Electronic Transactions on Numerical Analysis.
Volume 12, pp. 193-204, 2001.

ISSN 1068-9613.

ETNA
Kent State University
etna@mcs.kent.edu

MULTI-SYMPLECTIC FOURIER PSEUDOSPECTRAL METHOD FOR THE NONLINEAR SCHRÖDINGER EQUATION *

JING-BO CHEN † AND MENG-ZHAO QIN‡

Abstract. Bridges and Reich suggested the idea of multi-symplectic spectral discretization on Fourier space [4]. Based on their theory, we investigate the multi-symplectic Fourier pseudospectral discretization of the nonlinear Schrödinger equation (NLS) on real space. We show that the multi-symplectic semi-discretization of the nonlinear Schrödinger equation with periodic boundary conditions has N (the number of the nodes) semi-discrete multi-symplectic conservation laws. The symplectic discretization in time of the semi-discretization leads to N full-discrete multi-symplectic conservation laws. We also prove a result relating to the spectral differentiation matrix. Numerical experiments are included to demonstrate the remarkable local conservation properties of multi-symplectic spectral discretizations.

Key words. Multi-symplectic, Fourier pseudospectral method, nonlinear Schrödinger equation.

AMS subject classifications. 65M99.

1. Introduction. We consider the nonlinear Schrödinger equation

$$i\psi_t + \psi_{xx} + a|\psi|^2\psi = 0 \tag{1.1}$$

with the periodic boundary condition $\psi(0,t) = \psi(L,t)$. Here $a > 0$ is a constant parameter.

The equation (1.1) can be cast into a multi-symplectic Hamiltonian system [2,3,8]. A large class of PDEs (for simplicity, we only consider one space dimension) can be written as

$$Mz_t + Kz_x = \bigtriangledown_z S(z),\; z \in \mathbf{R}^n,\; (x,t) \in \mathbf{R}^2, \tag{1.2}$$

where M and K are skew-symmetric matrices on $\mathbf{R}^n, n \geq 3$ and $S : \mathbf{R}^n \to \mathbf{R}$ is a smooth function. We call the above system multi-symplectic Hamiltonian system, since it has a multi-symplectic conservation law

$$\frac{\partial}{\partial t}\omega + \frac{\partial}{\partial x}\kappa = 0, \tag{1.3}$$

where ω and κ are the pre-symplectic forms

$$\omega = \frac{1}{2}dz \wedge Mdz, \qquad \kappa = \frac{1}{2}dz \wedge Kdz.$$

The system (1.2) has an energy conservation law (ECL)

$$\frac{\partial}{\partial t}E + \frac{\partial}{\partial x}F = 0, \tag{1.4}$$

with energy density

$$E = S(z) - \frac{1}{2}z^T K z_x,$$

*Received April 26, 2000. Accepted for publication June 13, 2001. Recommended by V. Druskin.

† Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Sciences, Academia Sinica, P.O. Box 2719, Beijing 100080, P.R. China. This research was subsidized by the Special Funds for Major State Basic Research Projects (No. 1999032800). E-mail: `cjb@lsec.cc.ac.cn`

‡Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Sciences, Academia Sinica, P.O. Box 2719, Beijing 100080, P.R. China. This research was subsidized by the Special Funds for Major State Basic Research Projects (No. 19990328000). E-mail: `qmz@lsec.cc.ac.cn`

ETNA
Kent State University
etna@mcs.kent.edu

and energy flux

$$F = \frac{1}{2} z^T K z_t.$$

The system (1.2) also has a momentum conservation law (MCL)

$$\frac{\partial}{\partial t} I + \frac{\partial}{\partial x} G = 0, \tag{1.5}$$

with momentum density

$$I = \frac{1}{2} z^T M z_x,$$

and momentum flux

$$G = S(z) - \frac{1}{2} z^T M z_t.$$

Now consider the nonlinear Schrödinger equation (1.1). Using $\psi = p + iq$, we can rewrite (1.1) as a pair of real-valued equations

$$p_t + q_{xx} + a(p^2 + q^2)q = 0, \tag{1.6}$$

$$q_t - p_{xx} - a(p^2 + q^2)p = 0. \tag{1.7}$$

Next we introduce a pair of conjugate momenta $v = p_x, w = q_x$, and obtain the multi-symplectic PDE

$$\begin{aligned} q_t - v_x &= a(p^2 + q^2)p, \\ -p_t - w_x &= a(p^2 + q^2)q, \\ p_x &= v, \\ q_x &= w, \end{aligned} \tag{1.8}$$

with state variable $z = (p, q, v, w)^T$ and the Hamiltonian

$$S(z) = \frac{1}{2}(v^2 + w^2 + \frac{a}{2}(p^2 + q^2)^2).$$

In this case,

$$M = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

The corresponding multi-symplectic conservation law is

$$\frac{\partial}{\partial t}(-dp \wedge dq) + \frac{\partial}{\partial x}(dp \wedge dv + dq \wedge dw) = 0. \tag{1.9}$$

The corresponding energy conservation law is

$$\frac{\partial}{\partial t}[\frac{1}{2}(\frac{a}{2}(p^2 + q^2)^2 - v^2 - w^2)] + \frac{\partial}{\partial x}(vp_t + wq_t) = 0. \tag{1.10}$$

And the corresponding momentum conservation law is

$$\frac{\partial}{\partial t}(pw-qv)++\frac{\partial}{\partial x}[\frac{1}{2}(\frac{a}{2}(p^2+q^2)^2+v^2+w^2-pq_t+qp_t)]=0. \tag{1.11}$$

Bridges and Reich introduced the idea of a multi-symplectic Fourier transform for multi-symplectic PDEs with periodic boundary conditions [4]. The multi-symplectic Fourier transform leads to a semi-discretization on Fourier space and the concept of multi-symplecticity on Fourier space. Their theory lay a foundation of multi-symplectic spectral and pseudospectral methods. In this paper, we derive the semi-discrete and full-discrete multi-symplectic conservation laws directly on real space.

An outline of the paper is as follows. In section 2, we present the standard Fourier pseudospectral method for the nonlinear Schrödinger equation. Section 3 is devoted to the analysis of the multi-symplectic spectral discretization. Numerical experiments are reported in section 4. Section 5 contains some conclusions and comments.

2. Standard Fourier pseudospectral method for NLS. We begin with the pair of real-valued equations (1.6)-(1.7) with periodic boundary conditions $p(0,t) = p(L,t)$ and $q(0,t) = q(L,t)$. We follow the standard Fourier pseudospectral formulation [5-7]. Special attention is paid to the antisymmetry of the spectral differentiation matrix which plays a crucial role in what follows.

The Fourier pseudospectral method involves two basic steps. First, we construct the discrete representation of the solution through interpolating trigonometric polynomial of the solution at collocation points. Second, equations for the discrete values of the solution are obtained from the original equation. This second step involves finding an approximation for the differential operator in terms of the discrete values of the solution at collocation points.

We approximate $p(x,t)$ and $q(x,t)$ by $I_Np(x,t)$ and $I_Nq(x,t)$, respectively, which interpolate them at the following set of collocation points

$$x_j = \frac{L}{N}j, \quad j = 0, 1, \cdots, N-1.$$

Here N is an even number.

The approximations $I_Np(x,t)$ and $I_Nq(x,t)$ have the form

$$I_Np(x,t) = \sum_{j=0}^{N-1} p_j g_j(x), \tag{2.1}$$

$$I_Nq(x,t) = \sum_{j=0}^{N-1} q_j g_j(x), \tag{2.2}$$

where $p_j = p(x_j,t), q_j = q(x_j,t), g_j(x_k) = \delta_j^k$, and $g_j(x)$ is a trigonometric polynomial of degree $N/2$. In fact, $g_j(x)$ is given explicitly by

$$g_j(x) = \frac{1}{N}\sum_{l=-N/2}^{N/2}\frac{1}{c_l}e^{il\mu(x-x_j)}, \tag{2.3}$$

where $c_l = 1(|l| \neq N/2),\ c_{-N/2} = c_{N/2} = 2,\ \mu = \frac{2\pi}{L}$.

Substituting (2.3) into (2.1) and (2.2), we obtain

ETNA
Kent State University
etna@mcs.kent.edu

(2.4) $$I_N p(x,t) = \sum_{l=-N/2}^{N/2} \frac{1}{c_l} e^{il\mu x} \frac{1}{N} \sum_{j=0}^{N-1} p_j e^{-il\mu x_j},$$

(2.5) $$I_N q(x,t) = \sum_{l=-N/2}^{N/2} \frac{1}{c_l} e^{il\mu x} \frac{1}{N} \sum_{j=0}^{N-1} q_j e^{-il\mu x_j}.$$

Defining

(2.6) $$\widehat{p}_l = \frac{1}{Nc_l} \sum_{j=0}^{N-1} p_j e^{-il\mu x_j},$$

(2.7) $$\widehat{q}_l = \frac{1}{Nc_l} \sum_{j=0}^{N-1} q_j e^{-il\mu x_j},$$

(2.4) and (2.5) become, respectively,

(2.8) $$I_N p(x,t) = \sum_{l=-N/2}^{N/2} \widehat{p}_l e^{il\mu x},$$

(2.9) $$I_N q(x,t) = \sum_{l=-N/2}^{N/2} \widehat{q}_l e^{il\mu x}.$$

Therefore,

(2.10) $$p_j = \sum_{l=-N/2}^{N/2} \widehat{p}_l e^{il\mu x_j},$$

(2.11) $$q_j = \sum_{l=-N/2}^{N/2} \widehat{q}_l e^{il\mu x_j}.$$

In order to obtain the equations for p_j and q_j, we substitute (2.8) and (2.9) into (1.6)-(1.7), and require that (1.6)-(1.7) are satisfied exactly at collocation points, i.e.,

$$[(I_N p(x,t))_t + (I_N q(x,t))_{xx} + a((I_N p(x,t))^2 + (I_N q(x,t))^2) I_N q(x,t)] \,|_{x=x_j} = 0,$$
$$[(I_N q(x,t))_t - (I_N p(x,t))_{xx} - a((I_N p(x,t))^2 + (I_N q(x,t))^2) I_N p(x,t)] \,|_{x=x_j} = 0,$$

where $j = 0, 1, \cdots, N-1$.

The crucial step here is to obtain values for the derivatives $\partial^k I_N p(x,t)/\partial x^k$ and $\partial^k I_N q(x,t)/\partial x^k$ at the collocation points x_j in terms of the values p_j and q_j, respectively. This is done by differentiating (2.1)-(2.2) and evaluating the resulting expressions at the points x_j:

(2.12) $$\frac{\partial^k I_N p(x_j,t)}{\partial x^k} = \sum_{n=0}^{N-1} p_n \frac{d^k g_n(x_j)}{d\, x^k} = (D_k \mathbf{p})_j,$$

(2.13) $$\frac{\partial^k I_N q(x_j,t)}{\partial x^k} = \sum_{n=0}^{N-1} q_n \frac{d^k g_n(x_j)}{d\, x^k} = (D_k \mathbf{q})_j,$$

where D_k is an $N \times N$ matrix with elements

$$(D_k)_{j,n} = \frac{d^k g_n(x_j)}{d\,x^k},$$

and $\mathbf{p} = (p_0, \cdots, p_{N-1})^T$ and $\mathbf{q} = (q_0, \cdots, q_{N-1})^T$.

We can obtain explicitly

$$(D_1)_{j,n} = \begin{cases} \frac{1}{2}\mu(-1)^{j+n}\cot(\mu\frac{x_j - x_n}{2}), & j \neq n, \\ 0, & j = n, \end{cases}$$

$$(D_2)_{j,n} = \begin{cases} \frac{1}{2}\mu^2(-1)^{j+n+1}\frac{1}{\sin^2(\mu(x_j - x_n)/2)}, & j \neq n, \\ -\mu^2\frac{2(N/2)^2+1}{6}, & j = n, \end{cases}$$

and

$$(D_3)_{j,n} = \begin{cases} \mu^3(-1)^{j+n}\frac{\cos(\mu(x_j - x_n)/2)}{\sin^3(\mu(x_j - x_n)/2)} + \frac{\mu^3 N^2}{8}(-1)^{j+n+1}\cot(\mu\frac{x_j - x_n}{2}), & j \neq n, \\ 0, & j = n. \end{cases}$$

In general, we have the following result.

THEOREM 2.1. *For the spectral differentiation matrices D_k and $(D_1)^k$, the following equation holds*

$$(D_k)_{j,n} = (D_1^k)_{j,n} + (-1)^{j+n}\frac{\mu^k}{2N}\left[\left(i\frac{N}{2}\right)^k + \left(-i\frac{N}{2}\right)^k\right]. \tag{2.14}$$

In particular, $D_k = (D_1)^k$, if k is an odd number.

Proof. First, we have from (2.3)

$$(D_k)_{j,n} = \frac{d^k g_n(x_j)}{dx^k} = \frac{1}{N}\sum_{l=-N/2}^{N/2}\frac{(il\mu)^k}{c_l}e^{il\mu(x_j - x_n)}. \tag{2.15}$$

Now we compute $(D_1)^k$ directly. First, we have

$$\begin{aligned}(D_1^2)_{j,n} &= \sum_{m=0}^{N-1}(D_1)_{j,m}(D_1)_{m,n} \\ &= \sum_{m=0}^{N-1}\frac{1}{N}\sum_{l=-N/2}^{N/2}\frac{il\mu}{c_l}e^{il\mu(x_j - x_m)}\frac{1}{N}\sum_{p=-N/2}^{N/2}\frac{ip\mu}{c_p}e^{ip\mu(x_m - x_n)} \\ &= \frac{1}{N}\sum_{l=-N/2}^{N/2}\sum_{p=-N/2}^{N/2}\frac{-lp\mu^2}{c_l c_p}e^{i\mu(lx_j - px_n)}\frac{1}{N}\sum_{m=0}^{N-1}e^{i\mu(p-l)x_m}.\end{aligned}$$

Using the identity (see equation (2.7) in [7])

$$\sum_{m=0}^{N-1}e^{i\mu(p-l)x_m} = \begin{cases} 0, & p - l \neq nN, \quad n \ is \ an \ integer, \\ N, & p - l = nN, \end{cases} \tag{2.16}$$

ETNA
Kent State University
etna@mcs.kent.edu

and noting that

$$e^{-i\mu N(x_j-x_n)/2} = e^{i\mu N(x_j-x_n)/2} = (-1)^{j-n} = (-1)^{j+n},$$
$$e^{-i\mu N(x_j+x_n)/2} = e^{i\mu N(x_j+x_n)/2} = (-1)^{j+n} = (-1)^{j-n},$$
$$c_{-N/2} = c_{N/2} = 2, \quad c_l = 1 \ (|l| \neq N/2),$$

we obtain

$$\begin{aligned}
(D_1^2)_{j,n} &= \frac{1}{N}\sum_{l=-N/2}^{N/2}\left(\frac{-(l\mu)^2}{c_l^2}\right)e^{il\mu(x_j-x_n)} + 2(-1)^{j+n}\frac{\mu^2}{4N}\left(\frac{N}{2}\right)^2 \\
&= \frac{1}{N}\sum_{-N/2+1}^{N/2-1}\left(\frac{-(l\mu)^2}{c_l^2}\right)e^{il\mu(x_j-x_n)} \\
&= \frac{1}{N}\sum_{-N/2+1}^{N/2-1}\left(\frac{(il\mu)^2}{c_l}\right)e^{il\mu(x_j-x_n)}.
\end{aligned}$$

We rewrite $(D_1^2)_{j,n}$ as

$$(D_1^2)_{j,n} = \frac{1}{N}\sum_{l=-N/2}^{N/2} b_l(il\mu)^2 e^{il\mu(x_j-x_n)}, \tag{2.17}$$

where $b_{-N/2} = b_{N/2} = 0, b_l = \frac{1}{c_l} = 1 \ (|l| \neq N/2)$.

Using the same method, we have

$$\begin{aligned}
(D_1^3)_{j,n} &= \sum_{m=0}^{N-1}(D_1^2)_{j,m}(D_1)_{m,n} \\
&= \sum_{m=0}^{N-1}\frac{1}{N}\sum_{l=-N/2}^{N/2} b_l(il\mu)^2 e^{il\mu(x_j-x_m)}\frac{1}{N}\sum_{p=-N/2}^{N/2}\frac{ip\mu}{c_p}e^{ip\mu(x_m-x_n)} \\
&= \frac{1}{N}\sum_{l=-N/2}^{N/2}\sum_{p=-N/2}^{N/2}\frac{b_l(il\mu)^2 ip\mu}{c_p}e^{i\mu(lx_j-px_n)}\frac{1}{N}\sum_{m=0}^{N-1}e^{i\mu(p-l)x_m} \\
&= \frac{1}{N}\sum_{l=N/2}^{N/2}\frac{b_l(il\mu)^3}{c_l^3}e^{il\mu(x_j-x_n)} \\
&= \frac{1}{N}\sum_{l=N/2+1}^{N/2-1}\frac{(il\mu)^3}{c_l}e^{il\mu(x_j-x_n)}.
\end{aligned}$$

Applying induction on k leads to

$$(D_1^k)_{j,n} = \frac{1}{N}\sum_{l=-N/2+1}^{N/2-1}\frac{(il\mu)^k}{c_l}e^{il\mu(x_j-x_n)}. \tag{2.18}$$

Subtracting (2.18) from (2.15), we arrive at the equation (2.14). □

We note that D_1 is a real antisymmetric matrix. Using the spectral differentiation matrix, we obtain the standard Fourier pseudospectral semi-discretization for the nonlinear Schrödiger equation:

$$\frac{d}{dt}p_j + (D_2\mathbf{q})_j + a(p_j^2+q_j^2)q_j = 0, \tag{2.19}$$

$$\frac{d}{dt}q_j - (D_2\mathbf{p})_j - a(p_j^2+q_j^2)p_j = 0, \tag{2.20}$$

where $j = 0, 1, \cdots, N-1,\ \mathbf{p} = (p_0, \cdots, p_{N-1})^T, \mathbf{q} = (q_0, \cdots, q_{N-1})^T$.

Since D_2 is symmetric, (2.19)-(2.20) is a Hamiltonian system with Hamiltonian

$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}[\mathbf{p}^T D_2\mathbf{p} + \mathbf{q}^T D_2\mathbf{q}] + \frac{a}{4}\sum_{j=0}^{N-1}(p_j^2+q_j^2)^2.$$

Therefore, symplectic methods should be used to integrate in time.

Here we have presented the standard Fourier pseudospectral method in some detail in order to show that the first spectral differentiation matrix D_1 derived in the above way is antisymmetric. In the following slightly different way, the spectral differentiation matrix is not antisymmetric.

From (2.6), it is obvious that $\widehat{p}_{-N/2} = \widehat{p}_{N/2}$ and $e^{iN\mu x_j/2} = e^{-iN\mu x_j/2}$. Thus we can rewrite (2.10) as

$$p_j = \sum_{l=-N/2}^{N/2-1} \bar{\widehat{p}}_l e^{il\mu x_j}, \tag{2.21}$$

where $\bar{\widehat{p}}_l = \widehat{p}_l\ (l = -N/2+1, \cdots, N/2-1), \bar{\widehat{p}}_{-N/2} = 2\widehat{p}_{-N/2}$.

Similarly, we have

$$q_j = \sum_{l=-N/2}^{N/2-1} \bar{\widehat{q}}_l e^{ilx_j}, \tag{2.22}$$

where $\bar{\widehat{q}}_l = \widehat{q}_l\ (l = -N/2+1, \cdots, N/2-1), \bar{\widehat{q}}_{-N/2} = 2\widehat{q}_{-N/2}$.

It is more efficient to implement Fast Fourier Transform using (2.21) and (2.22) instead of (2.10) and (2.11). However, the following fact should be noted.

Let

$$\bar{I}_N p(x,t) = \sum_{l=-N/2}^{N/2-1} \bar{\widehat{p}}_l e^{il\mu x}, \tag{2.23}$$

$$\bar{I}_N q(x,t) = \sum_{l=-N/2}^{N/2-1} \bar{\widehat{q}}_l e^{il\mu x}. \tag{2.24}$$

It is obvious that $\bar{I}_N p(x,t) \neq I_N p(x,t), \bar{I}_N q(x,t) \neq I_N q(x,t)$. In fact,

$$I_N p(x,t) = \bar{I}_N p(x,t) + \widehat{p}_{N/2}(e^{iN\mu x/2} - e^{-iN\mu x/2}), \tag{2.25}$$

$$I_N q(x,t) = \bar{I}_N q(x,t) + \widehat{q}_{N/2}(e^{iN\mu x/2} - e^{-iN\mu x/2}). \tag{2.26}$$

The spectral differentiation matrix is not antisymmetric if we use (2.23) and (2.24) instead of (2.8) and (2.9) when deriving the spectral differentiation matrix. In fact, the resulting spectral differentiation matrix has diagonal entries $-i/2$.

ETNA
Kent State University
etna@mcs.kent.edu

3. The multi-symplectic Fourier pseudospectral method for NLS. As was mentioned in the Introduction, Bridges and Reich introduced the idea of multi-symplectic Fourier transform and obtained multi-symplectic semi-discretization on Fourier space. They showed that the resulting semi-discretization leads automatically to a finite dimensional Hamiltonian system in time when truncated. They also used the 1D shallow-water equations and the Z-K equation as examples to demonstrate the local conservation property of the multi-symplectic spectral discretization. Their theory applies to both spectral and pseudospectral methods [4]. Here we derive the multi-symplectic structure of the Fourier pseudospectral method for the NLS directly from the real space.

Applying the Fourier pseudospectral method to the multi-symplectic system (1.8) and using the notations

$$\mathbf{p} = (p_0, \cdots, p_{N-1})^T, \mathbf{q} = (q_0, \cdots .q_{N-1})^T,$$
$$\mathbf{v} = (v_0, \cdots, v_{N-1})^T, \mathbf{w} = (w_0, \cdots .w_{N-1})^T,$$

we obtain

$$\begin{aligned} \frac{dq_j}{dt} - (D_1\mathbf{v})_j &= a(p_j^2 + q_j^2)p_j, \\ -\frac{dp_j}{dt} - (D_1\mathbf{w})_j &= a(p_j^2 + q_j^2)q_j, \\ (D_1\mathbf{p})_j &= v_j, \\ (D_1\mathbf{q})_j &= w_j. \end{aligned} \tag{3.1}$$

Here $j = 0, 1, \cdots, N-1$ and D_1 is the first order spectral differentiation matrix.

THEOREM 3.1. *The Fourier pseudospectral semi-discretization (3.1) has N semi-discrete multi-symplectic conservation laws*

$$\frac{d}{dt}\omega_j + \sum_{k=0}^{N-1} (D_1)_{j,k}\kappa_{jk} = 0, \quad j = 0, 1, \cdots, N-1, \tag{3.2}$$

where

$$\omega_j = \frac{1}{2}(dz_j \wedge M dz_j), \quad \kappa_{jk} = \frac{1}{2}[dz_j \wedge K dz_k + dz_k \wedge K dz_j],$$

and $z_j = (p_j, q_j, v_j, w_j)^T, j = 0, 1, \cdots, N-1$. M and $K$are the antisymmetric matrices in the Introduction.

Proof. We rewrite (3.1) in the compact form

$$M\frac{d}{dt}z_j + K\sum_{k=0}^{N-1} (D_1)_{j,k} z_k = \bigtriangledown_z S(z_j). \tag{3.3}$$

The variational equation associated with (3.3) is

$$M\frac{d}{dt}dz_j + K\sum_{k=0}^{N-1} (D_1)_{j,k} dz_k = S_{zz}(z_j)dz_j. \tag{3.4}$$

Taking the wedge product with dz_k and noting the fact

$$dz_j \wedge S_{zz}(z_j)dz_j = 0,$$

we obtain the N multi-symplectic conservation laws (3.2). □

Since D_1 is antisymmetric and $\kappa_{jk} = \kappa_{kj}$, we can sum (3.2) over the spatial index and obtain

$$\frac{d}{dt}\sum_{j=0}^{N-1}\omega_j = 0, \tag{3.5}$$

which implies conservation of the total symplecticity over time [4]. Thus it is natural to integrate with respect to time using a symplectic integrator. We discretize (3.1) with respect to time by the midpoint rule and obtain

$$\begin{aligned}
&\frac{q_j^1 - q_j^0}{\Delta t} - (D_1\mathbf{v}^{1/2})_j - a((p_j^{1/2})^2 + (q_j^{1/2})^2)p_j^{1/2} = 0,\\
&\frac{p_j^1 - p_j^0}{\Delta t} + (D_1\mathbf{w}^{1/2})_j + a((p_j^{1/2})^2 + (q_j^{1/2})^2)q_j^{1/2} = 0,\\
&(D_1\mathbf{p}^{1/2})_j = v_j^{1/2},\\
&(D_1\mathbf{q}^{1/2})_j = w_j^{1/2}.
\end{aligned} \tag{3.6}$$

Here, without loss of generality, we take the time index as 0 and 1 instead of n and $n+1$. Δt is the time step length. $\mathbf{p}^{1/2} = \frac{1}{2}(\mathbf{p}^0 + \mathbf{p}^1)$, etc.

THEOREM 3.2. *The scheme (3.6) has N full-discrete multi-symplectic conservation laws*

$$\frac{\omega_j^1 - \omega_j^0}{\Delta t} - \sum_{k=0}^{N-1}(D_1)_{j,k}\kappa_{j,k}^{1/2} = 0, \tag{3.7}$$

where $\omega_j^n = \frac{1}{2}dz_j^n \wedge M dz_j^n, n = 0, 1,$ *and* $\kappa_{j,k}^{1/2} = \frac{1}{2}(dz_j^{1/2} \wedge K dz_k^{1/2} + dz_k^{1/2} \wedge K dz_j^{1/2})$, $j = 0, 1, \cdots, N-1$.

Proof. From Theorem 3.1, we know that (3.6) can be rewritten in the compact form

$$M\frac{z_j^1 - z_j^0}{\Delta t} + K\sum_{k=0}^{N-1}(D_1)_{j,k}z_k^{1/2} = \bigtriangledown_z S(z_j^{1/2}). \tag{3.8}$$

The variational equation associated with (3.8) is

$$M\frac{dz_j^1 - dz_j^0}{\Delta t} + K\sum_{k=0}^{N-1}(D_1)_{j,k}dz_k^{1/2} = S_{zz}(z_j^{1/2})dz_j^{1/2}. \tag{3.9}$$

Taking the wedge product with $dz_j^{1/2}$ and noting the fact

$$dz_j^{1/2} \wedge S_{zz}(z_j^{1/2})dz_j^{1/2} = 0, \quad dz_j^{1/2} = \frac{1}{2}(dz_j^0 + dz_j^1),$$

we obtain the full-discrete multi-symplectic conservation laws (3.7) after slightly complicated but trivial derivations. □

The full-discrete multi-symplectic conservation laws are completely local, and therefore the scheme (3.6) has remarkable local conservation properties [8]. In the next section, we shall demonstrate this observation.

ETNA
Kent State University
etna@mcs.kent.edu

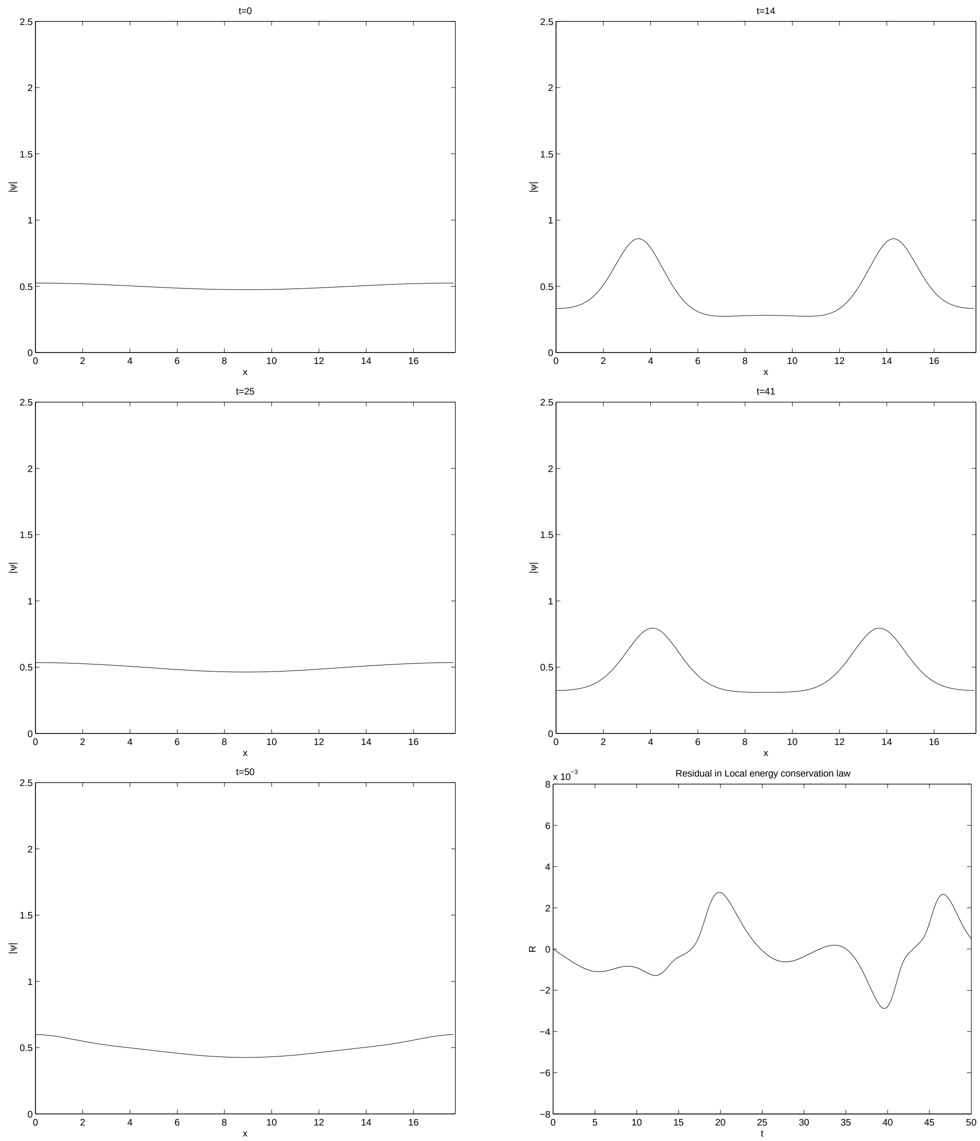

Fig.1 Waveforms at $t = 0, 14, 25, 41, 50$ and the residual in local ECL

4. Numerical experiments. For the numerical experiments, we consider the cubic NLS

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0, \tag{4.1}$$

with initial condition

$$\psi(x, 0) = 0.5 + 0.025\cos(\mu x), \tag{4.2}$$

and periodic boundary condition $\psi(0, t) = \psi(L, t)$. Here $L = 4\sqrt{2}\pi$, $\mu = 2\pi/L$. The initial condition (4.2) is in the vicinity of the homoclinic orbit [1].

Now we perform numerical experiments using the scheme (3.6). Special attention is paid to monitoring the local energy conservation law (1.10). First, we consider the discrete version of (1.10). Corresponding to the scheme (3.6), the discrete local energy conservation law is

$$\begin{aligned} &\frac{E_i^1 - E_i^0}{\Delta t} + (D_1 \mathbf{F}^{\frac{1}{2}})_i = R_i, \\ &E_i^n = \frac{1}{2}[((p_i^n)^2 + (q_i^n)^2)^2 - (v_i^n)^2 - (w_i^n)^2], \quad n = 0, 1, \\ &\mathbf{F}^{\frac{1}{2}} = \mathbf{v}^{\frac{1}{2}}(\frac{\mathbf{p}^1 - \mathbf{p}^0}{\Delta t}) + \mathbf{w}^{\frac{1}{2}}(\frac{\mathbf{q}^1 - \mathbf{q}^0}{\Delta t}). \end{aligned} \tag{4.3}$$

Here $i = 0, 1, \cdots, N-1$ and R_i is the residual in the local energy conservation law due to the discretization.

We take $N = 256, \Delta t = 0.01$ and compute for $0 \leq t \leq 50$. In Figure 1, the waveforms at different time levels and the residual in the local energy conservation law are showed. From the waveforms, we can clearly observe the recurrence of the state. The residual in the discrete local energy conservation law (ECL) is summed over the spatial index i from $i = 100$ to $i = 150$. That is, $R = \sum_{i=100}^{150} R_i$. We note that the scheme (3.6) exhibits a good local energy conservation property. The reason behind this performance is that the scheme (3.6) satisfies the multi-symplectic conservation laws. The local ECL is a useful indicator of spatial discretization errors. The large fluctuations in local ECL when using a multi-symplectic spectral discretization indicate a coarse discretization, since the local ECL is a natural part of the multi-symplectic spectral discretizations [4].

5. Conclusions. Using the multi-symplectic formulation of the NLS, we show that the Fourier pseudospectral semi-discretization of the nonlinear Schrödinger equation with periodic boundary conditions has N semi-discrete multi-symplectic conservation laws. The symplectic discretization in time of the semi-discretization leads to N full-discrete multi-symplectic conservation laws. These results have helped us to gain a deeper understanding of the Fourier pseudospectral method. We also prove a result on the spectral differentiation matrix. The numerical experiments show that the multi-symplectic spectral discretizations have remarkable local conservation properties.

For other multi-symplectic Hamiltonian systems, such as Sine-Gordon equation and KdV equation, we can arrive at the same conclusions.

REFERENCES

[1] M. J. Ablowitz and B. M. Herbst, *On homoclinic structure and numerically induced chaos for the nonlinear Schrödinger equation,* SIAM J. Appl. Math., 50 (1990), pp. 339–351.

[2] T. J. Bridges, *Multi-symplectic structures and wave propagation,* Math. Proc. Cambridge Philos. Soc., 121 (1997), pp. 147–190.

[3] T. J. Bridges and S. Reich, *Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity,* Technical Report.

[4] T. J. Bridges and S. Reich, *Multi-symplectic spectral discretizations for the Zakharov-Kuznetsov and shallow water equations*, Technical Report.

[5] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. Zang, *Spectral Methods in Fluid Dynamics*, Springer-Verlag, New York, 1988.

[6] B. Fornberg, *A Practical Guide to Pseudospectral Methods*, Cambridge University Press, 1996.

[7] D. Gottlib, M. Y. Hussaini, and S. A. Orszag, *Theory and applications of spectral methods,* in Spectral Methods for Partial Differential Equations, R. G. Voigt, D. Gottlieb, and M. Y. Hussaini, eds., SIAM-CBMS, Philadelphia, 1984, pp. 1–54.

ETNA
Kent State University
etna@mcs.kent.edu

[8] S. REICH, *Multi-Symplectic Runge-Kutta Collocation Methods for Hamiltonian Wave Equations*, J. Comput. Phys., 157 (2000), pp. 473–499.