DOI: 10.4208/aamm.09-m0929 October 2009

Symplectic Euler Method for Nonlinear High Order Schrödinger Equation with a Trapped Term

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Received 03 April 2009; Accepted (in revised version) 09 June 2009 Available online 30 July 2009

Abstract. In this paper, we establish a family of symplectic integrators for a class of high order Schrödinger equations with trapped terms. First, we find its symplectic structure and reduce it to a finite dimensional Hamilton system via spatial discretization. Then we apply the symplectic Euler method to the Hamiltonian system. It is demonstrated that the scheme not only preserves symplectic geometry structure of the original system, but also does not require to resolve coupled nonlinear algebraic equations which is different with the general implicit symplectic schemes. The linear stability of the symplectic Euler scheme and the errors of the numerical solutions are investigated. It shows that the semi-explicit scheme is conditionally stable, first order accurate in time and $2l^{th}$ order accuracy in space. Numerical tests suggest that the symplectic integrators are more effective than non-symplectic ones, such as backward Euler integrators.

AMS subject classifications: 65M06, 65M12, 65Z05, 70H15

Key words: Symplectic Euler integrator, high order Schrödinger equation, stability, trapped term.

1 Introduction

In this paper, we consider a class of high order nonlinear Schrödinger equation with a trapped term (HNSET)

$$iu_{t} + (-1)^{m} \frac{\partial^{2m} u}{\partial x^{2m}} + h'(|u|^{2})u + \beta g(x)u = 0,$$
(1.1)

together with the prescribed initial and periodic boundary conditions

$$u(x,0) = u_0(x),$$
 $x \in [0,L],$ (1.2)

$$\frac{\partial^s u(x,t)}{\partial x^s} = \frac{\partial^s u(x+L,t)}{\partial x^s}, \quad t \in [0,T], \quad s = 0,1,2,\cdots, m-1, \tag{1.3}$$

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where $i=\sqrt{-1}$, $m\in\mathbb{N}$, β is a given constant, $\hbar(|u|^2)$ is a bounded real differentiable function of $|u(x,t)|^2\in\mathbb{R}$, and g(x) is a real-valued bounded function with period L, $u_0(x)$ is a given complex-valued function. The trapped term g(x) is to position the solutions near x=0. The initial-boundary value problem (1.1)-(1.3) admits at least two conserved quantities:

(1) The charge is invariant

$$Q(t) = \int_0^L |u(x,t)|^2 dx = \int_0^L |u_0(x)|^2 dx = Q(0); \tag{1.4}$$

(2) The energy is conserved

$$\mathcal{E}(t) = \int_0^L \left(\left| \frac{\partial^m u(x,t)}{\partial x^m} \right|^2 + \hbar (|u(x,t)|^2) + \beta g(x) |u(x,t)|^2 \right) dx = \mathcal{E}(0). \tag{1.5}$$

Symplectic geometric integrators have been very popular for the Hamiltonian system since the method was proposed by Feng in [1–3]. It has been applied to many practical physics problems, such as quantum mechanics [4]. Eq. (1.1) can be reformulated into Hamiltonian system. In fact, let

$$u(x,t) = p(x,t) + iq(x,t),$$

where p(x,t), q(x,t) are real-valued functions, we have

$$\begin{cases}
 p_t = -\left((-1)^m \frac{\partial^{2m} q}{\partial x^{2m}} + \hbar'(p^2 + q^2)q + \beta g(x)q\right), \\
 q_t = (-1)^m \frac{\partial^{2m} p}{\partial x^{2m}} + \hbar'(p^2 + q^2)p + \beta g(x)p.
\end{cases} (1.6)$$

Suppose

$$z(x,t) = [p(x,t),q(x,t)]^{T}.$$

The infinite dimensional Hamiltonian system (1.6) can be written into the standard Hamiltonian system

$$\frac{d}{dt}z = J^{-1}Az, (1.7)$$

where

$$J^{-1} = \left[\begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right],$$

and

$$A = (-1)^m \begin{bmatrix} \triangle^{2m} & 0 \\ 0 & \triangle^{2m} \end{bmatrix} + \left(\frac{\partial}{\partial |u|^2} \hbar(|u|^2) + \beta g(x) \right) I_2,$$

with the identity matrix I_2 and the $2m^{th}$ order differential operator \triangle^{2m} . The Hamiltonian function is

$$H(p,q) = \frac{1}{2} \int_0^L \left[\left(\frac{\partial^m p}{\partial x^m} \right)^2 + \left(\frac{\partial^m q}{\partial x^m} \right)^2 + \hbar (p^2 + q^2) + \beta g(x) (p^2 + q^2) \right] dx.$$

The system is non-separable, and we can only devise completely implicit symplectic Runge-Kutta (SRK) for such kinds of Hamiltonian systems [2,5–7]. It needs to solve a coupled nonlinear algebraic system at every marching time step. To overcome the drawback and to absorb the advantages of symplectic integrator, we resort to the symplectic partitioned Runge-Kutta (SPRK) method in the work [2,4]. To the purposes, the spatial direction is firstly discretized to reduce the infinite dimensional Hamiltonian system to a finite one. The key point here is the discretization of $\partial^{2m}/\partial x^{2m}$.

The outline of the work is organized as follows: In Section 2, we devise a family of symplectic Euler scheme for HNLSET (1.1). Linear stability and error estimations for the schemes are investigated in Section 3. In Section 4, we present some numerical results. Some remarks will be made in the last section.

2 Construction of symplectic Euler scheme

We partition the spatial-temporal domain $[0, L] \times [0, T]$ with two families of parallel lines

$$x_j = jh(j = 0, 1, \dots, N),$$
 and $t^n = n\tau(n = 0, 1, \dots, M),$

where N, $M \in \mathbb{N}$ and h, τ are spatial and temporal mesh-step sizes, respectively. We let u_j^n to be an approximation of $u(x_j, t^n)$. To simplify the theoretical analysis, we employ the following notations:

$$(U^n, V^n) = h \sum_{j=0}^N u_j^n \overline{v_j^n}, \qquad \|U^n\| = \sqrt{(U^n, U^n)},$$

where $\overline{v_j^n}$ is the complex conjugate of v_j^n .

2.1 Spatial discretization

As mentioned above, the key point to convert an infinite-dimensional Hamiltonian system into a finite one, is the disretization of the differential operator $\partial^{2m}/\partial x^{2m}$. Here we use the discretization in [12]:

Second order accuracy difference quotient operator is given by

$$\Delta_2^{(2m)} v_j = \frac{\delta_x^{2m} v_j}{h^{2m}} = \frac{1}{h^{2m}} \left[\sum_{k=0}^{m-1} (-1)^k C_{2m}^k (v_{j-(m-k)} + v_{j+(m-k)}) + (-1)^m C_{2m}^m v_j \right]. \tag{2.1}$$

Fourth order accuracy difference quotient operator is given by

$$\Delta_4^{(2m)} v_j = \frac{\delta_x^{2m} v_j}{h^{2m}} + \beta_m \frac{\delta_x^{2(m+1)} v_j}{h^{2m}}, \tag{2.2}$$

where

$$\beta_m = \frac{2}{(2m+2)!} \Big[m^{2m+2} - C_{2m}^1 (m-1)^{2m+2} + C_{2m}^2 (m-2)^{2m+2} + \dots + (-1)^m C_{2m}^{m-1} \Big].$$

Table 1: The coefficients of $\Delta_2^{(2m)}v_i$.

m j	j – 2	j-1	j	j+1	j + 2
1		1	-2	1	
2	1	-4	6	-4	1

Table 2: The coefficients of $\Delta_4^{(2m)}v_i$.

m j	<i>j</i> – 3	<i>j</i> – 2	j-1	j	j+1	<i>j</i> + 2	j+3
1		-1/12	16/12	-30/12	16/12	-1/12	
2	-1/6	12/6	-39/6	56/6	-39/6	12/6	-1/6

We give some coefficients of $\Delta_2^{(2m)}v_j$ and $\Delta_4^{(2m)}v_j$ in Tables 1 and 2, respectively.

The matrices to $\Delta_{2l}^{(2m)}$, l=1,2, are denoted by \mathcal{B}_{2l}^{2m} . According to above tables, we conclude that \mathcal{B}_{2l}^{2m} are symmetric. Moreover, by Fourier analysis, their eigenvalues are

$$\lambda_{2l,k}^{2m} = \left\{ egin{array}{ll} \dfrac{(-1)^m}{h^{2m}} (4s_k^2)^m, & l = 1, \ \dfrac{(-1)^m}{h^{2m}} (1+4eta_m s_k^2) (4s_k^2)^m, & l = 2, \end{array}
ight.$$

where $s_k = \sin(k\pi/2N)$. Assume

$$P = [p_1, p_2, \cdots, p_N]^T, \qquad Q = [q_1, q_2, \cdots, q_N]^T,$$

we replace the partial derivative $\partial^{2m}/\partial x^{2m}$ by the $2l^{th}$ order accuracy difference quotient $\Delta_{2l}^{(2m)}$, l=1,2. Then it leads to a semi-discretization system

$$\frac{d}{dt} \begin{bmatrix} P \\ Q \end{bmatrix} = \begin{bmatrix} \mathbf{0} & -I_N \\ I_N & \mathbf{0} \end{bmatrix} \begin{bmatrix} M_{2l}(2m) & \mathbf{0} \\ \mathbf{0} & M_{2l}(2m) \end{bmatrix} \begin{bmatrix} P \\ Q \end{bmatrix}, \tag{2.3}$$

where I_N is the identity matrix, and

$$M_{2l}(2m) = (-1)^m \mathcal{B}_{2l}^{2m} + D.$$

Here

$$D = diag(h'(P^2 + Q^2) + \beta g(X)),$$

is a diagonal matrix with diagonal elements

$$D_{ij} = \hbar'(p_i^2 + q_i^2) + \beta g(x_i), \qquad j = 1, 2, \dots, N.$$

2.2 Time discretization

Applying the symplectic Euler scheme to the semi-discretization system (2.3), we obtain the full-discrete symplectic Euler scheme:

$$\frac{p_j^{n+1} - p_j^n}{\tau} + (-1)^m (\mathcal{B}_{2l}^{2m} Q^n)_j + \left[\hbar' \left((p_j^{n+1})^2 + (q_j^n)^2 \right) + \beta g(x_j) \right] q_j^n = 0, \tag{2.4}$$

$$\frac{q_j^{n+1} - q_j^n}{\tau} - (-1)^m (\mathcal{B}_{2l}^{2m} P^{n+1})_j - \left[\hbar' \left((p_j^{n+1})^2 + (q_j^n)^2 \right) + \beta g(x_j) \right] p_j^{n+1} = 0.$$
 (2.5)

From the expressions (2.4) and (2.5), it is observed that we can update p_j^{n+1} from p_j^n and q_j^n by (2.4) at the first step. In the step, we are only required to solve some uncoupled nonlinear algebraic system by iterative methods. That is, this step is explicit in nature. At the second step, we can update q_j^{n+1} from p_j^{n+1} and q_j^n by (2.5) which is completely explicit, and no iteration is desired. In a word, the symplectic Euler scheme (2.4)-(2.5) is explicit in essence. To illustrate the superiorities and efficiency of our scheme (2.4)-(2.5), we enumerate the backward Euler scheme for the semi-discrete Hamiltonian system (2.3) which reads

$$\frac{i}{\tau}(u_{j}^{n+1} - u_{j}^{n}) + (-1)^{m}(\mathcal{B}_{2l}^{2m}U^{n+1})_{j} + \hbar'(|u_{j}^{n+1}|^{2})u_{j}^{n+1} + \beta g(x_{j})u_{j}^{n+1} = 0.$$
 (2.6)

The scheme is completely implicit and is of first-order accuracy in time and $2l^{th}$ order in space which is just the same as symplectic Euler scheme (2.4)-(2.5).

2.3 Conservation laws of the symplectic Euler scheme

Theorem 1. The symplectic scheme (2.4)-(2.5) has the following implicit discrete invariant:

$$||P^{n+1}||^{2} + ||Q^{n+1}||^{2} - ||P^{n}||^{2} - ||Q^{n}||^{2} + (-1)^{m-1}\tau \left[(P^{n+1})^{T}\mathcal{B}_{2l}^{2m}Q^{n+1} - (P^{n})^{T}\mathcal{B}_{2l}^{2m}Q^{n} \right] - h\tau \sum_{j=1}^{N} \left[h'(|p_{j}^{n+1}|^{2} + |q_{j}^{n}|^{2}) + \beta g(x_{j}) \right] (p_{j}^{n+1}q_{j}^{n+1} - p_{j}^{n}q_{j}^{n}) = 0.$$

$$(2.7)$$

Proof: Computing inner product of (2.4) and (2.5) with $P^{n+1} + P^n$, $Q^{n+1} + Q^n$, respectively, then adding the two resulted equations up, we obtain the implicit invariant (2.7).

Remark 1. The discrete invariant (2.7) is an approximation of the charge conservation law (1.4).

3 Theoretical analysis

3.1 Error estimation

To estimate the error, we first show some notations:

$$\psi_i^n = \gamma_i^n + i\mu_i^n,$$

denote the exact solution at (x_i, t^n) , and

$$\gamma^n = [\gamma_1^n, \gamma_2^n, \cdots, \gamma_N^n]^T, \qquad \mu^n = [\mu_1^n, \mu_2^n, \cdots, \mu_N^n]^T.$$

The point-wise error of the scheme (2.4)-(2.5) is denoted by

$$E_j^n = \psi_j^n - u_j^n$$
, $e_j^n = \gamma_j^n - p_j^n$, $\varepsilon_j^n = \mu_j^n - q_j^n$.

and

$$||E^n||^2 = ||e^n||^2 + ||\epsilon^n||^2.$$

From the conservation laws (1.4), (1.5) and Theorem 1, we can assume that

$$\|\psi^n\|^2 \le \mathcal{Q}(u_0(x)), \qquad \|E^n\|^2 \le 4\mathcal{Q}(u_0(x)).$$
 (3.1)

By Taylor expansion, we can find the truncation error of symplectic Euler scheme (2.4)-(2.5) is

$$Tr = \frac{\gamma_{j}^{n+1} - \gamma_{j}^{n}}{\tau} + (-1)^{m} (\mathcal{B}_{2l}^{2m} \mu^{n})_{j} + \left[\hbar' \left((\gamma_{j}^{n+1})^{2} + (\mu_{j}^{n})^{2} \right) + \beta g(x_{j}) \right] \mu_{j}^{n}$$

$$= \mathcal{O}(\tau + h^{2l}), \qquad (3.2a)$$

$$Tm = \frac{\mu_{j}^{n+1} - \mu_{j}^{n}}{\tau} - (-1)^{m} (\mathcal{B}_{2l}^{2m} \gamma^{n+1})_{j} - \left[\hbar' \left((\gamma_{j}^{n+1})^{2} + (\mu_{j}^{n})^{2} \right) + \beta g(x_{j}) \right] \gamma_{j}^{n+1}$$

$$= \mathcal{O}(\tau + h^{2l}). \qquad (3.2b)$$

Lemma 1. (Gronwall's inequality) [13] *Suppose the mesh functions* $w^n(n=0,1,2,\cdots,M)$ *satisfy the relationship*

$$w^n - w^{n-1} \le A\tau w_n + B\tau w_{n-1} + \tau C_n,$$

where $M = T/\tau$, T is the length of time, A, B, C_n are non-negative constants. Then the sequence w^n satisfies

$$||w||_{\infty} \leq (w^0 + \tau \sum_{k=1}^{M} C_k)e^{2(A+B)T},$$

where τ is sufficiently small, such that

$$(A+B)\tau \le \frac{M-1}{2M}, \quad M > 1.$$

For convenience, *C* is a general constant in what follows, in other words, it can be different in different occurrences.

Theorem 2. There exists a positive constant C depending only on the initial value $u_0(x)$, such that the errors of the symplectic scheme (2.4)-(2.5) satisfy

$$||E^{n+1}||^2 \le (||E^0||^2 + \tau \mathcal{O}(\tau + h^{2l})^2) e^{4CT},$$
 (3.3)

where τ is sufficiently small such that

$$2CT \leq \frac{M-1}{2M}$$
.

Proof: Subtracting (2.4)-(2.5) from (3.2a) and (3.2b), respectively, gives

$$Tr = \frac{e_{j}^{n+1} - e_{j}^{n}}{\tau} + (-1)^{m} \left(\mathcal{B}_{2l}^{2m} \varepsilon^{n} \right)_{j} + \hbar' \left((\gamma_{j}^{n+1})^{2} + (\mu_{j}^{n})^{2} \right) \varepsilon_{j}^{n}$$

$$+ \left[\hbar' \left((\gamma_{j}^{n+1})^{2} + (\mu_{j}^{n})^{2} \right) - \hbar' \left((p_{j}^{n+1})^{2} + (q_{j}^{n})^{2} \right) \right] q_{j}^{n} + \beta g(x_{j}) \varepsilon_{j}^{n}, \quad (3.4)$$

$$Tm = \frac{\varepsilon_{j}^{n+1} - \varepsilon_{j}^{n}}{\tau} - (-1)^{m} \left(\mathcal{B}_{2l}^{2m} e^{n+1} \right)_{j} - \hbar' \left((\gamma_{j}^{n+1})^{2} + (\mu_{j}^{n})^{2} \right) e_{j}^{n+1}$$

$$- \left[\hbar' \left((\gamma_{j}^{n+1})^{2} + (\mu_{j}^{n})^{2} \right) - \hbar' \left((p_{j}^{n+1})^{2} + (q_{j}^{n})^{2} \right) \right] p_{j}^{n+1} - \beta g(x_{j}) e_{j}^{n+1}. \quad (3.5)$$

By the assumptions on $\hbar(|u|^2)$, g(x) and (3.1), there exists a constant C such that

$$\begin{split} & \left\| \left[\hbar' \left((\gamma^{n+1})^2 + (\mu^n)^2 \right) - \hbar' \left((P^{n+1})^2 + (Q^n)^2 \right) \right] Q^n \right\| \\ & \leq |\hbar''(\xi)| \left(\|\gamma^{n+1} + P^{n+1}\| \|e^{n+1}\| + \|\mu^n + Q^n\| \|\varepsilon^n\| \right) \\ & \leq \max |\hbar''(|u|^2)| \max(\|\gamma^{n+1} + P^{n+1}\|, \|\mu^n + Q^n\|) (\|e^{n+1}\| + \|\varepsilon^n\|) \\ & \leq C(\|e^{n+1}\| + \|\varepsilon^n\|). \end{split}$$

Computing inner product of (3.4),(3.5) by multiplying $(e^{n+1} + e^n)$ and $(\varepsilon^{n+1} + \varepsilon^n)$, respectively, and adding the two resulting equations up, yield

$$\begin{split} &\frac{1}{\tau} \left(\|e^{n+1}\|^2 + \|\varepsilon^{n+1}\|^2 - \|e^n\|^2 - \|\varepsilon^n\|^2 \right) \\ &\leq \frac{1}{2} \|Tr\|^2 + \frac{1}{2} \left(\|e^{n+1}\|^2 + \|e^n\|^2 \right) + \frac{1}{2} \|Tm\|^2 + \frac{1}{2} \left(\|\varepsilon^{n+1}\|^2 + \|\varepsilon^n\|^2 \right) \\ &+ \frac{1}{2} \|\mathcal{B}_{2l}^{2m}\|_{\infty} \left(\|e^{n+1}\|^2 + \|\varepsilon^{n+1}\|^2 + \|e^n\|^2 + \|\varepsilon^n\|^2 \right) \\ &+ \max_{j} \left| \hbar' \left((\gamma_j^{n+1})^2 + (\mu_j^n)^2 \right) \right| \left| (\varepsilon^n, e^{n+1} + e^n) + (e^{n+1}, \varepsilon^{n+1} + \varepsilon^n) \right| \\ &+ \left| \left(\left[\hbar' \left((\gamma^{n+1})^2 + (\mu^n)^2 \right) - \hbar' \left((P^{n+1})^2 + (Q^n)^2 \right) \right] Q^n, e^{n+1} + e^n \right) \right| \\ &+ \left| \left(\left[\hbar' \left((\gamma^{n+1})^2 + (\mu^n)^2 \right) - \hbar' \left((P^{n+1})^2 + (Q^n)^2 \right) \right] P^{n+1}, \varepsilon^{n+1} + \varepsilon^n \right) \right| \\ &+ \max_{j} \left| \beta g(x_j) \right| \left| (\varepsilon^n, e^{n+1} + e^n) + (e^{n+1}, \varepsilon^{n+1} + \varepsilon^n) \right| \end{split}$$

$$\leq \mathcal{O}(\tau + h^{2l})^2 + C(\|e^{n+1}\|^2 + \|\varepsilon^{n+1}\|^2 + \|e^n\|^2 + \|\varepsilon^n\|^2),$$

which leads to

$$||E^{n+1}||^2 - ||E^n||^2 \le \tau C(||E^{n+1}||^2 + ||E^n||^2) + \tau \mathcal{O}(\tau + h^{2l})^2.$$

By Gronwall's inequality, we arrive at the conclusion (3.3).

3.2 Linear stability analysis

In the subsection, we investigate the linear stability of the symplectic Euler scheme (2.4)-(2.5). To this end, we rewrite the scheme in the matrix form

$$\begin{bmatrix} I & \mathbf{0} \\ -\tau[(-1)^m \mathcal{B}_{2l}^{2m} + G] & I \end{bmatrix} \begin{bmatrix} P^{n+1} \\ Q^{n+1} \end{bmatrix} = \begin{bmatrix} I & -\tau[(-1)^m \mathcal{B}_{2l}^{2m} + G] \\ \mathbf{0} & I \end{bmatrix} \begin{bmatrix} P^n \\ Q^n \end{bmatrix}, \quad (3.6)$$

where *G* is a diagonal matrix with diagonal elements:

$$G_{ii} = \beta g(x_i), \qquad j = 1, 2, \cdots, N.$$

Let

$$M = (-1)^m \mathcal{B}_{21}^{2m} + G.$$

Then the amplification matrix of (3.6) is

$$F = \begin{bmatrix} I & \mathbf{0} \\ -\tau M & I \end{bmatrix}^{-1} \begin{bmatrix} I & -\tau M \\ \mathbf{0} & I \end{bmatrix} = \begin{bmatrix} I & -\tau M \\ \tau M & I - \tau^2 M^2 \end{bmatrix}.$$

We have to discuss the eigenvalues of F according to the specific expression of G. For simplicity, we consider the special case that $\beta g(x) \equiv 0$. Recalling the eigenvalues of \mathcal{B}_{2l}^{2m} , we can conclude that when l=1, the eigenvalues of F satisfy

$$\lambda^2 + \left[r^2 (4s_k^2)^{2m} - 2\right]\lambda + 1 = 0, (3.7)$$

where $r=\tau/h^{2m}$ represents the mesh ratio. For Eq. (3.7), we have

$$|\lambda| \le 1 \Leftrightarrow |r^2(4s_k^2)^{2m} - 2| \le 1 - (-1) = 2.$$
 (3.8)

Similarly, when l=2, the eigenvalues of F satisfy

$$|\lambda| \le 1 \Leftrightarrow |r^2(1 + 4\beta_m s_k^2)^2 (4s_k^2)^{2m} - 2| \le 1 - (-1) = 2.$$
(3.9)

Form (3.8) and (3.9), it is easy to obtain the following theorem.

Theorem 3. The necessary and sufficient condition for stability of the scheme (3.6) is

$$r \le 1/2^{2m-1} \ (l=1), \quad r \le 0.375 \ (m=1,l=2), \quad r \le 0.075 \ (m=2,l=2).$$

in the case of $\beta g(x) \equiv 0$. Other cases can be discussed with similar procedures as above.

4 Numerical experiments

In this section, we present some numerical results of the symplectic approximation for the HNLSET equation (1.1) in different cases, including linear problem and nonlinear problem with trapped terms. For convenience, we employ the following notations:

$$e_2 = h \sqrt{\sum_{j=0}^{N} |u_j^n - \psi_j^n|^2}, \qquad e_\infty = \max_j |u_j^n - \psi_j^n|.$$

4.1 Linear problem

First, we consider the linear problem

$$\begin{cases} iu_t + (-1)^m \frac{\partial^{2m}}{\partial x^{2m}} u = 0, \\ u(x,t) = u(x+2\pi,t), \\ u(x,0) = e^{-i\frac{\pi}{4}} \sin x. \end{cases}$$
(4.1)

The exact solution of the problem (4.1) reads

$$u(x,t) = e^{i(t-\frac{\pi}{4})}\sin x.$$

We check the linear stability of symplectic Euler scheme (2.4)-(2.5). The numerical errors with different mesh ratios are listed in Table 3. We find that the scheme is unstable and the solution blows up as the mesh ratio does not satisfy the stability condition of Theorem 3, which agrees with the theoretical analysis.

4.2 Nonlinear Schrödinger equation with a trapped term

Next, we study the following fourth-order Schrödinger equation with a *sine* trapped term

$$\begin{cases} iu_t + u_{xxxx} - 150(\sin^2 x)u + 6|u|^2 u = 0, \\ u(x,0) = 5e^{i\frac{\pi}{4}}\sin x, \\ u(x,t) = u(x+2\pi,t). \end{cases}$$
(4.2)

The problem (4.2) admits the exact solution

$$u(x,t) = 5e^{i(t+\frac{\pi}{4})}\sin x.$$

We fix τ =2 × 10⁻⁶ and take different spatial step sizes to investigate the behavior of the symplectic scheme (2.4)-(2.5). Moreover, it makes a comparison with the backward Euler method (2.6). The results presented in Table 4 show that the symplectic Euler scheme is more efficient than the backward Euler scheme (2.6). Under the same mesh partition, the symplectic Euler scheme (2.4)-(2.5) is more effective and more rapid than

m	τ	l	$r = \tau/h^{2m}$	e_2	e_{∞}
		1	0.4053	7.133×10^{-4}	1.436×10^{-3}
1	0.0005	1	0.6333	blow up	blow up
1	0.0025	2	0.2594	1.2620×10^{-3}	2.2725×10^{-3}
		2	0.3853	blow up	blow up
		1	0.0821	5.7386×10^{-3}	8.1690×10^{-3}
_	0.0000	1	0.2005	blow up	blow up
2 0.00005	2	0.0336	3.9375×10^{-5}	5.0133×10^{-5}	
		4	0.0821	blow up	blow up

Table 3: Stability of the scheme with different mesh ratios at t=2.

Table 4: The errors with different mesh grid divisions at t=1 and CPU (sec).

Scheme	1	h	e_2	e_{∞}	CPU
(2.4)(2.5)	1	$\pi/20$	1.4919×10^{-2}	2.1236×10^{-2}	80
		$\pi/40$	2.9091×10^{-3}	5.8579×10^{-3}	95
	2	$\pi/20$	5.6754×10^{-4}	8.1056×10^{-4}	83
		$\pi/40$	3.6017×10^{-4}	7.2782×10^{-4}	99
(2.6)	1	$\pi/20$	3.4867×10^{-1}	4.9596×10^{-1}	149
		$\pi/40$	2.4279×10^{-1}	4.8880×10^{-1}	422
	2	$\pi/20$	3.4145×10^{-1}	4.8592×10^{-1}	149
		$\pi/40$	2.4149×10^{-1}	4.8598×10^{-1}	390

the backward Euler method (2.6). Besides, we also present the exact and numerical solutions in Fig. 1. The residuals of charge and energy are presented in Fig. 2.

It is observed from Fig. 2 that the symplectic Euler scheme (2.4)-(2.5) can not conserve discrete charge and energy conservation exactly for nonlinear cases, however, their residuals are very small, especially for charge.

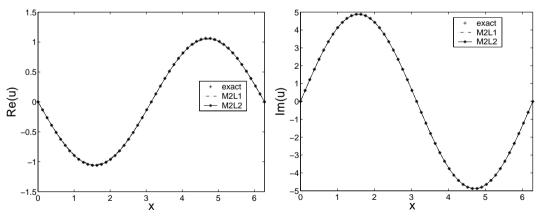


Figure 1: The exact and numerical solutions: Left for real part; Right for imaginary part.

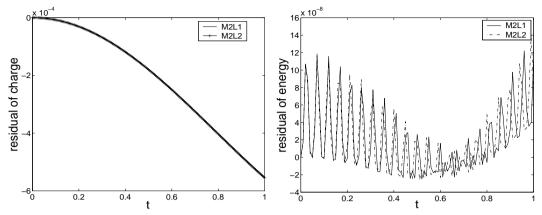


Figure 2: The residuals of charge and energy: Left for charge; Right for energy.

5 Summary

In this paper, we mainly develop a family of symplectic Euler schemes to simulate high order Schrödinger equation with trapped terms. The schemes are of first order in time and of $2l^{th}$ order in space. Moreover, the symplectic Euler scheme not only preserves symplectic geometry structure, but also is essentially explicit with some iteration. Therefore, this scheme speeds more quickly than the general implicit symplectic schemes and non-symplectic ones, such as backward Euler scheme. As a price, the scheme is conditionally stable. Numerical experiments demonstrate that the proposed schemes are efficient. The symplectic Euler scheme can not preserve the discrete charge or energy conservation exactly in general; however, their residual is very small. We can construct high order SPRK methods to improve its accuracy in time. We will investigate high order SPRK methods, such as multi-stage symplectic schemes, for HNLSET in future works.

Acknowledgement

This work is supported by the Provincial Natural Science Foundation of Jiangxi (No. 2008GQS0054), the Foundation of Department of Education Jiangxi province (No. GJJ09147), the Foundation of Jiangxi Normal University (Nos. 2057 and 2390), and State Key Laboratory of Scientific and Engineering Computing, CAS. This work is partially supported by the Provincial Natural Science Foundation of Anhui (No. 090416227).

References

[1] K. FENG, On difference schemes and symplectic geometry, In: Feng K., ed, Proceeding of the

- 1984 Beijing Symposium on Differential Geometry and Differential Equations, Computation of Partial Differential Equations, Science Press, Beijing (1985), pp. 42–58.
- [2] K. FENG AND M.Z. QIN, Symplectic geometric algorithms for Hamiltonian system, Sci. and Tech. Press of Zhejiang: Hangzhou (in Chinese), 2002.
- [3] E.HAIRER, C. LUBICH AND G. WANNER, Geometric Numerical Integration Structure-Preserving Algorithms for Ordinary Differential Equations, 2nd ed., Springer-Verlag. Berlin, 2006.
- [4] X. S. LIU, Y. Y. QI, J. F. HE AND P. Z. DING, Recent progress in symplectic algorithms for use in quantum systems, Commun. Comput. Phys., 2 (2007), pp. 1–53.
- [5] P.J. CHANNEL AND C. SCOVEL, Symplectic integration of Hamiltonian system, Nonlinearity, 3 (1990), pp. 231–259.
- [6] J.B. CHEN, M.Z. QIN AND Y.F. TANG, Symplectic and multi-symplectic methods for the non-linear Schrödinger equations, Comput. Math. with Appl., 43 (2002), pp. 1095–1106.
- [7] L.H. KONG, J.L. HONG AND R.X. LIU, Long-term numerical simulation of the interaction between a neutron field and a neutral meson field by a symplectic-preserving scheme, J. Phys. A: Math. Theor., 41 (2008) pp. 255207.
- [8] L.H. KONG, J.L. HONG, L. WANG AND F.F. Fu, Symplectic integrator for nonlinear high order Schrödinger equation with a trapped term, J. Comput. Appl. Math., in press.
- [9] J.L. HONG AND L.H. KONG, Novel multi-symplectic integrators for nonlinear fourth-order Schrödinger equation with trapped term, Commun. Comput. Phys., in press.
- [10] ISLAS AL AND SCHOBER CM, On the preservation of phase space structure under multisymplectic discretization, J. Comput. Phys., 197 (2004), pp. 585–609.
- [11] H.Y. CHAO, A difference scheme for a class of nonlinear Schrödinger equation, J. Comput. Math., 5 (1987), pp. 272–280.
- [12] W.P. ZENG, *Leap-frog schemes for Hamiltonian systems for higher-order Schrödinger equations*, Numer. Math. J. Chinese Univ., 17 (1995), pp. 305–317.
- [13] Y. L. Zhou, Application of discrete functional analysis to the finite difference method, International Academic Publishers, Hong Kong, 1990.