A conservative Fourier pseudospectral algorithm for the nonlinear Schrödinger equation*

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In this paper, we derive a new method for a nonlinear Schrödinger system by using the square of the first-order Fourier spectral differentiation matrix D_1 instead of the traditional second-order Fourier spectral differentiation matrix D_2 to approximate the second derivative. We prove that the proposed method preserves the charge and energy conservation laws exactly. A deduction argument is used to prove that the numerical solution is second-order convergent to the exact solutions in $\|\cdot\|_2$ norm. Some numerical results are reported to illustrate the efficiency of the new scheme in preserving the charge and energy conservation laws.

Keywords: Fourier pseudospectral method, Schrödinger equation, conservation law, convergence

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1. Introduction

The nonlinear Schrödinger equation (NLSE) describes a wide range of physical phenomena, such as hydrodynamics, plasma physics, nonlinear optics, self-focusing in laser pulses, propagation of heat pulses in crystals, description of the dynamics of Bose–Einstein condensate at extremely low temperatures.[1,2] It plays an essential role in mathematical and physical context, and more and more focus is concentrated upon its numerical solvers in recent years.[3,4] Fruitful results about the structure in the algorithm and theoretical analysis have been achieved for the Schrödinger system.[5–12]

The general form of the nonlinear Schrödinger equation with the initial value and the periodic boundary condition is

$$\begin{aligned} &\mathrm{i}\psi_t + \psi_{xx} + a|\psi|^2\psi = 0, \\ &\psi(x_\mathrm{L}, t) = \psi(x_\mathrm{R}, t), \end{aligned} \tag{1}$$

where a is a real parameter. Now using $\psi = p + \mathrm{i}q$, we can rewrite Eq. (1) as a pair of real-valued equations as follows:

$$\begin{aligned} &p_t + q_{xx} + a(p^2+q^2)q = 0, \\ &q_t - p_{xx} - a(p^2+q^2)p = 0. \end{aligned} \tag{2}$$

Equation (2) can be expressed in the Hamilton form

$$\frac{\mathrm{d}z}{\mathrm{d}t} = J\frac{\delta H(z)}{\delta z}, \tag{3}$$

where $z = (p,q) \in R^2$, and the Hamiltonian function, which is the system energy, is

$$H(z) = \int \frac{1}{2}(p_x^2 + q_x^2 - \frac{\alpha}{2}(p^2+q^2)^2)\,\mathrm{d}x, \tag{4}$$

and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The NLS system admits charge conservation law

$$Q(t) = \int_{x_\mathrm{L}}^{x_\mathrm{R}} |\psi|^2\,\mathrm{d}x = Q(0) \tag{5}$$

and the energy conservation law

$$\varepsilon(t) = \int_{x_\mathrm{L}}^{x_\mathrm{R}} \left[\frac{a}{4}|\psi|^4 - \frac{1}{2}|\psi_x|^2\right]\mathrm{d}x = \varepsilon(0). \tag{6}$$

The idea of space–time separation can transform the infinite-dimensional system into the finite-dimensional system, then by using the numerical scheme in the finite-dimensional Hamilton system, the fully discrete scheme can be obtained. The fascinating merit of spectral methods is the high accuracy, the so-called convergence of "infinite order". Even though the spectral methods have many advantages, they were not used widely for a long time. The main reason is the expensive cost of computational time. However, the discovery of the Fast Fourier Transformation (FFT), see Cooley and Turey,[13] removed this obstacle. With spatial discretization, spectral or pseudo-spectral methods not only improve the accuracy, but also preserve the geometric structure of the original partial differential equations (PDEs); besides this, they perform quite well in long-time integrations. In this paper, we derive a new method for a nonlinear Schrödinger system

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by using the square of first-order Fourier spectral differentiation matrix D_1 instead of the traditional second-order Fourier spectral differentiation matrix D_2 to approximate the second derivative for spatial discretization.[5]

The paper is organized as follows. In Section 2, a new scheme is proposed for the NLS system. We prove that the method conserves the charge and energy conservation laws simultaneously. In Section 3, a deduction argument is used to prove that the numerical solution is convergent to the exact solutions in $\|\cdot\|_2$ norm. Numerical experiments are reported in Section 4. Some conclusions are given in Section 5.

2. Construction of conservative algorithm for the Schrödinger equation

Let inner product and norm of $I=(0,2\pi)$, $L^2(I)$ respectively be $(\cdot,\cdot)$ and $\|\cdot\|$, for any real $r\geq 0$ and $1\leq q<+\infty$, we use $H^r(I):=W^{r,2}(I)$ to represent commonly defined Sobolev space, whose norm and semi-norm are respectively denoted by $\|\cdot\|_r$ and $|\cdot|_r$, $H_p^r(I)$ is a subspace composed by functions whose period is 2π on $H^r(I)$. Let equivalent norm and semi-norm respectively be

$$\|u\|_r=\left\{\sum_{l=-\infty}^{\infty}(1+|l|^2)^r|a_l|^2\right\}^{1/2},$$
$$|u|_r=\left\{\sum_{l=-\infty}^{\infty}|l|^{2r}|a_l|^2\right\}^{1/2},$$

where

$$u(x)=\sum_{l=-\infty}^{\infty}a_l\mathrm{e}^{\mathrm{i}lx},\quad a_l=\frac{1}{2\pi}\int_I u(x)\mathrm{e}^{-\mathrm{i}lx}\mathrm{d}x.$$

For even N, the approximation space of two $N/2$ order real trigonometric polynomial is defined by

$$V_N=\left\{u(x)=\sum_{|k|\leq N/2}\hat{u}_k\mathrm{e}^{\mathrm{i}kx}:\overline{\hat{u}_k}=\hat{u}_{-k},|k|\leq N/2\right\},$$
$$V_N''=\left\{u(x)=\sum_{|l|\leq N/2}{}''\hat{u}_l\mathrm{e}^{\mathrm{i}lx}:\overline{\hat{u}_l}=\hat{u}_{-l},|l|\leq N/2,\hat{u}_{N/2}=\hat{u}_{-N/2}\right\},$$

where $\sum''$ denotes that coefficient of the highest order term is divided by 2 when performing summation.

Let Fourier collocation points be

$$x_j=x_{\mathrm{L}}+jh,\quad j=0,1,2,\ldots,N-1,$$

where $h=2\pi/N$ and N is an even number.

We also need to define the inner product and p-norm $(1<p<\infty)$ of vectors as

$$(u,v)=\int_{2\pi}u\bar{v}\mathrm{d}x,$$

$$(u,v)_N=h\sum_{j=0}^{N\text{-}1}u(x_j)\overline{v(x_j)},$$
$$\|u\|_p=\left(h\sum_{j=0}^{N\text{-}1}u(x_j)\overline{v(x_j)}\right)^{1/p}.$$

We start our work with the pair of real-valued Eq. (2) by the periodic boundary conditions $p(0,t)=p(2\pi,t)$ and $q(0,t)=q(2\pi,t)$. We discrete the solution through trigonometric polynomial at collocation points and approximate $p(x,t)$, $q(x,t)$ by $I_Np(x,t)$, $I_Nq(x,t)$, respectively. As an example, we interpolate $p(x,t)$ at a series of collocation points x_j.

The approximation $I_Np(x,t)$ has the form

$$I_Np(x,t)=\sum_{j=0}^{N\text{-}1}p_jg_j(x)$$

with $p_j=p(x_j,t)$, $g_j(x_k)=\delta_j^k$. Here $g_j(x)$ is a trigonometric polynomial and is given explicitly by

$$g_j(x)=\frac{1}{N}\sum_{l=-N/2}^{N/2}\frac{1}{c_l}\mathrm{e}^{\mathrm{i}l\mu(x-x_j)},$$

where $c_l=1$ $(|l|\neq N/2)$, $c_{-N/2}=c_{N/2}=2$, $\mu=2\pi/2\pi$. Substituting it into the expression of $I_Np(x,t)$, we get

$$I_Np(x,t)=\sum_{l=-N/2}^{N/2}\frac{1}{c_l}\mathrm{e}^{\mathrm{i}l\mu x}\frac{1}{N}\sum_{j=0}^{N\text{-}1}p_j\mathrm{e}^{-\mathrm{i}l\mu x_j}.$$

Therefore

$$p_i=I_Np(x_i,t)=\sum_{l=-N/2}^{N/2}\frac{1}{c_l}\mathrm{e}^{\mathrm{i}l\mu x_i}\frac{1}{N}\sum_{j=0}^{N\text{-}1}p_j\mathrm{e}^{-\mathrm{i}l\mu x_j}.$$

The derivative $\partial I_Np(x,t)/\partial x$ at the collocation points x_i in terms of the values p_i is a key step, the resulting expression at the points x_i is

$$\frac{\partial I_Np(x_i,t)}{\partial x}=\sum_{j=0}^{N\text{-}1}p_j\frac{\mathrm{d}g_j(x_i)}{\mathrm{d}x}=(D_1\boldsymbol{p})_i,$$

where D_1 is an $N\times N$ matrix with elements given by

$$(D_1)_{i,j}=\frac{\mathrm{d}g_j(x_i)}{\mathrm{d}x}$$

and $\boldsymbol{p}=(p_0,\ldots,p_{N\text{-}1})^{\mathrm{T}}$.

In the same way, we can easily conclude that

$$\frac{\partial I_Nq(x_i,t)}{\partial x}=\sum_{j=0}^{N\text{-}1}q_j\frac{\mathrm{d}g_j(x_i)}{\mathrm{d}x}=(D_1\ \boldsymbol{q})_i.$$

From the above analysis, we can also obtain a Fourier spectral differentiation matrix D_2 for the second-order differential operator ∂_{xx}. For the ordinary differential equation $u_{xx}=f$, we set $u_x=v$ and $v_x=f$. Applying the first-order Fourier pseudospectral method to the two equations leads to $D_1u=v$ and $D_1v=f$. Eliminating vector v gives $D_1^2u=f$.

In this work, in order to construct a charge-preserving and energy-preserving method for the NLS system, we use $D_1^2 u$ to approximate u_{xx} instead of $D_2 u$. Using the spectral differentiation matrix $D_1^2 u$, we obtain the standard Fourier pseudospectral semi-discretization for the nonlinear Schrödinger equation (1) as follows:

$$\mathrm{i}\psi_t + (D_1^2\Psi)_i + a(|\psi_i|^2)\psi_i = 0, \tag{7}$$

equation (7) can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}p_i + (D_1^2 q)_i + \alpha((p_i)^2 + (q_i)^2)q_i = 0, \tag{8}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}q_i - (D_1^2 p)_i - \alpha((p_i)^2 + (q_i)^2)p_i = 0, \tag{9}$$

where $i = 0,1,\ldots,N\text{-}1$, $\boldsymbol{p} = (p_0, p_1, \ldots, p_{N\text{-}1})^{\mathrm{T}}, \boldsymbol{q} = (q_0, q_1, \ldots, q_{N\text{-}1})^{\mathrm{T}}$. Since D_1^2 is symmetric, equations (8) and (9) construct a Hamiltonian system with the following form of Hamiltonian

$$H(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{2}[\boldsymbol{p}^{\mathrm{T}} D_1^2 \boldsymbol{p} + \boldsymbol{q}^{\mathrm{T}} D_1^2 \boldsymbol{q}] + \frac{\alpha}{4}\sum_{i=0}^{N\text{-}1}((p_i)^2 + (q_i)^2)^2.$$

We discretize Eq. (7) with respect to time by the midpoint rule and obtain

$$\mathrm{i}\delta_t \psi_i^n + A_t(D_1^2\Psi^n)_i + aA_t(|\psi_i^n|^2)A_t(\psi_i^n) = 0, \tag{10}$$

where $\Psi^n = (\psi_0^n, \psi_1^n, \psi_2^n, \cdots, \psi_{N\text{-}1}^n,)$, and $i = 0,1,\ldots,N-1$.

Obviously, the scheme (10) can be reformed as a vector form

$$\mathrm{i}\delta_t \Psi^n + A_t(D_1^2\Psi^n) + aA_t(|\Psi^n|^{.2})\cdot A_t(\Psi^n) = 0, \tag{11}$$

where '$\cdot$' denotes point multiplication between vectors, that is

$$\boldsymbol{p}^n \cdot \boldsymbol{q}^n = (p_0^n q_0^n, p_1^n q_1^n, p_2^n q_2^n, \ldots, p_{N\text{-}1}^n q_{N\text{-}1}^n)^{\mathrm{T}}.$$

Equation (10) can also be rewritten as

$$\delta_t p_i^n + A_t(D_1^2 q^n)_i + \alpha A_t((p_i^n)^2 + (q_i^n)^2)A_t(q_i^n) = 0, \tag{12}$$

$$\delta_t q_i^n - A_t(D_1^2 p^n)_i - \alpha A_t((p_i^n)^2 + (q_i^n)^2)A_t(p_i^n) = 0, \tag{13}$$

where $i = 0,1,\ldots,N-1$, $\boldsymbol{p}^n = (p_0^n, p_1^n, \ldots, p_{N-1}^n)^{\mathrm{T}}, \boldsymbol{q}^n = (q_0^n, q_1^n, \ldots, q_{N-1}^n)^{\mathrm{T}}$.

Theorem 1 With periodic boundary condition $\psi(0,t) = \psi(2\pi,t)$, the scheme (11) preserves the charge conservation law exactly, namely,

$$Q^{n+1} = Q^n = \cdots = Q^1 = Q^0, \tag{14}$$

where $Q^n = \|\Psi^n\|_2^2$. The algorithm is unitary, thus the method is unconditionally stable with respect to the initial value.

Proof By taking the inner product of Eq. (11) with $\Psi^{n+1} + \Psi^n$ yields

$$\mathrm{i}\langle\delta_t\Psi^n, \Psi^{n+1} + \Psi^n\rangle + \langle A_t(D_1^2\Psi^n), \Psi^{n+1} + \Psi^n\rangle + a\langle A_t(|\Psi^n|^{.2})\cdot A_t(\Psi^n), \Psi^{n+1} + \Psi^n\rangle = 0, \tag{15}$$

the first term becomes

$$\begin{aligned}&\frac{\mathrm{i}}{\tau}\langle\Psi^{n+1} - \Psi^n, \Psi^{n+1} + \Psi^n\rangle\\ &= \frac{\mathrm{i}}{\tau}(\|\Psi^{n+1}\|_2^2 - \|\Psi^n\|_2^2) - \frac{2}{\tau}\varsigma\langle\Psi^{n+1}, \Psi^n\rangle,\end{aligned} \tag{16}$$

where ς stands for the imaginary part.

The second term can be reduced to

$$\begin{aligned}&\frac{1}{2}\langle D_1^2(\Psi^{n+1} + \Psi^n), \Psi^{n+1} + \Psi^n\rangle\\ &= -\frac{1}{2}\langle D_1(\Psi^{n+1} + \Psi^n), D_1(\Psi^{n+1} + \Psi^n)\rangle\\ &= -\frac{1}{2}\|D_1(\Psi^{n+1} + \Psi^n)\|_2^2,\end{aligned} \tag{17}$$

this is a real function.

The last term

$$\begin{aligned}&a\langle A_t(|\Psi^n|^{.2})\cdot A_t(\Psi^n), \Psi^{n+1} + \Psi^n\rangle\\ &= 2ah\sum_{i=0}^{N\text{-}1} A_t(|\psi_i^n|^2)A_t(\psi_i^n)A_t(\overline{\psi_i^n})\\ &= 2ah\sum_{i=0}^{N\text{-}1} A_t(|\psi_i^n|^2)|A_t(\psi_i^n)|^2,\end{aligned} \tag{18}$$

this is also a real function.

Therefore, the imaginary part of Eq. (15) implies

$$\|\Psi^{n+1}\|_2^2 = \|\Psi^n\|_2^2. \tag{19}$$

So equation (19) gives the charge conservation law (14). □

Theorem 2 With periodic boundary condition $\psi(0,t) = \psi(2\pi,t)$, the scheme (11) possesses the discrete global energy conservation law exactly, namely,

$$\varepsilon^{n+1} = \varepsilon^n = \cdots = \varepsilon^1 = \varepsilon^0, \tag{20}$$

where

$$\varepsilon^n = \frac{a}{4}\|\Psi^n\|_4^4 - \frac{1}{2}\|D_1\Psi^n\|_2^2.$$

Proof Taking the inner product of Eq. (11) with $\Psi^{n+1} - \Psi^n$ yields

$$\begin{aligned}&\mathrm{i}\langle\delta_t\Psi^n, \Psi^{n+1} - \Psi^n\rangle + \langle A_t(D_1^2\Psi^n), \Psi^{n+1} - \Psi^n\rangle\\ &+ a\langle A_t(|\Psi^n|^{.2})\cdot A_t(\Psi^n), \Psi^{n+1} - \Psi^n\rangle = 0,\end{aligned} \tag{21}$$

the first term becomes

$$\frac{\mathrm{i}}{\tau}\langle\Psi^{n+1} - \Psi^n, \Psi^{n+1} - \Psi^n\rangle = \frac{\mathrm{i}}{\tau}\|\Psi^{n+1} - \Psi^n\|_2^2, \tag{22}$$

and it is purely imaginary.

The second term can be reduced to

$$\begin{aligned}&\frac{1}{2}\langle D_1^2(\Psi^{n+1} + \Psi^n), \Psi^{n+1} - \Psi^n\rangle\\ &= -\frac{1}{2}(\|D_1\Psi^{n+1}\|_2^2 - \|D_1\Psi^n\|_2^2) + \mathrm{i}\varsigma\langle D_1\Psi^{n+1}, D_1\Psi^n\rangle.\end{aligned} \tag{23}$$

The last term

$$\begin{aligned}&a\langle A_t(|\Psi^n|^{\cdot 2})\cdot A_t(\Psi^n),\Psi^{n+1}-\Psi^n\rangle\\ =&\frac{a}{4}[\|\Psi^{n+1}\|_4^4-\|\Psi^n\|_4^4-2i\varsigma\langle|\Psi^{n+1}|^2\cdot\Psi^{n+1},\Psi^n\rangle\\&-2i\varsigma\langle|\Psi^n|^2\cdot\Psi^{n+1},\Psi^n\rangle].\end{aligned}\tag{24}$$

Therefore, the real part of Eq. (21) is

$$\begin{aligned}&-\frac{1}{2}(\|D_1\Psi^{n+1}\|_2^2-\|D_1\Psi^n\|_2^2)\\&+\frac{a}{4}(\|\Psi^{n+1}\|_4^4-\|\Psi^n\|_4^4)=0.\end{aligned}\tag{25}$$

So equation (25) gives the energy conservation law (20).

□

3. The convergent analysis of full-discrete Fourier pseudo-spectral scheme

In this section, we use an important inequality and a deduction argument to prove the convergence of the numerical solution.

We first introduce a series of useful lemma.

Lemma 1[14] For $u\in V_N''$,

$$\|u\|\le\|u\|_N\le\sqrt{2}\|u\|.$$

Lemma 2[14] For $u,v\in V_N''$,

$$(\partial_{xx}u,v)_N=(u,\partial_{xx}v)_N.$$

Denote $P_N: L^2(I)\to V_N$ orthogonal projector of L^2, whose truncate and differential can be exchanged, i.e.,

$$P_N\partial_x u=\partial_x P_N u.$$

Note that

$$P_{N-1}\partial_x u(x_j)=\partial_x u(x_j),\forall u\in V_N'',$$

this conclusion is often used in error analysis.

Denote $P_N'': L^2(I)\to V_N''$ as another orthogonal projector of L^2, the following conclusions can be proved.

Lemma 3[15] Let $r\ge 0, u\in H_p^r(I)$,

$$\|P_N u-u\|_l\le CN^{l-r}|u|_r, 0\le l\le r,$$

$$\|P_N'' u-u\|_l\le CN^{l-r}|u|_r, 0\le l\le r.$$

Lemma 4[14] For $u,v\in V_N''$,

$$(\partial_x u,v)_N=-(u,\partial_x v)_N.$$

Denote interpolation of $u(x)$ at node $x_j=2j\pi/N, j=0,1,2,\ldots,N-1$ by $P_c''u(x)\in V_N''$, i.e., $P_c''u(x_j)=u(x_j)$.

It can be denoted by Lagrange as

$$P_c''u(x)=\sum_{j=0}^{N-1}u_jL_j(x),$$

where $u_j=u(x_j)$, $L_j(x_k)=\delta_j^k$, $L_j(x)$ is $N/2$ order trigonometric polynomial, denoted as

$$L_j(x)=\frac{1}{N}{\sum_{|l|\le N/2}}''\mathrm{e}^{\mathrm{i}l(x-x_j)}.$$

The approximation result of this interpolation operator is described as follows:

Lemma 5[15] Let $u\in H_p^r(I)$ and $1/2<r\le 1$,

$$\|P_c''u\|\le C(\|u\|+N^{-r}|u|_r).$$

Lemma 6[15] Let $u\in H_p^r(I)$ and $r>1/2$,

$$\|P_c''u-u\|_l\le CN^{l-r}|u|_r, 0\le l\le r.$$

Lemma 7[14] Let $u\in C(\bar{I}), v\in V_N''$ and $r>1/2$,

$$|(u,v)-(u,v)_N|\le C(\|u-P_{N-1}u\|+\|u-P_c''u\|)\|v\|.$$

Lemma 8 (Gronwall's inequality)[16] Suppose that the discrete function $\{w^n|n=0,1,2,\ldots,N;N\tau=T\}$ satisfies the inequality

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

where A, B, and C_n $(n=0,1,2,\ldots,N)$ are nonnegative constants. Then

$$\max_{1\le n\le N}|w^n|\le\left(w^0+\sum_{l=1}^{N}C_l\right)\mathrm{e}^{2(A+B)T},$$

where τ is sufficiently small, such that $(A+B)\tau\le(N-1)/2N$, $(N>1)$.

Temporal direction employs a midpoint scheme, an equivalent form of full-discrete Fourier pseudo-spectral schemes (12) and (13) for the system of Eq. (3) is looking for $(p_c^n,q_c^n)^{\mathrm{T}}\in(V_N'')^2$, so that for any $\Phi^n=(\Phi_1^n,\Phi_2^n)^{\mathrm{T}}\in(V_N'')^2$, then

$$\begin{aligned}&\left(\frac{p_c^{n+1}-p_c^n}{\tau},\Phi_1^n\right)_N+(\partial_{xx}q_c^{n+1/2}),\Phi_1^n)_N\\=&\left(-\frac{a}{2}[(p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2]q_c^{n+1/2},\Phi_1^n\right)_N,\end{aligned}\tag{26}$$

$$\begin{aligned}&\left(\frac{q_c^{n+1}-q_c^n}{\tau},\Phi_2^n)_N-(\partial_{xx}p_c^{n+1/2}),\Phi_2^n\right)_N\\=&\left(\frac{a}{2}[(p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2]p_c^{n+1/2},\Phi_2^n\right)_N.\end{aligned}\tag{27}$$

Let $\mathrm{e}^n=z_c^n-z^{*n}$, where $z^{*n}=P_{N-2}z^n=(p^{*n},q^{*n})^{\mathrm{T}}$.

According to Eq. (2), we can get

$$\begin{aligned}&p_t^*+q_{xx}^*+P_{N-2}[a(p^2+q^2)q]=0,\\&q_t^*-p_{xx}^*-P_{N-2}[a(p^2+q^2)p]=0.\end{aligned}\tag{28}$$

Then

$$\left(\frac{p_c^{n+1}-p_c^n}{\tau}-\frac{p^{*n+1}-p^{*n}}{\tau},\Phi_1^n\right)_N$$

$$
\begin{aligned}
&+(\partial_{xx}(q_c^{n+1/2}-q^{*n+1/2}),\Phi_1^n)_N\\
=&\left(-\frac{a}{2}[(p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2]q_c^{n+1/2}\right.\\
&\left.+P_{N-2}[a(p^2+q^2)q]+p_t^{*n+1/2}-\frac{p^{*n+1}-p^{*n}}{\tau},\Phi_1^n\right)_N, \quad (29)\\
&\left(\frac{q_c^{n+1}-q_c^n}{\tau}-\frac{q^{*n+1}-q^{*n}}{\tau},\Phi_2^n\right)_N\\
&-(\partial_{xx}(p_c^{n+1/2}-p^{*j+1/2}),\Phi_2^n)_N\\
=&\left(\frac{a}{2}[(p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2]p_c^{n+1/2}\right.\\
&\left.-P_{N-2}[a(p^2+q^2)p]+q_t^{*n+1/2}-\frac{q^{*n+1}-q^{*n}}{\tau},\Phi_2^n\right)_N. \quad (30)
\end{aligned}
$$

Let $\Phi^n=(p_c^{n+1/2}-p^{*n+1/2},q_c^{n+1/2}-q^{*n+1/2})^{\mathrm{T}}$, then

$$
\begin{aligned}
&\frac{1}{2\tau}(\|q_c^{n+1}-q^{*n+1}\|_N^2+\|p_c^{n+1}-p^{*n+1}\|_N^2\\
&-\|q_c^n-q^{*n}\|_N^2-\|p_c^n-p^{*n}\|_N^2)=G_f, \quad (31)
\end{aligned}
$$

where

$$
\begin{aligned}
G_f=&\left(\frac{a}{2}[(p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2]p_c^{n+1/2}\right.\\
&-P_{N-2}[a(p^2+q^2)p]\\
&\left.+q_t^{*n+1/2}-\frac{q^{*n+1}-q^{*n}}{\tau},q_c^{n+1/2}-q^{*n+1/2}\right)_N\\
&+\left(-\frac{a}{2}[(p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2]q_c^{n+1/2}\right.\\
&+P_{N-2}[a(p^2+q^2)q]+p_t^{*n+1/2}\\
&\left.-\frac{p^{*n+1}-p^{*n}}{\tau},p_c^{n+1/2}-p^{*n+1/2}\right)_N.
\end{aligned}
$$

Let

$$
\begin{aligned}
G_f=&(\widetilde{gp_c}+\widetilde{gp^*}+\widetilde{gq_t},q_c^{n+1/2}-q^{*n+1/2})_N\\
&+(\widetilde{gq_c}+\widetilde{gq^*}+\widetilde{gp_t},p_c^{n+1/2}-p^{*n+1/2})_N,\\
\widetilde{gp_c}=&\frac{a}{2}((p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2)p_c^{n+1/2}\\
&-a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2},\\
\widetilde{gp^*}=&a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2}\\
&-P_{N-2}(a(p^2+q^2)p),\\
\widetilde{gq_t}=&q_t^{*n+1/2}-\frac{q^{*n+1}-q^{*n}}{\tau},\\
\widetilde{gq_c}=&-\frac{a}{2}((p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2)q_c^{n+1/2}\\
&+a((p^{*n+1/2})^2+(q^{*n+1/2})^2)q^{*n+1/2},\\
\widetilde{gq^*}=&-a((p^{*n+1/2})^2+(q^{*n+1/2})^2)q^{*n+1/2}\\
&+P_{N-2}(a(p^2+q^2)q),\\
\widetilde{gp_t}=&p_t^{*n+1/2}-\frac{p^{*n+1}-p^{*n}}{\tau},
\end{aligned}
$$

then

$$
\begin{aligned}
\|\widetilde{gp_c}\|_N=&\|\frac{a}{2}((p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2)p_c^{n+1/2}\\
&-a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2}\|_N\\
=&\|\frac{a}{2}((p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2)p_c^{n+1/2}\\
&-a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p_c^{n+1/2}\\
&+a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p_c^{n+1/2}\\
&-a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2}\|_N\\
\le&\|(\frac{a}{2}((p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2)\\
&-a((p^{*n+1/2})^2+(q^{*n+1/2})^2))\|_N\|p_c^{n+1/2}\|_\infty\\
&+\|a((p^{*n+1/2})^2+(q^{*n+1/2})^2)\|_\infty\|p_c^{n+1/2}-p^{*n+1/2}\|_N\\
\le&C_1(\|p_c^{n+1/2}-p^{*n+1/2}\|_N+\|q_c^{n+1/2}-q^{*n+1/2}\|_N)\\
\le&C_2(\|p_c^{n+1}-p^{*n+1}\|_N+\|p_c^n-p^{*n}\|_N\\
&+\|q_c^{n+1}-q^{*n+1}\|_N+\|q_c^n-q^{*n}\|_N).\\
\|\widetilde{gp^*}\|_N=&\|a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2}\\
&-P_{N-2}(a(p^2+q^2)p)\|_N\\
=&\|a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2}-a(p^2+q^2)p\\
&+a(p^2+q^2)p-P_{N-2}(a(p^2+q^2)p)\|_N\\
\le&\|a((p^{*n+1/2})^2+(q^{*n+1/2})^2)p^{*n+1/2}-a(p^2+q^2)p\|_N\\
&+\|a(p^2+q^2)p-P_{N-2}(a(p^2+q^2)p)\|_N\\
\le&C_3(\|p^{*n+1/2}-p\|_N+\|q^{*n+1/2}-q\|_N)\\
&+\|P_c''(a(p^2+q^2)p)-P_{N-2}(a(p^2+q^2)p)\|_N\\
\le&C_4N^{-r}(|p|_r+|q|_r)\\
&+\|P_c''(a(p^2+q^2)p)-a(p^2+q^2)p+a(p^2+q^2)p\\
&-P_{N-2}(a(p^2+q^2)p)\|_N\\
\le&C_4N^{-r}(|p|_r+|q|_r)\\
&+\sqrt{2}(\|P_c''(a(p^2+q^2)p)-a(p^2+q^2)p\|_N\\
&+\|P_{N-2}(a(p^2+q^2)p)-a(p^2+q^2)p\|_N)\\
\le&C_4N^{-r}(|p|_r+|q|_r)+C_5N^{-r}|a(p^2+q^2)p|_r,\\
\|\widetilde{gq_t}\|_N=&\left\|q_t^{*n+1/2}-\frac{q^{*n+1}-q^{*n}}{\tau}\right\|_N\\
=&\left\|-\frac{\tau^2}{12}\partial_{ttt}q^*(t_n+\theta_1\tau)\right\|_N\le C_6\tau^2.
\end{aligned}
$$

So in the same way,

$$
\begin{aligned}
\|\widetilde{gq_c}\|_N=&\left\|\frac{a}{2}((p_c^{n+1})^2+(p_c^n)^2+(q_c^{n+1})^2+(q_c^n)^2)q_c^{n+1/2}\right.\\
&\left.-a((p^{*n+1/2})^2+(q^{*n+1/2})^2)q^{*n+1/2}\right\|_N\\
\le&C_7(\|p_c^{n+1}-p^{*n+1}\|_N+\|p_c^n-p^{*n}\|_N\\
&+\|q_c^{n+1}-q^{*n+1}\|_N+\|q_c^n-q^{*n}\|_N),\\
\|\widetilde{gq^*}\|_N=&\|a((p^{*n+1/2})^2+(q^{*n+1/2})^2)q^{*n+1/2}\\
&-P_{N-2}(a(p^2+q^2)q)\|_N\\
\le&C_8N^{-r}(|p|_r+|q|_r)+C_9N^{-r}|a(p^2+q^2)q|_r,
\end{aligned}
$$

$$\|\widetilde{gp_t}\|_N = \left\| p_t^{*n+1/2} - \frac{p^{*n+1}-p^{*n}}{\tau} \right\|_N = \left\| -\frac{\tau^2}{12}\partial_{ttt}p^*(t_n+\theta_2\tau) \right\|_N \le C_{10}\tau^2,$$

then

$$\begin{aligned}
&\frac{1}{2\tau}(\|q_c^{n+1}-q^{*n+1}\|_N^2+\|p_c^{n+1}-p^{*n+1}\|_N^2 \\
&-\|q_c^n-q^{*n}\|_N^2-\|p_c^n-p^{*n}\|_N^2) \\
\le\ & C_{11}(\|p_c^{n+1}-p^{*n+1}\|_N^2+\|p_c^n-p^{*n}\|_N^2 \\
&+\|q_c^{n+1}-q^{*n+1}\|_N^2+\|q_c^n-q^{*n}\|_N^2) \\
&+C_{12}N^{-2r}(|p|_r^2+|q|_r^2+|a(p^2+q^2)p|_r^2 \\
&+|a(p^2+q^2)q|_r^2)+C_{13}\tau^4.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\|q_c^{n+1}-q^{*n+1}\|_N^2+\|p_c^{n+1}-p^{*n+1}\|_N^2 \\
&-\|q_c^n-q^{*n}\|_N^2-\|p_c^n-p^{*n}\|_N^2 \\
\le\ & C_{14}\tau(\|p_c^{n+1}-p^{*n+1}\|_N^2+\|q_c^{n+1}-q^{*n+1}\|_N^2) \\
&+C_{14}\tau(\|p_c^n-p^{*n}\|_N^2+\|q_c^n-q^{*n}\|_N^2) \\
&+C_{14}\tau(N^{-2r}+\tau^4).
\end{aligned}$$

Based on Lemma (8), we can obtain

$$\begin{aligned}
&\|q_c^k-q^{*k}\|_N^2+\|p_c^k-p^{*k}\|_N^2 \\
\le\ & (\|q_c^0-q^{*0}\|_N^2+\|p_c^0-p^{*0}\|_N^2 \\
&+C_{15}(\tau^4+N^{-2r}))\,\mathrm{e}^{4C_{14}T}. \qquad (32)
\end{aligned}$$

For the initial error, there are

$$\|p_c^0-p^{*0}\|_N = \|P_c''p(0)-P_{N-2}p(0)\|_N \le C_{16}N^{-r}|p(0)|_r,$$
$$\|q_c^0-q^{*0}\|_N = \|P_c''q(0)-P_{N-2}q(0)\|_N \le C_{16}N^{-r}|q(0)|_r.$$

According to the initial error, we can obtain

$$\|q_c^k-q^{*k}\|_N+\|p_c^k-p^{*k}\|_N \le C(N^{-r}+\tau^2). \qquad (33)$$

According to the above analysis and derivation, we give the following theorem.

Theorem 3 Suppose that $p,q \in H^1(0,T;H_p^r(I)) \cap H^3(0,T;L^2(I))$, $r>1/2$, and τ are small enough, then the solution of the full-discrete Fourier pseudo-spectral schemes (12) and (13) converges to the solution of problems Eq. (3) with order $O(N^{-r}+\tau^2)$ in the $|\cdot|$ norm.

4. Numerical experiments

In this section, we conduct some tentative numerical experiments for this new scheme (11) to verify the theoretical conclusions, including the accuracy, the ability to preserve the first integrals of the nonlinear Schrödinger equation for long-time integration.

First we take the parameter $a=2$. Then, we get the equation

$$\mathrm{i}\psi_t+\psi_{xx}+2|\psi|^2\psi=0.$$

The space interval is $[x_\mathrm{L},x_\mathrm{R}]$ with the periodic boundary condition $\psi(-15,t)=\psi(15,t)$ and the initial condition

$$\psi(x,0)=\mathrm{sech}(x)\exp(2x\mathrm{i}). \qquad (34)$$

We take $N=200$, and the time step $\tau=10^{-3}$ for the new scheme (11). We check the ability of this new scheme preserving the first integral which is one of the important criterion to judge numerical schemes. The nonlinear Schrödinger equation with periodic boundary condition has two conservation laws:

$$F_1(\psi)=\int_{x_\mathrm{L}}^{x_\mathrm{R}}|\psi|^2\mathrm{d}x,$$
$$F_2(\psi)=\int_{x_\mathrm{L}}^{x_\mathrm{R}}[\frac{a}{4}|\psi|^4-\frac{1}{2}|\psi_x|^2]\mathrm{d}x.$$

If the approximate solution of $\psi(x,t=j\tau)$ is $\psi^j=(\psi_0,\psi_1,\ldots,\psi_N)^\mathrm{T}$, then the discrete conservation law F_1 and F_2 are

$$F_1^h(\psi)=\sum_{i=1}^{N}|\psi_i|^2h,$$
$$F_2^h(\psi)=\sum_{i=1}^{N}\frac{1}{2}(|\psi_i|^4-|D_1\Psi|_i^2)h.$$

We define the errors of the discrete conservation law on the j-th time level as

$$Err_{F_1}(j\tau)=F_1^h(\psi^j)-F_1^h(\psi^0),$$
$$Err_{F_2}(j\tau)=F_2^h(\psi^j)-F_2^h(\psi^0),$$

where ψ^j is the numerical solution on the j-th time level and ψ^0 is the discrete initial value. The waveforms at different time levels and the changes of Err_{F_1} and Err_{F_2} with time are shown in Fig. 1.

The discrete L^2 norm of complex-valued function ψ is defined as

$$\|\psi\|_2=\left(\sum_{i=1}^{N}|\psi_i|^2h\right)^{1/2}.$$

We consider that the problem is solved in $[-15,15]$ till time $t=1$ for accuracy test. Note that in Table 1, the spatial error $(N=100)$ is negligible and the error is dominated by the time discretization error. It shows that accuracy of space is very large. Table 1 clearly indicates that the new scheme (11) is of the second order in time.

Table 1. Time accuracy of the new scheme (11) with the initial condition (34) $(N=100)$.

τ	L_2 error	Order
4×10^{-2}	1.1850×10^{-4}	–
2×10^{-2}	2.9580×10^{-5}	2.0022
1×10^{-2}	7.3583×10^{-6}	2.0072
5×10^{-3}	1.8040×10^{-6}	2.0282
2.5×10^{-3}	4.1898×10^{-7}	2.1062
1.25×10^{-3}	9.2257×10^{-8}	2.1832

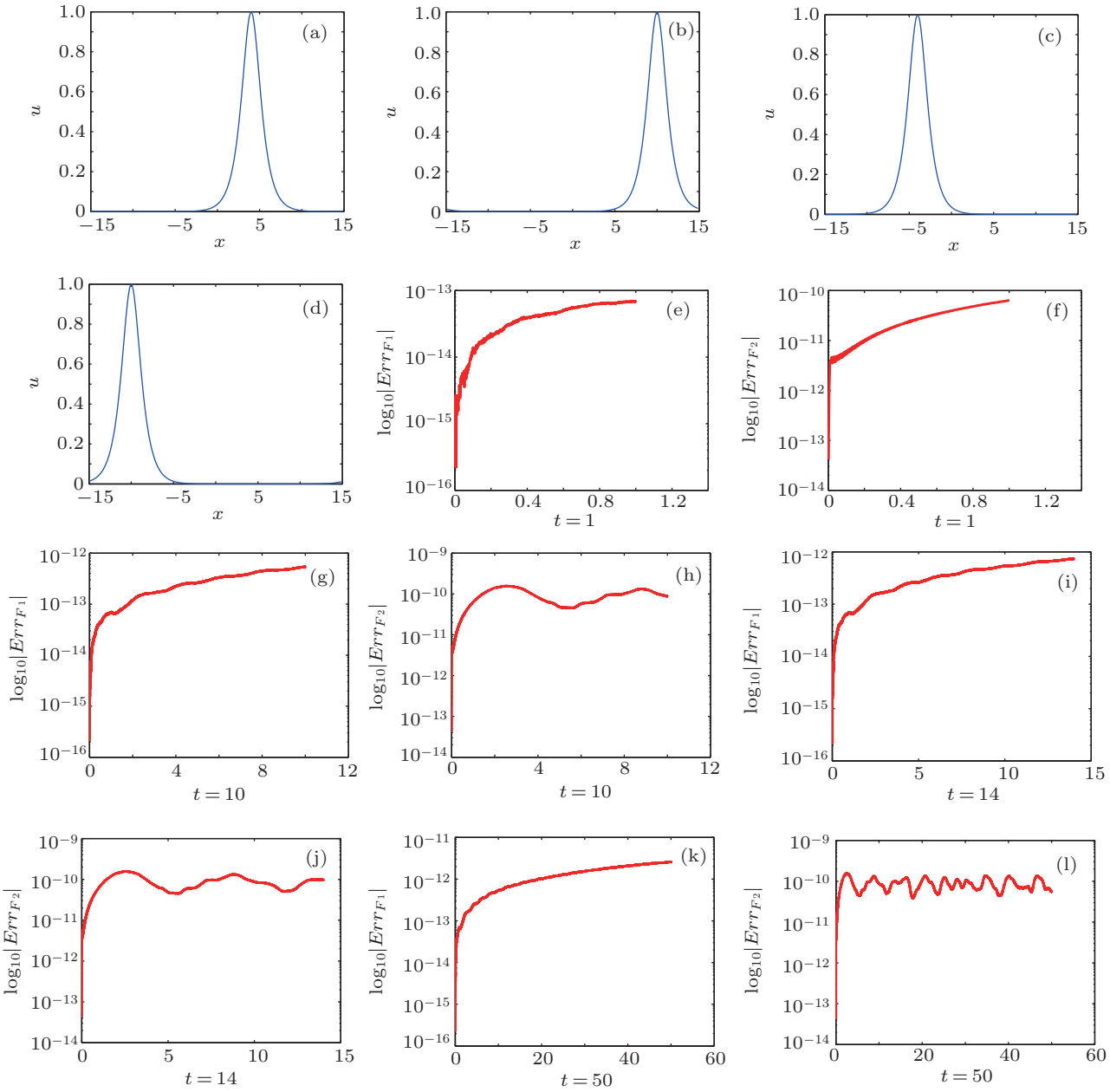


Fig. 1. (color online) The numerical solutions at $t = 1$ (a), 10 (b), 14 (c), (50) (d) and the changes of Err_{F_1} (e), (g), (i), (k) and Err_{F_2} (f), (h), (j), (l) with time.

In the traditional method, we use the second-order Fourier spectral differentiation matrix D_2 to approximate the second derivative for spatial discretization. Moreover, we discretize the time by the midpoint rule. So we obtain the standard Fourier pseudospectral discretization for the nonlinear Schrödinger equation (1) as follows:

$$\delta_t p_i^n + A_t(D_2 \boldsymbol{q}^{\boldsymbol{n}})_i + \alpha((A_t(p_i^n))^2 + (A_t(q_i^n))^2)A_t(q_i^n) = 0, \quad (35)$$

$$\delta_t q_i^n - A_t(D_2 \boldsymbol{p}^{\boldsymbol{n}})_i - \alpha((A_t(p_i^n))^2 + (A_t(q_i^n))^2)A_t(p_i^n) = 0, \quad (36)$$

where $i = 0, 1, \ldots, N-1$, $\boldsymbol{p}^{\boldsymbol{n}} = (p_0^n, p_1^n, \ldots, p_{N-1}^n)^{\mathrm{T}}$, $\boldsymbol{q}^{\boldsymbol{n}} = (q_0^n, q_1^n, \ldots, q_{N-1}^n)^{\mathrm{T}}$.

We take the same parameter to Eqs. (35) and (36). Comparing the solutions between the two methods, the errors are shown in Fig. 2 when $t = 1, 10, 25, 50$. Obviously we find that the errors are very small. Thus, we provide a new choice for solving the nonlinear Schrödinger equation.

We also test our new scheme on the following initial condition $\psi(x,0) = 0.5 + 0.025\cos(\mu x)$ with the periodic boundary condition $\psi(0,t) = \psi(4\sqrt{2}\pi, t)$. We take $L = 4\sqrt{2}\pi$, $\mu = 2\pi/L$. The initial condition is in the vicinity of the homoclinic orbit in Ref. [3].

In this case, we also take $N = 200$, and the time step $\tau = 10^{-3}$ for the new scheme (11). The corresponding waveforms at different time levels and the changes of errors of discrete conservation law F_1 and F_2 with time are shown in Fig. 3. We find that the numerical results we presented in the paper show that the new scheme is very robust and stable.

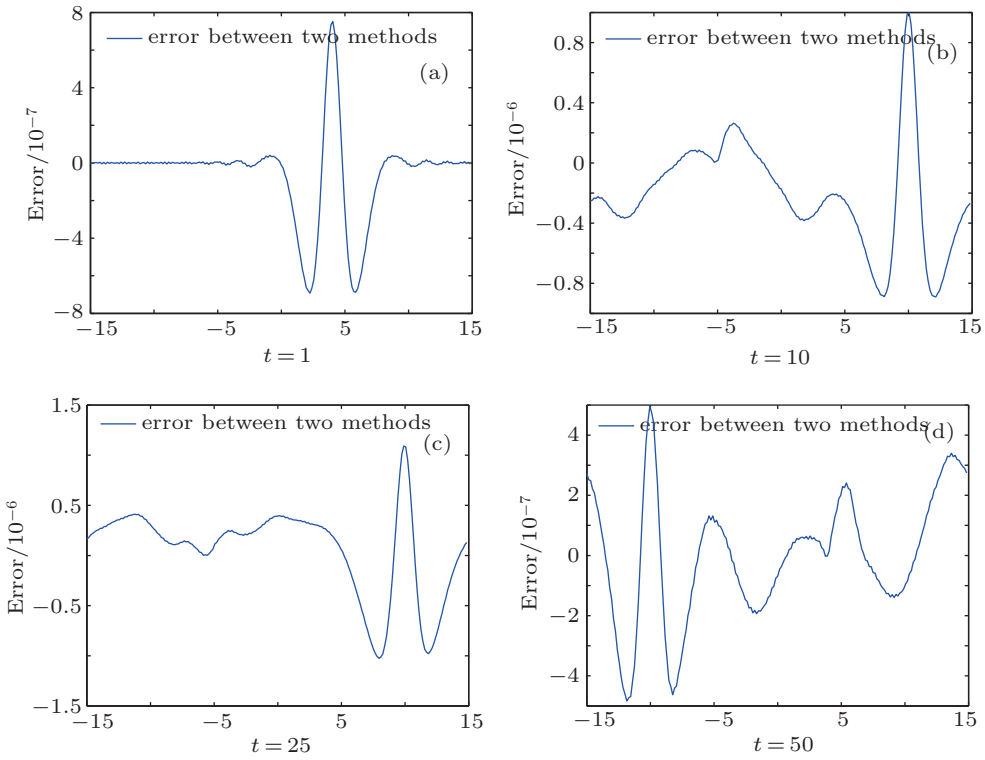
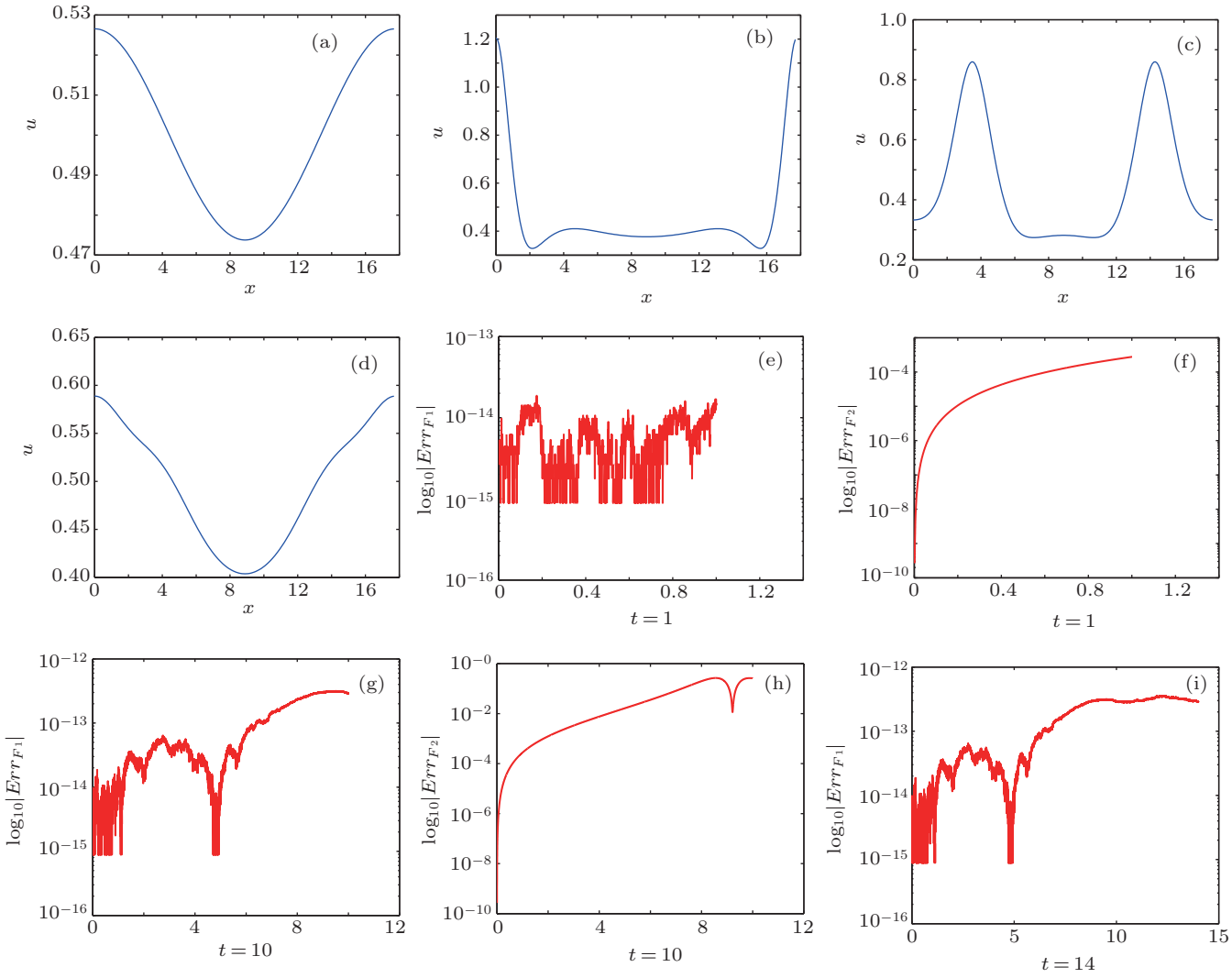


Fig. 2. (color online) The errors at $t = 1$ (a), 10 (b), 25 (c), and 50 (d).



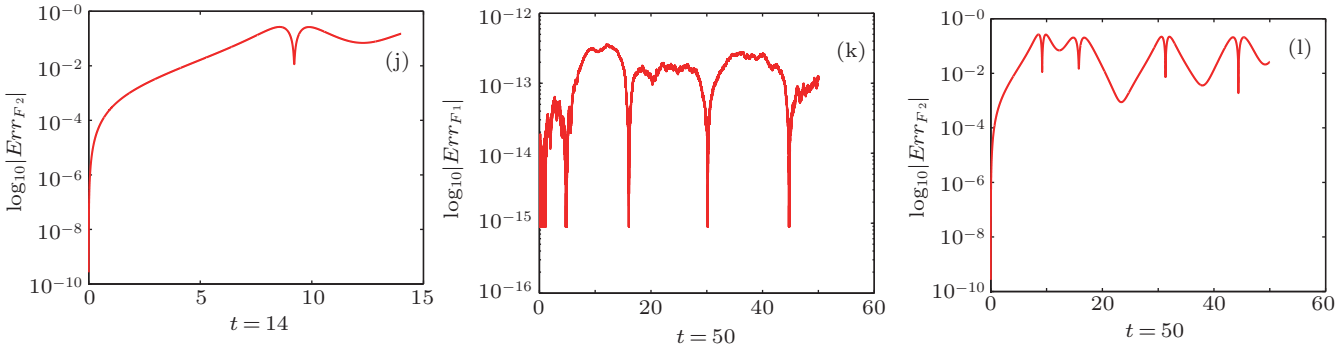


Fig. 3. (color online) The numerical solutions at $t = 1$ (a), 10 (b), 14 (c), 50 (d) and the changes of Err_{F_1} and Err_{F_2} (f), (h), (j), (l) with time.

5. Conclusion

In this paper, we derive a new method for the nonlinear Schrödinger system. We proved that the proposed method can preserve the charge and energy conservation laws exactly. A deduction argument demonstrates that the numerical solution is second-order convergent to the exact solutions in $\|\cdot\|_2$ norm. The numerical experiments with different initial conditions show that the new scheme is effective. Furthermore, the new scheme can also preserve the discrete charge and energy very well. Therefore, it will be a good choice for solving the nonlinear Schrödinger equation in computation especially with high spatial dimensions.

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