparison we use the classical first order Lie and second order Strang splitting which are known for their near energy preservation over long times, see, e.g., [10].

In the numerical examples we plot the deviation of the exact Hamiltonian and the modified Hamiltonian \tilde{H} , i.e., $e_{\tilde{H}} = |H(t^k) - \tilde{H}^k|$, the error between the exact Hamiltonian and the discrete non-modified Hamiltonian $e_H = |H(u(t^k)) - H(U^k)|$, as well as the L^2 error $e_u = \||U^k| - |u(t^k)|\|_{L^2(\Omega)}$. We choose the potential $V = 0$ in the Schrödinger equation (1.1).

6.1 First test case: cubic nonlinearity

In a first example we consider the nonlinear Schrödinger equation (1.1) with a cubic nonlinearity i.e.

$$f(|u|^2) = \beta |u|^2$$

on the spatial domain $\Omega = [-32, 32]$. In Figure 1 we choose a mesh size $h = 1/32$ and approximate the soliton solution [5, 2]

$$u(x, t) = \frac{a}{\sqrt{-\beta}} \operatorname{sech}(a(x - vt)) \exp(ivx - 0.5(v^2 - a^2)t),$$

with the parameters $a = 1$, $\beta = -1$ and $v = 1$ up to $T = 10$. Figure 1 numerically confirms the second-order convergence of the SAV method. The numerical findings also suggest that the error constant of the Strang splitting method is slightly better than the one of the SAV method in this example. In Figure 2 we simulate the solitary wave

$$u(t, x) = \frac{\sqrt{2}e^{it}}{\cosh(x)}$$

on the domain $[-\frac{\pi}{0.11}, \frac{\pi}{0.11}]$ with $N = 256$ collocation points and time step size $\tau = 0.01$. We illustrate the evolution of the errors e_H , e_u and $e_{\tilde{H}}$ over long times, i.e., up to $T = 1000$. Our numerical findings confirm the conservation of the modified Hamiltonian by the SAV method, see Figure 2. We also observe that the SAV method preserves well the exact energy and L^2 norm over long times. Even though, the error e_H of the Strang splitting seems favorable in this example, we have to stress that the modified Hamiltonian is closer to the value of the real Hamiltonian (see error $e_{\tilde{H}}$ on Figure 2).

6.2 Second test case: cubic nonlinearity with non-smooth initial condition

In this example we analyse the error behaviour of the SAV scheme in case of non-smooth initial data. For this purpose we solve the NLS equation with cubic nonlinearity with initial data of various regularity. More precisely, we choose $f(|u|^2) = \beta |u|^2$ with $\beta = 1$ and consider $u^0 \in H^\alpha$ with $\alpha =$

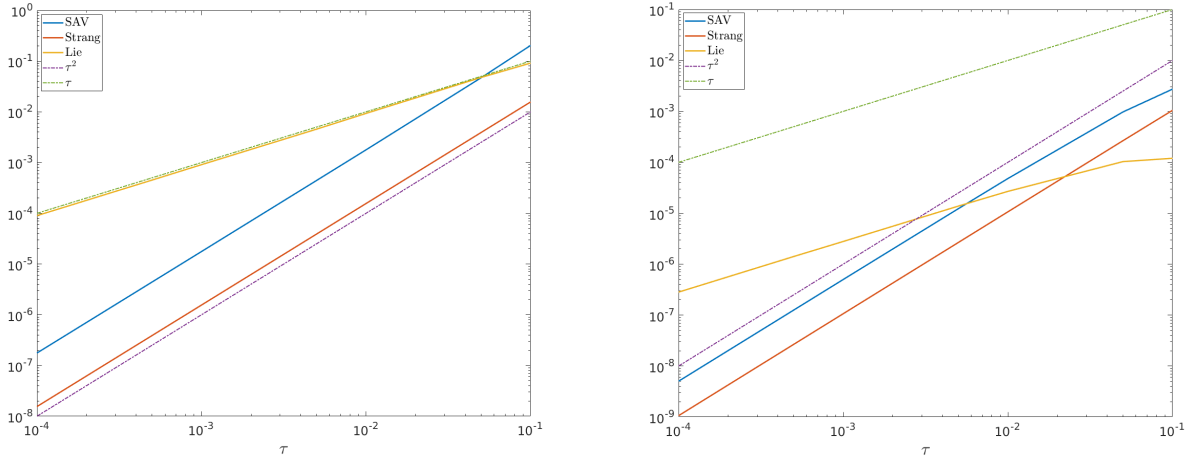


Figure 1: Error e_u (left) and e_H (right) versus step size τ at time $T = 10$.

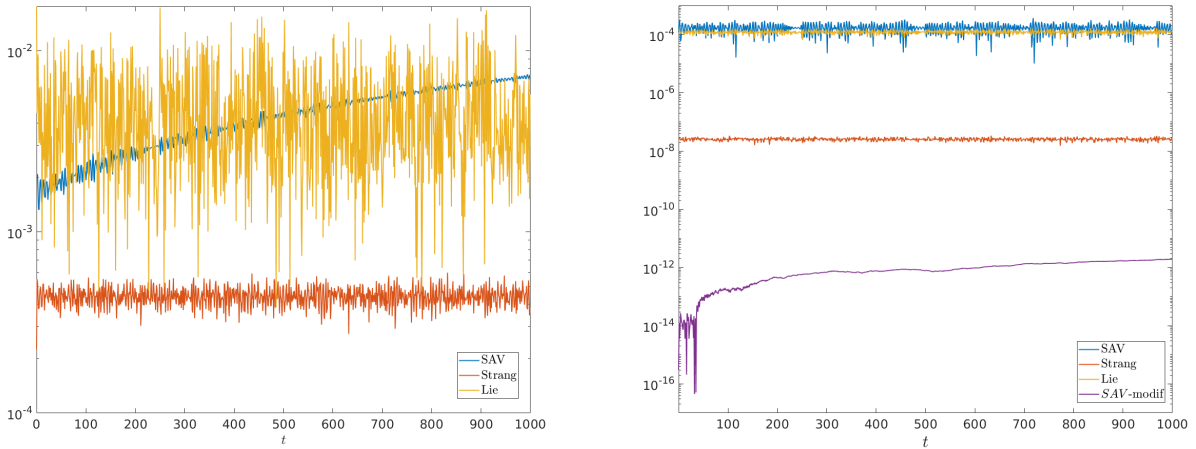


Figure 2: Left Figure: error e_u (left) through time. Right Figure: e_H (blue, red, yellow) and $e_{\tilde{H}}$ (purple) through time.

$3/2, 2, 3, 5$ on the spatial domain $\Omega = [-\pi, \pi]$ with $N = 1024$ gridpoints. The discrete initial data of various regularity is generated as proposed in [14].

Figure 3 shows the convergence behaviour of the SAV scheme, and the two splitting methods for the initial data of different regularity. We find that if $\alpha < 3$, the SAV method does not maintain its second order convergence rate and for $\alpha = 2$, the SAV scheme reduces to first order. Decreasing the regularity of the initial condition even more, the convergence worsens and becomes less than order 1. A similar order reduction is observed for the splitting schemes, however, for the latter the error starts to oscillate for $\alpha < 3$. Again, the error e_H is favorable for the Strang splitting for all α . However, the modified Hamiltonian is closer to the real Hamiltonian (see Figure 4 for $\alpha = \frac{2}{3}$).

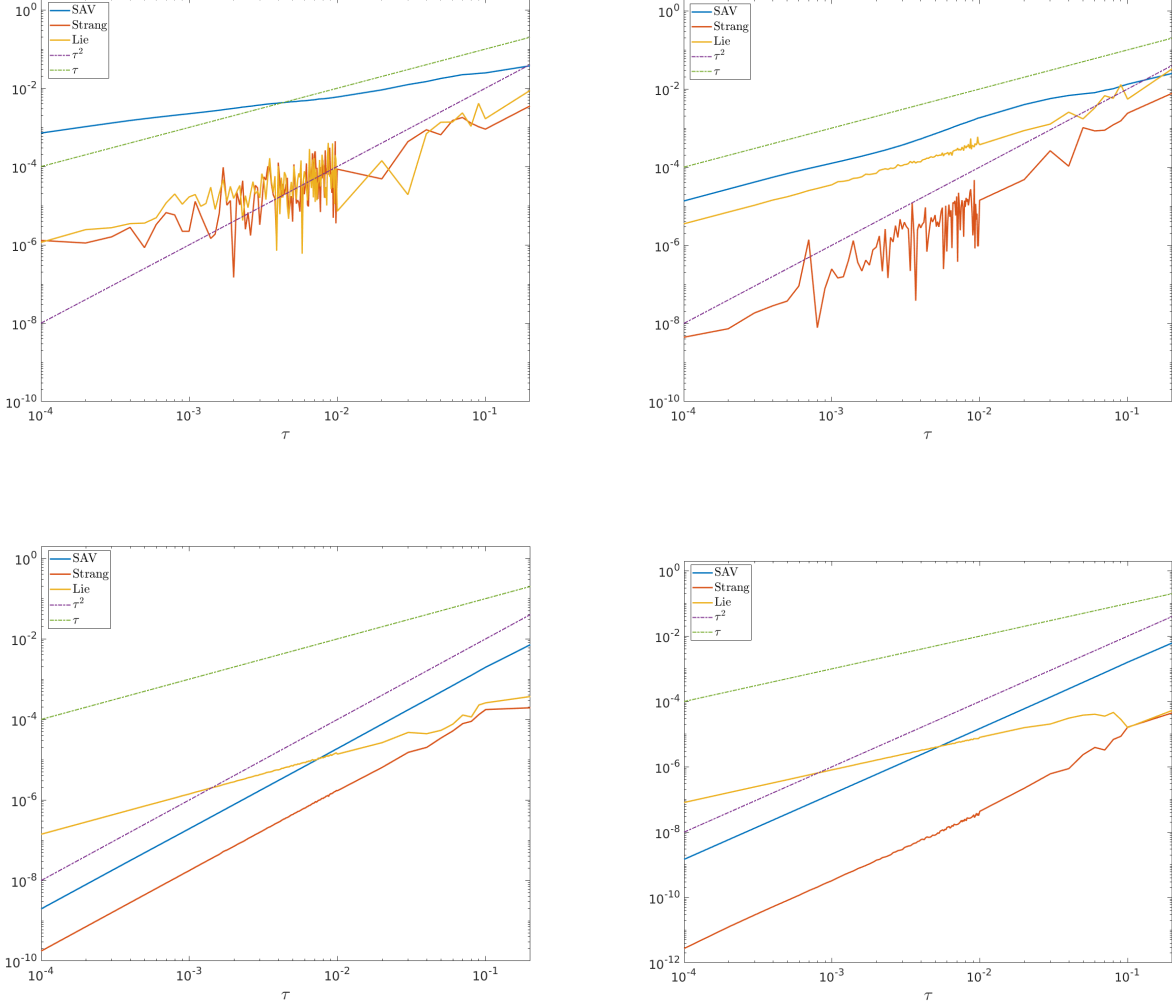


Figure 3: Error e_H versus step size τ for the nonlinear Schrödinger equation starting from different initial conditions in H^α ($\alpha = \frac{2}{3}$ top-left, $\alpha = 2$ top-right, $\alpha = 3$ bottom left and $\alpha = 5$ bottom-right). The dotted lines represent order τ (green) and τ^2 (purple), respectively.

6.3 Third test case: non-integer exponent

In this example we consider the periodic nonlinear Schrödinger equation (1.1) with nonlinearities with non-integer exponents ([9])

$$f(|u|^2) = \beta |u|^{4/\gamma}, \quad \gamma > 0$$

where the Hamiltonian takes the form

$$H(u) = \int_{\Omega} \frac{1}{2} |\nabla u|^2 + \beta \frac{\gamma}{(4 + 2\gamma)} |u|^{\frac{4}{\gamma} + 2} dx.$$

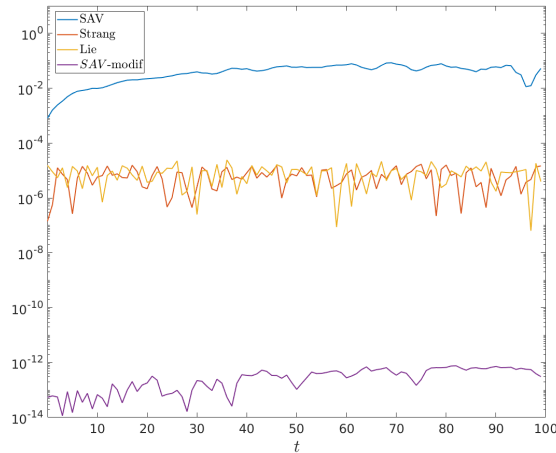


Figure 4: Error e_H (blue, red, yellow) through time and $e_{\bar{H}}$ (purple) through time for initial condition in $H^{\frac{2}{3}}$.

We carry out simulations for various exponents $\gamma = 2, 8/3, 4, 8$ up to time $T = 10$ with smooth initial value

$$u(0, x) = \sin(x) \in C^\infty([-\pi, \pi]).$$

The error e_H for different exponents γ is plotted in Figure 5. Our numerical findings suggest that as γ increases the splitting methods suffer from sever order reduction. This loss of convergence of splitting methods was also observed in [14]. The SAV method, on the other hand, retains its second order convergence for non-integer exponents.

References

- [1] R. A. ADAMS, *Sobolev spaces*, Academic Press, New York-London, 1975. Pure and Applied Mathematics, Vol. 65.
- [2] X. ANTOINE, J. SHEN, AND Q. TANG, *Scalar Auxiliary Variable/Lagrange multiplier based pseudospectral schemes for the dynamics of nonlinear Schrödinger/Gross-Pitaevskii equations*. preprint, Sept. 2020.
- [3] W. BAO, *The nonlinear Schrödinger equation and applications in Bose-Einstein condensation and plasma physics*, in Dynamics in models of coarsening, coagulation, condensation and quantization, vol. 9 of Lect. Notes Ser. Inst. Math. Sci. Natl. Univ. Singap., World Sci. Publ., Hackensack, NJ, 2007, pp. 141–239.
- [4] W. BAO, S. JIN, AND P. A. MARKOWICH, *On time-splitting spectral approximations for the Schrödinger equation in the semiclassical regime*, J. Comput. Phys., 175 (2002), pp. 487–524.
- [5] W. BAO, Q. TANG, AND Z. XU, *Numerical methods and comparison for computing dark and bright solitons in the nonlinear Schrödinger equation*, J. Comput. Phys., 235 (2013), pp. 423–445.

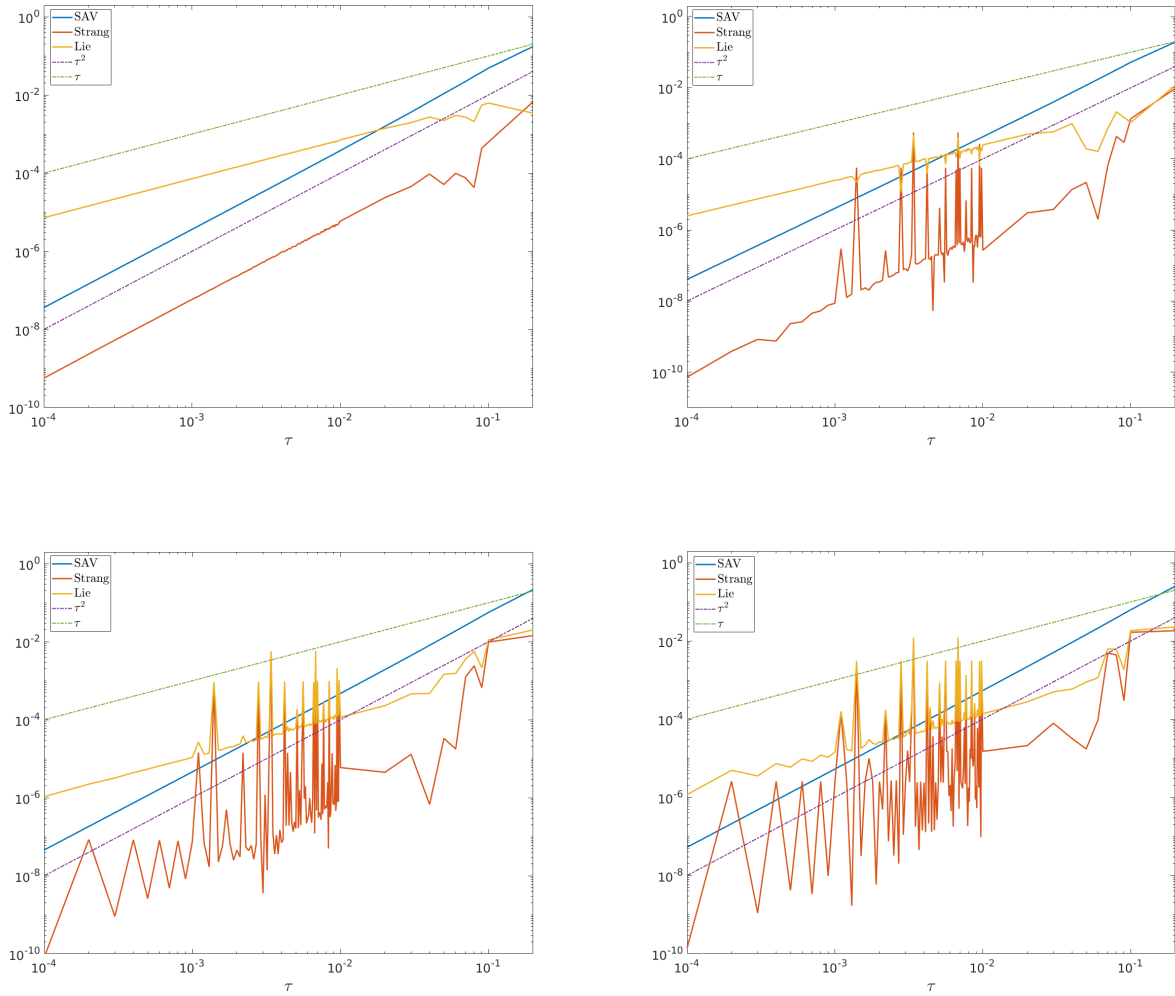


Figure 5: Error e_H versus step size τ for the nonlinear Schrödinger equation with different non-integer exponents ($\gamma = 2$ top-left, $\gamma = \frac{8}{3}$ top-right, $\gamma = 4$ bottom left and $\gamma = 8$ bottom-right). The dotted lines represent order τ (green) and τ^2 (purple), respectively.

- [6] C. BESSE, B. BIDÉGARAY, AND S. DESCOMBES, *Order estimates in time of splitting methods for the nonlinear Schrödinger equation*, SIAM J. Numer. Anal., 40 (2002), pp. 26–40.
- [7] W. CAI, C. JIANG, Y. WANG, AND Y. SONG, *Structure-preserving algorithms for the two-dimensional sine-Gordon equation with Neumann boundary conditions*, J. Comput. Phys., 395 (2019), pp. 166–185.
- [8] C. CANUTO, M. Y. HUSSAINI, A. QUARTERONI, AND T. A. ZANG, *Spectral methods*, Scientific Computation, Springer-Verlag, Berlin, 2006. Fundamentals in single domains.

- [9] S. H. CRUTCHER AND A. OSEI, *Derivation of the Effective Nonlinear Schrödinger Equations for Dark and Power Law Spatial Plasmon-Polariton Solitons Using Nano Self-Focusing*, Progress In Electromagnetics Research, 29 (2011), pp. 83–103. Publisher: EMW Publishing.
- [10] E. FAOU, *Geometric numerical integration and Schrödinger equations*, Zurich Lectures in Advanced Mathematics, European Mathematical Society (EMS), Zürich, 2012.
- [11] Y. FU, W. CAI, AND Y. WANG, *A structure-preserving algorithm for the fractional nonlinear Schrödinger equation based on the sav approach*, arXiv preprint arXiv:1911.07379, (2019).
- [12] G. H. GOLUB AND C. F. VAN LOAN, *Matrix computations*, Johns Hopkins Studies in the Mathematical Sciences, Johns Hopkins University Press, Baltimore, MD, fourth ed., 2013.
- [13] E. P. GROSS, *Structure of a quantized vortex in boson systems*, Il Nuovo Cimento (1955-1965), 20 (1961), pp. 454–477.
- [14] A. OSTERMANN AND K. SCHRATZ, *Low regularity exponential-type integrators for semilinear Schrödinger equations*, Found. Comput. Math., 18 (2018), pp. 731–755.
- [15] J. SHEN AND J. XU, *Convergence and error analysis for the scalar auxiliary variable (SAV) schemes to gradient flows*, SIAM J. Numer. Anal., 56 (2018), pp. 2895–2912.
- [16] J. SHEN, J. XU, AND J. YANG, *The scalar auxiliary variable (SAV) approach for gradient flows*, J. Comput. Phys., 353 (2018), pp. 407–416.
- [17] ———, *A new class of efficient and robust energy stable schemes for gradient flows*, SIAM Rev., 61 (2019), pp. 474–506.