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MULTISYMPLECTIC FOURIER PSEUDOSPECTRAL METHOD FOR THE NONLINEAR SCHRÖDINGER EQUATIONS WITH WAVE OPERATOR *1)

Jian Wang
(*Department of Mathematics, Shanghai Jiaotong University, Division of Computational Science, E-Institute of Shanghai Universities, Shanghai 200240, China*
Email: math_wangjian@sohu.com)

Abstract

In this paper, the multisymplectic Fourier pseudospectral scheme for initial-boundary value problems of nonlinear Schrödinger equations with wave operator is considered. We investigate the local and global conservation properties of the multisymplectic discretization based on Fourier pseudospectral approximations. The local and global spatial conservation of energy is proved. The error estimates of local energy conservation law are also derived. Numerical experiments are presented to verify the theoretical predications.

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Key words: Multisymplecticity, Fourier pseudospectral method, Local conservation laws.

1. Introduction

The nonlinear Schrödinger equations with wave operator (NSEW)

$$\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} + i\frac{\partial\psi}{\partial t} + g(|\psi|^2)\psi = 0, \tag{1.1}$$

is one of the most important models of mathematical physics, with applications in different fields such as plasma physics, nonlinear optics, water waves and biomolecular dynamics. In this work, we will concentrate on equation (1.1) subject to initial-boundary conditions

$$\begin{aligned} &\psi(0,t) = \psi(L,t), \\ &\psi(x,0) = \psi_0, \quad \psi_t(x,0) = \psi_1. \end{aligned} \tag{1.2}$$

The important feature of problem (1.1)-(1.2) is the following energy conservation law

$$\|\psi_t\|^2 + \|\psi_x\|^2 + \int_0^L Q(|\psi|^2)dx = const., \tag{1.3}$$

where Q is a primitive function of g, defined by

$$Q(s) = \int_0^s g(x)dx.$$

Several numerical methods have been investigated for solving equation (1.1), such as finite difference methods with conservative type [1, 2].

Bridge and Reich presented a multisymplectic integrator based on a multisymplectic structure of some Hamiltonian PDEs, such as Schrödinger equations and Klein-Gordon equations [3, 4]. The theoretical results indicated that significant features of the multisymplectic integrator are excellent for local invariant properties. Many numerical experiments demonstrated

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that the multisymplectic-preserving methods can preserve local and global conservation properties for long time computations [3, 4, 6, 9, 10, 11, 12, 13]. Moreover, when the Hamiltonian function is quadratic, the multisymplectic integrators preserve discrete local energy and local momentum exactly. However, error estimates of energy and momentum conservation laws for the multisymplectic integrator in the literature remain very limited. Recently, Hong and Li [10] used Runge-Kutta methods to construct multisymplectic schemes for the nonlinear Dirac equations and presented the error estimates of local and global conservation laws of energy and momentum.

Fourier pseudospectral methods have been proven very powerful for periodic initial value problems with constant coefficients. The well known results include spectral accuracy for smooth solutions and dispersion free. These properties are important in the numerical simulation of some physical phenomena.

The NSEW admits a multisymplectic Hamiltonian formulation. It is our objective in this paper to apply the multisymplectic Fourier pseudospectral method [9] to the equation and discuss properties of energy conservation law.

This paper is structured as follows. In Section 2, the multisymplectic Hamiltonian formulation for NSEW is established and some conservation properties are obtained. Section 3 is concerned with multisymplectic Fourier pseudospectral discretizations and spatial conservation laws of energy. Section 4 involves the construction of fully discretizations scheme and error estimates of energy conservation law. Numerical experiments are given in Section 5. Finally, Section 6 contains concluding remarks.

2. Multisymplecticity and Local Conservation Law

A Hamiltonian differential equation is said to be multisymplectic if it can be written as

$$\mathbf{M}\partial_t \mathbf{z} + \mathbf{K}\partial_x \mathbf{z} = \nabla_z S(\mathbf{z}), \tag{2.1}$$

where ∂_t and ∂_x are the operators of total differentiation with respect to t and x, respectively; $\mathbf{M}$, $\mathbf{K} \in R^{d\times d}$ are skew-symmetric; $\mathbf{z}(x,t)$ is the vector of state variables and $S\colon R^d \to R^1$ is a smooth function; $\nabla_z S(\mathbf{z})$ denotes the gradient of the function $S = S(\mathbf{z})$ with respect to variable $\mathbf{z}$.

According to [3, 4], an important consequence of multisymplecticity is that the system (2.1) has a multisymplectic conservation law (MSCL):

$$\partial_t \omega + \partial_x \kappa = 0, \tag{2.2}$$

where ω and κ are pre-symplectic forms

$$\omega = dz \wedge \mathbf{M}_+ dz, \quad \kappa = dz \wedge \mathbf{K}_+ dz, \tag{2.3}$$

which define a symplectic space-time structure. Here $\wedge$ is the exterior multiplication of the two vectors, and $\mathbf{M}_+$ and $\mathbf{K}_+$ satisfy

$$\mathbf{M} = \mathbf{M}_+ + \mathbf{M}_- \quad \textit{and} \quad \mathbf{K} = \mathbf{K}_+ + \mathbf{K}_-,$$

with

$$\mathbf{M}_+^T = -\mathbf{M}_- \quad \textit{and} \quad \mathbf{K}_+^T = -\mathbf{K}_-.$$

For example, $\mathbf{M}_+$ and $\mathbf{K}_+$ can be taken as the upper triangular part of matrix $\mathbf{M}$ and $\mathbf{K}$, respectively [8].

The MSCL (2.2) is a local property which indicates that symplecticity for Hamiltonian PDEs can be vary locally over the spatial domain.

The system (2.1) has local energy conservation law (LECL)

$$\partial_t E + \partial_x F = 0, \tag{2.4}$$

with energy density

$$E = S(\mathbf{z}) + \mathbf{z}_x^T \mathbf{K}_+ \mathbf{z},$$

and energy flux

$$F = -\mathbf{z}_t^T \mathbf{K}_+ \mathbf{z}.$$

The system (2.1) also has momentum conservation law (LMCL)

$$\partial_t I + \partial_x G = 0, \tag{2.5}$$

with momentum density

$$I = -\mathbf{z}_x^T \mathbf{M}_+ \mathbf{z},$$

and momentum flux

$$G = S(\mathbf{z}) + \mathbf{z}_t^T \mathbf{M}_+ \mathbf{z}.$$

For periodic boundary conditions, the local conservation laws can be integrated in x to obtain global conservation of energy and momentum [6].

In order to multisymplectify the system (1.1), let $\psi = a + ib$, $\psi_t = u + iv$, $\psi_x = p + iq$, where a, b, u, v, p, q are real functions. In terms of these functions, the system (1.1) can be rewritten as the following first-order system

$$\begin{cases} u_t - b_t - p_x = -g(a^2 + b^2)a, \\ -a_t = -u, \\ a_x = p, \\ a_t + v_t - q_x = -g(a^2 + b^2)b, \\ -b_t = -v, \\ b_x = q, \end{cases} \tag{2.6}$$

which can be formulated as multisymplectic Hamiltonian system (2.1) with state variable $\mathbf{z} = (a, u, p, b, v, q)^T$ and two skew-symmetric matrices

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

The Hamiltonian function $S : R^6 \to R$, is given by

$$\begin{aligned} S &= \frac{1}{2}(p^2 + q^2 - u^2 - v^2) - \frac{1}{2}Q(a^2 + b^2) \\ &= \frac{1}{2}(|\psi_x|^2 - |\psi_t|^2) - \frac{1}{2}Q(|\psi|^2). \end{aligned}$$

By direct calculations, we can prove that with above two skew-symmetric matrices the system (2.6) satisfies the multisymplectic conservation law

$$\begin{aligned} \omega &= d\mathbf{z} \wedge \mathbf{M}_+ d\mathbf{z} = da \wedge du + db \wedge da + db \wedge dv, \\ \kappa &= d\mathbf{z} \wedge \mathbf{K}_+ d\mathbf{z} = dp \wedge du + dq \wedge dv. \end{aligned}$$

The system (2.6) has a local energy conservation law (2.4) with energy density

$$E = -\frac{1}{2}Q(a^2 + b^2) - \frac{1}{2}(p^2 + q^2 + u^2 + v^2) \tag{2.7}$$

and energy flux

$$F = up + vq. \tag{2.8}$$

The system (2.6) also has local momentum conservation law (2.5) with momentum density

$$I = -pu - qv + pb \tag{2.9}$$

and momentum flux

$$G = -\frac{1}{2}Q(a^2 + b^2) + \frac{1}{2}(p^2 + q^2 + u^2 + v^2) - ub. \tag{2.10}$$

The LECL and LMCL are the local properties because they are independent of boundary conditions. However, under appropriate assumptions, such as periodic boundary condition or zero boundary condition, we can obtain the corresponding global conservation laws of local properties.

Proposition 2.1. *Under the assumptions of periodic boundary condition* (1.2)*, the system* (1.1) *has global energy and momentum conservation laws*

$$\frac{d}{dt}\mathcal{E}(\psi) = 0, \tag{2.11}$$

and

$$\frac{d}{dt}\mathcal{P}(\psi) = 0, \tag{2.12}$$

where

$$\begin{aligned} &\mathcal{E}(\psi) = \|\psi_t\|^2 + \|\psi_x\|^2 + \textstyle\int_0^L Q(|\psi|^2)dx, \\ &\mathcal{P}(\psi) = \textstyle\int_0^L (\Im(\psi)\Re(\psi_x) - \frac{1}{2}(\psi_x\overline{\psi_t} + \overline{\psi_x}\psi_t))dx. \end{aligned} \tag{2.13}$$

In (2.13)*, $\Re(u), \Im(u)$ and $\overline{u}$ denote the real, imaginary part and the conjugate of the complex function u respectively.*

Proof. First, we note that

$$\mathcal{E}(\psi) = -2\int_R E dx, \qquad \mathcal{P}(\psi) = \int_R I dx. \tag{2.14}$$

Integrating (2.4) over interval $[0, L]$ yields

$$\int_0^L \partial_t E dx + \int_0^L \partial_x F dx = 0. \tag{2.15}$$

The periodic boundary condition (1.2) implies

$$\int_0^L \partial_x F dx = F|_0^L = 0. \tag{2.16}$$

Substituting (2.16) into (2.15) and using the expression of E give

$$\tfrac{d}{dt}[-\tfrac{1}{2}\textstyle\int_0^L Q(a^2 + b^2)dx - \int_0^L (u^2 + v^2 + p^2 + q^2)dx] = 0,$$

which shows that (2.11) holds. Similarly, combining (2.14) and the local momentum conservation law (2.5), we can obtain the momentum conservation law (2.12).

3. Semi-discrete Approximation and Spatial Conservation Laws

The multisymplectic integrator was first introduced by Bridge [3]. The discretization of the multisymplectic PDE (2.1) and the multisymplectic conservation law (2.2) can be solved numerically by

$$\mathbf{M}\partial_t^{j,k}\mathbf{z}_j^k + \mathbf{K}\partial_x^{j,k}\mathbf{z}_j^k = (\nabla_z S(\mathbf{z}))_j^k, \tag{3.1}$$

and

$$\partial_t^{j,k}\omega_j^k + \partial_x^{j,k}\kappa_j^k = 0, \tag{3.2}$$

where $(\nabla_z S(\mathbf{z}))_j^k = (\nabla_z S(\mathbf{z}_j^k))$, $\partial_t^{j,k}$ and $\partial_x^{j,k}$ are discretizations of the corresponding derivatives ∂_t and ∂_x respectively, and

$$\omega_j^k = \frac{1}{2}(dz)_j^k \wedge \mathbf{M}(dz)_j^k, \quad \kappa_j^k = \frac{1}{2}(dz)_j^k \wedge \mathbf{K}(dz)_j^k.$$

The numerical schemes (3.1) is said to be multisymplectic if (3.2) is a discrete conservation law of (3.1) [3, 4].

Bridge and Reich [5] introduced the multisymplectic Fourier transform for multisymplectic PDEs with periodic boundary conditions. Multisymplectic Fourier transform leads to the multisymplecticity on Fourier space. Chen and Qin [9] demonstrated that the Fourier pseudospectral discretization applied to the periodic nonlinear Schrödinger equation lead to a multisymplectic integrator. In this section, we will apply Fourier pseudospectral discretizations to the NSEW (1.1), which yields a multisymplectic integrator. We start by introducing some basic properties of the Fourier pseudospectral method that will be used in the remaining of the paper. For simplicity, we will consider the spatial domain $\Lambda = [0, L]$.

For any integer $N > 0$, denote by

$$S_N = \{g_j(x); -N/2 \le j \le N/2 - 1\}$$

the interpolation space, where $g_j(x)$ is a trigonometric polynomial of degree $N/2$ given explicitly by

$$g_j(x) = \frac{1}{N} \sum_{l=-N/2}^{N/2} \frac{1}{c_l} e^{il\mu(x-x_j)}. \tag{3.3}$$

In (3.3), $c_l = 1$ ($|l| \neq N/2$), $c_{-N/2} = c_{N/2} = 2$, $\mu = \frac{2\pi}{L}$.

Let $h = \frac{L}{N}$ be spatial step. Consider the set of points

$$x_j = hj, \quad j = 0, 1, \cdots, N-1,$$

referred as collocation nodes. The discrete Fourier coefficients of a function u in Λ with respect to these points are

$$\widetilde{u}_l = \frac{1}{Nc_l} \sum_{j=0}^{N-1} u(x_j) e^{-il\mu x_j}. \tag{3.4}$$

Due to the orthogonality relation

$$\frac{1}{N} \sum_{m=0}^{N-1} e^{i\mu p x_m} = \begin{cases} 1, & p = nN, n \text{ is an integer} \\ 0, & p \neq nN \end{cases}, \tag{3.5}$$

we have the inversion formula

$$u_j = u(x_j) = \sum_{l=-N/2}^{N/2} \widetilde{u}_l e^{il\mu x_j}. \tag{3.6}$$

The interpolation operator I_N is defined as follows. For a function $u(x) \in C^0(\Lambda)$, $N/2$-degree trigonometric interpolation operator I_N at the nodes satisfies

$$I_N u(x_j) = u(x_j), \quad j = 0, 1, \cdots, N-1.$$

For $u, v \in C^0(\Lambda)$, define the bilinear form

$$(u, v)_N = h \sum_{j=0}^{N-1} u(x_j)\overline{v(x_j)}. \tag{3.7}$$

Associate with (3.7) is the discrete norm

$$\|u\|_N = (u,u)_N^{1/2}. \tag{3.8}$$

It is easy to verify that

$$(I_N u, v)_N = (u,v)_N, \quad \forall u, v \in S_N. \tag{3.9}$$

As a consequence, (3.7) is an inner product on S_N, and the interpolation operator I_N can be regarded as an orthogonal projection on S_N with respect to the inner product (3.7).

The values for the derivatives $\frac{d}{dx} I_N u(x)$ at the collocation points x_j are obtained in terms of the values of u_j and the differential matrix D_N, i.e.

$$\frac{d}{dx} I_N u(x)|_{x=x_j} = (D_N u)_j,$$

where D_N represents Fourier pseudospectral differential matrix with the elements

$$d_{j,s} = \begin{cases} (-1)^{j+s} \frac{\pi}{L} \cot \frac{(x_j - x_s)\pi}{L}, & s \neq j, \\ 0, & s = j. \end{cases}$$

We introduce the notation of the Hadamard product of vectors and state its properties.

Definition 3.1. *Let $u = (u_0, u_1, \cdots, u_{N-1})^T$ and $v = (v_0, v_1, \cdots, v_{N-1})^T$. The Hadamard product of vectors is defined by*

$$u \circ v = (u_0 v_0, u_1 v_1, \cdots, u_{N-1} v_{N-1})^T.$$

According to the definition of the discrete inner product and the discrete norm, following identities can be derived easily.

Lemma 3.1. (1) $h \sum_{j=0}^{N-1} (u \circ v)_j = (u,v)_N$, *and* (2) $h \sum_{j=0}^{N-1} (u \circ u)_j = \|u\|_N^2$.

Lemma 3.2. *Let $u(x), v(x) \in S_N$, $u = (u_0, u_1, \cdots, u_{N-1})^T, v = (v_0, v_1, \cdots, v_{N-1})^T$, where $u_j = u(x_j), v_j = v(x_j)$, with x_j being the Fourier collocation points. Then*

$$D_N(u \circ v) = D_N u \circ v + u \circ D_N v. \tag{3.10}$$

Proof. Let D_x represent the differential operator $\frac{d}{dx}$. Since $u \in S_N$, we have

$$\begin{aligned} D_x u(x) = D_x(I_N u(x)) &= D_x[\sum_{l=-N/2}^{N/2} (\frac{1}{N c_l} \sum_{n=0}^{N-1} u(x_n) e^{-il\mu x_n}) e^{il\mu x}] \\ &= \sum_{l=-N/2}^{N/2} \sum_{n=0}^{N-1} \frac{il\mu}{N c_l} u(x_n) e^{il\mu(x - x_n)}. \end{aligned}$$

On the other hand, by the definition of D_N

$$\begin{aligned} (D_N u)_j = \sum_{n=0}^{N-1} d_{j,n} u(x_n) &= \sum_{n=0}^{N-1} \frac{1}{N} (D_x \sum_{l=-N/2}^{N/2} \frac{1}{c_l} e^{il\mu(x - x_n)})|_{x=x_j} u(x_n) \\ &= \sum_{n=0}^{N-1} \sum_{l=-N/2}^{N/2} \frac{il\mu}{N c_l} u(x_n) e^{il\mu(x_j - x_n)} \\ &= (D_x u(x))|_{x=x_j}. \end{aligned}$$

Thus, we get

$$(D_x u(x))|_{x=x_j} = (D_N u)_j. \tag{3.11}$$

From the definition of Hadamard product, (3.11) implies

$$[D_x(u(x)\cdot v(x))]|_{x=x_j} = [D_N(u\circ v)]_j. \tag{3.12}$$

Combining (3.12) and the following identity

$$[D_x(u(x)\cdot v(x))]|_{x=x_j} = [D_x u(x)]|_{x=x_j}\cdot v(x_j) + u(x_j)\cdot [D_x v(x)]|_{x=x_j},$$

we obtain

$$[D_N(u\circ v)]_j = [D_x u(x)]_{x=x_j}\cdot v(x_j) + u(x_j)\cdot [D_x v(x)]_{x=x_j},$$

which is equivalent to (3.10). The proof is completed.

Lemma 3.3. *Let* $u=(u_0,u_1,\cdots,u_{N-1})^T$ *and* $v=(v_0,v_1,\cdots,v_{N-1})^T$. *Then*

$$h\sum_{j=0}^{N-1}[D_N(u\circ v)]_j = 0. \tag{3.13}$$

Proof. By virtue of Lemmas 3.1 and 3.2, and note that D_N is skew-symmetric, we have

$$h\sum_{j=0}^{N-1}[D_N(u\circ v)]_j = (D_N u, v)_N + (u, D_N v)_N = 0,$$

which complete the proof.

The semi-discrete Fourier pseudospectral approximation for system (2.6) is constructed as follows: Find $a(t),b(t),u(t),v(t),p(t),q(t)\in S_N$, such that

$$\begin{cases} u_t(x_j,t) - b_t(x_j,t) - (D_N p)(x_j,t) = -g[a^2(x_j,t)+b^2(x_j,t)]a(x_j,t),\\ -a_t(x_j,t) = -u(x_j,t),\\ (D_N a)(x_j,t) = p(x_j,t),\\ a_t(x_j,t) + v_t(x_j,t) - (D_N q)(x_j,t) = -g[a^2(x_j,t)+b^2(x_j,t)]b(x_j,t),\\ -b_t(x_j,t) = -v(x_j,t),\\ (D_N b)(x_j,t) = q(x_j,t). \end{cases} \tag{3.14}$$

Rewrite (3.14) as complex function: Find $\psi(t),\phi(t),w(t)\in S_N$, such that

$$\begin{cases} \phi_t(x_j,t) - (D_N w)(x_j,t) + i\psi_t(x_j,t) = -g(|\psi(x_j,t)|^2)\psi(x_j,t),\\ \psi_t(x_j,t) = \phi(x_j,t),\\ (D_N\psi)(x_j,t) = w(x_j,t). \end{cases} \tag{3.15}$$

The system (3.14) is called the multisymplectic Fourier pseudospectral discretization for system (2.6), because it satisfies the following multisymplectic conservation law.

Theorem 3.1. *The multisymplectic Fourier pseudospectral discretization* (3.14) *has* N *semi-discrete multisymplectic conservation laws*

$$\frac{d}{dt}\omega_j + \sum_{k=0}^{N-1}(D_N)_{jk}\kappa_{jk} = 0, \quad (j=0,1,\cdots,N-1), \tag{3.16}$$

and satisfies the total symplecticity in time

$$\frac{d}{dt}\sum_{j=0}^{N-1}\omega_j = 0, \tag{3.17}$$

where

$$\omega_j = d\mathbf{z}_j\wedge\mathbf{M}_+ d\mathbf{z}_j = da_j\wedge du_j + db_j\wedge da_j + db_j\wedge dv_j; \tag{3.18}$$

$$\begin{aligned}\kappa_{jk} &= d\mathbf{z}_j\wedge\mathbf{K}_+ dz_k + d\mathbf{z}_k\wedge\mathbf{K}_+ d\mathbf{z}_j\\ &= dp_j\wedge du_k + dq_j\wedge dv_k + dp_k\wedge du_j + dq_k\wedge dv_j.\end{aligned} \tag{3.19}$$

Proof. First, rewrite (3.14) as a compact form

$$\mathbf{M}\frac{d}{dt}\mathbf{z}_j + \mathbf{K}\sum_{k=0}^{N-1}(D_N)_{j,k}\mathbf{z}_k = \nabla_z S(\mathbf{z}_j). \tag{3.20}$$

The variational equation associated with (3.20) is

$$\mathbf{M}\frac{d}{dt}d\mathbf{z}_j + \mathbf{K}\sum_{k=0}^{N-1}(D_N)_{j,k}d\mathbf{z}_k = \nabla_{zz} S(\mathbf{z}_j)d\mathbf{z}_j. \tag{3.21}$$

Taking the wedge product with $d\mathbf{z}_j$ on both sides of (3.21) and noting that

$$\begin{gathered} d\mathbf{z}_j \wedge \nabla_{zz} S(\mathbf{z}_j)d\mathbf{z}_j = 0, \\ \tfrac{1}{2}d\mathbf{z}_j \wedge \mathbf{M}d\mathbf{z}_j = d\mathbf{z}_j \wedge \mathbf{M}_+ d\mathbf{z}_j, \\ \tfrac{1}{2}d\mathbf{z}_j \wedge \mathbf{K}d\mathbf{z}_j = d\mathbf{z}_j \wedge \mathbf{K}_+ d\mathbf{z}_j, \end{gathered}$$

we can obtain (3.16). Summing the semi-discrete multisymplectic conservation law (3.16) over all spatial grid points, and noting that

$$\sum_{j=0}^{N-1}\sum_{k=0}^{N-1}(D_N)_{jk}\kappa_{jk} = 0, \tag{3.22}$$

we can reach the desired result (3.17). The proof is completed.

Theorem 3.1 indicates in addition to conservation of local symplecticity (3.16), it also has conservation of total symplecticity in time (3.17). This partially explains that the multisymplectic integrators can well approximate the energy and momentum conservation of the system over long time [13]. Furthermore, it is found that the spatial conservation property of energy to the NSWE when the Fourier pseudospectral discretizations is used.

Theorem 3.2. *The multisymplectic Fourier pseudospectral discretization* (3.14) *satisfies the local spatial energy conservation law*

$$\frac{d}{dt}E_j(t) + (D_N F(t))_j = 0, \quad j = 0, 1, \cdots, N-1, \tag{3.23}$$

where

$$\begin{aligned} &E_j(t) = -\tfrac{1}{2}Q[a_j^2(t) + b_j^2(t)] - \tfrac{1}{2}[u_j^2(t) + v_j^2(t) + p_j^2(t) + q_j^2(t)], \\ &F(t) = u(t) \circ p(t) + v(t) \circ q(t); \end{aligned} \tag{3.24}$$

and the spatial energy conservation law

$$\frac{d}{dt}\mathcal{E}(t) = 0, \tag{3.25}$$

where

$$\mathcal{E}(t) = -2h\sum_{j=0}^{N-1}E_j(t) = h\sum_{j=0}^{N-1}Q(|\psi_j|^2) + (\|\psi_t(t)\|_N^2 + \|\psi_x(t)\|_N^2). \tag{3.26}$$

Proof. We consider the abstract form of (3.14)

$$\mathbf{M}\frac{d}{dt}\mathbf{z}_j(t) + \mathbf{K}(D_N\mathbf{z}(t))_j = \nabla_z S(\mathbf{z}_j(t)). \tag{3.27}$$

Let $\mathbf{K} = \mathbf{K}_+ + \mathbf{K}_-$ with $\mathbf{K}_+^T = -\mathbf{K}_-$. Taking inner product with $\frac{d}{dt}\mathbf{z}_j(t)$ on both sides of (3.27) and noting that $(\frac{d}{dt}\mathbf{z}_j(t), \mathbf{M}\frac{d}{dt}\mathbf{z}_j(t)) = 0$, we obtain

$$(\tfrac{d}{dt}\mathbf{z}_j(t), \mathbf{K}_+(D_N\mathbf{z}(t))_j) + (\tfrac{d}{dt}\mathbf{z}_j(t), \mathbf{K}_-(D_N\mathbf{z}(t))_j) = \tfrac{d}{dt}S(\mathbf{z}_j(t)).$$

It follows

$$\begin{array}{l}\frac{d}{dt}[S(\mathbf{z}_j(t)+(D_N\mathbf{z}(t))_j,\mathbf{K}_+\mathbf{z}_j(t))]\\ -(\frac{d}{dt}\mathbf{z}_j(t),\mathbf{K}_+(D_N\mathbf{z}(t))_j)-(\mathbf{K}_+\mathbf{z}_j(t),(D_N\frac{d}{dt}\mathbf{z}(t))_j)=0.\end{array} \tag{3.28}$$

By some computations, it is not difficult to show that

$$\begin{array}{l}S(\mathbf{z}_j(t))+(D_N\mathbf{z}(t))_j,\mathbf{K}_+\mathbf{z}_j(t))]\\ =-\frac{1}{2}Q[a_j^2(t)+b_j^2(t)]-\frac{1}{2}[u_j^2(t)+v_j^2(t)+p_j^2(t)+q_j^2(t)],\end{array} \tag{3.29}$$

and

$$\begin{array}{l}(\frac{d}{dt}\mathbf{z}_j(t),\mathbf{K}_+(D_N\mathbf{z}(t))_j)+(\mathbf{K}_+\mathbf{z}_j(t),(D_N\frac{d}{dt}\mathbf{z}(t))_j)\\ =-u_j(t)(D_Np(t))_j-v_j(t)(D_Nq(t))_j-p_j(t)(D_Nu(t))_j-q_j(t)(D_Nv(t))_j\\ =-(D_N(u(t)\circ p(t))_j-(D_N(v(t)\circ q(t))_j.\end{array} \tag{3.30}$$

Substituting (3.29) and (3.30) into (3.28) and using Hadamard product and Lemma 3.1, we can obtain (3.23).

According to Lemma 3.3 and (3.24), we have

$$h\sum_{j=0}^{N-1}(D_NF(t))_j=0. \tag{3.31}$$

Multiplying (3.23) by $-2h$, summing over the spatial index and by using (3.31), we can obtain the desired result (3.25). The proof of this theorem is then complete.

4. Fully Discrete Scheme and Error Estimation of Energy Conservation Law

To obtain a multisymplectic integrator, symplectic time integrator methods, such as implicit midpoint method and symplectic Störmer-Verlet method, should be used.

Let $\mathbf{z}^n=(z_1^n,z_2^n,\cdots,z_{N-1}^n)^T$, where $\mathbf{z}_j^n$ denotes the numerical approximation of $\mathbf{z}(x_j,t_n)$. Let $\Delta t=t_{n+1}-t_n$ be the temporal step. In addition, define the average operator

$$\mu_t\mathbf{z}_j^n=\tfrac{1}{2}(\mathbf{z}_j^{n+1}+\mathbf{z}_j^n),$$

and the difference operator

$$\delta_t^+\mathbf{z}_j^n=\tfrac{1}{\Delta t}(\mathbf{z}_j^{n+1}-\mathbf{z}_j^n).$$

For difference operator δ_t^+ and average operator μ_t, we have the following lemma (see[14]).

Lemma 4.1. *Let $B(v,w)$ be a bilinear form. Then a discrete chain rule holds for $B(v,w)$*

$$B(\delta_x^+\mathbf{v}_i^n,\mu_x\mathbf{w}_i^n)+B(\mu_x\mathbf{v}_i^n,\delta_x^+\mathbf{w}_i^n)=\delta_x^+B(\mathbf{v}_i^n,\mathbf{w}_i^n).$$

Applying the implicit midpoint rule to discretize (3.14) in time yields a simple second-order Fourier pseudospectral scheme

$$\left\{\begin{array}{l}\delta_t^+u_j^n-\delta_t^+b_j^n-(D_N\mu_tp^n)_j=-g[(\mu_ta_j^n)^2+(\mu_tb_j^n)^2]\mu_ta_j^n,\\ -\delta_t^+a_j^n=-\mu_tu_j^n,\\ (D_N\mu_ta^n)_j=\mu_tp_j^n,\\ \delta_j^+a_j^n+\delta_t^+v_j^n-(D_N\mu_tq^n)_j=-g[\mu_ta_j^n)^2+(\mu_tb_j^n)^2]\mu_tb_j^n,\\ -\delta_t^+b_j^n=-\mu_tv_j^n,\\ (D_N\mu_tb^n)_j=\mu_tq_j^n.\end{array}\right. \tag{4.1}$$

The abstract form of (4.1) is

$$\mathbf{M}\delta_t^+\mathbf{z}_j^n+\mathbf{K}(D_N\mu_t\mathbf{z}^n)_j=\nabla_zS(\mu_t\mathbf{z}_j^n). \tag{4.2}$$

Following the argument similar to the proof of Theorem 3.1, we can obtain the fully discrete multisymplectic conservation law.

Theorem 4.1. *The integrator* (4.1) *has N fully-discrete multisymplectic conservation laws*

$$\delta_t^+ \omega_j^n + \sum_{k=0}^{N-1} (D_N)_{jk} \mu_t \kappa_{jk}^n = 0, \quad (j = 0, 1, \cdots, N-1), \tag{4.3}$$

and also satisfies the total symplecticity in time

$$\sum_{j=0}^{N-1} \omega_j^{n+1} = \sum_{j=0}^{N-1} \omega_j^n, \tag{4.4}$$

where

$$\begin{array}{ll} \omega_j^n & = d\mathbf{z}_j^n \wedge \mathbf{M}_+ d\mathbf{z}_j^n \\ & = da_j^n \wedge du_j^n + db_j^n \wedge da_j^n + db_j^n \wedge dv_j^n; \\ \kappa_{jk}^n & = d\mathbf{z}_j^n \wedge \mathbf{K}_+ d\mathbf{z}_j^n \\ & = dp_j^n \wedge du_k^n + dq_j^n \wedge dv_k^n + dp_k^n \wedge du_j^n + dq_k^n \wedge dv_j^n. \end{array} \tag{4.5}$$

Islas and Schober [13] have proved that if $S(\mathbf{z})$ is the quadratic functional in $\mathbf{z}$, then the multisymplectic Fourier pseudospectral method (4.2) conserves the LECL and LMCL exactly. Since the equation (1.1) is nonlinear and $S(\mathbf{z})$ is not a quadratic function, we use the discretization of the forms

$$(R_E)_j^{n+1/2} = \delta_t^+ E_j^n + (D_N \mathbf{F}^{n+1/2})_j, \tag{4.6}$$

$$(R_M)_j^{n+1/2} = \delta_t^+ I_j^n + (D_N \mathbf{G}^{n+1/2})_j, \tag{4.7}$$

to evaluate the local conservation laws of energy and momentum, where

$$E_j^n = -\frac{1}{2} Q[(a_j^n)^2 + (b_j^n)^2] - \frac{1}{2}[(u_j^n)^2 + (v_j^n)^2 + (p_j^n)^2 + (q_j^n)^2],$$

$$\mathbf{F}^{n+1/2} = \mu_t \mathbf{u}^n \circ \mu_t \mathbf{p}^n + \mu_t \mathbf{v}^n \circ \mu_t \mathbf{q}^n, \quad I_j^n = p_j^n \cdot b_j^n - p_j^n \cdot u_j^n - q_j^n \cdot v_j^n,$$

$$\mathbf{G}^{n+1/2} = -\frac{1}{2} Q[(\mu_t \mathbf{a}^n)^2 + (\mu_t \mathbf{b}^n)^2] + \frac{1}{2}[(\mu_t \mathbf{u}^n)^2 + (\mu_t \mathbf{v}^n)^2 + (\mu_t \mathbf{p}^n)^2 + (\mu_t \mathbf{q}^n)^2] - \mu_t \mathbf{u}^n \circ \mu_t \mathbf{b}^n.$$

$(R_E)_j^{n+1/2}$ and $(R_M)_j^{n+1/2}$ are called the residual of LECL and LMCL, respectively. If $(R_E)_j^{n+1/2} = 0$, for all spatial index j and temporal index n, then we say the solutions of (4.2) satisfies discrete LECL.

In addition, we define the discrete energy and momentum as follows

$$\mathcal{E}^n = -2h \sum_{j=0}^{N-1} E_j^n, \quad \mathcal{P}^n = h \sum_{j=0}^{N-1} I_j^n. \tag{4.8}$$

Lemma 4.2. *The residual* $(R_E)_j^{n+1/2}$ *of the LECL has the expression:*

$$(R_E)_j^{n+1/2} = \delta_t^+ S(\mathbf{z}_j^n) - (\delta_t^+ \mathbf{z}_j^n, \nabla_z S(\mu_t \mathbf{z}_j^n)). \tag{4.9}$$

Proof. Taking inner product with $\delta_t^+ \mathbf{z}_j^n$ on both sides of (4.2) and noting that

$$(\delta_t^n \mathbf{z}_j^n, \mathbf{M} \delta_t^+ \mathbf{z}_j^n) = 0,$$

we have

$$(\delta_t^+ \mathbf{z}_j^n, \mathbf{K}(D_N \mu_t \mathbf{z}^n)_j) = (\delta_t^+ \mathbf{z}_j^n, \nabla_z S(\mu_t \mathbf{z}_j^n)). \tag{4.10}$$

Since matrix $\mathbf{K} = \mathbf{K}_+ + \mathbf{K}_-$ with $\mathbf{K}_+^T = -\mathbf{K}_-$, by Lemma 4.1, we can deduce

$$\begin{array}{l} (\delta_t^+ \mathbf{z}_j^n, \mathbf{K}_+(D_N \mu_t \mathbf{z}^n)_j) + (\delta_t^+ \mathbf{z}_j^n, \mathbf{K}_-(D_N \mu_t \mathbf{z}^n)_j) \\ = \delta_t^+ (\mathbf{z}_j^n, \mu_t \mathbf{z}_j^n) - (\mu_t \mathbf{z}_j^n, \delta_t^n \mathbf{K}_+(D_N \mathbf{z}^n)_j) - ((D_N \mu_t \mathbf{z}^n)_j, \mathbf{K}_+ \delta_t^n \mathbf{z}_j^n). \end{array} \tag{4.11}$$

Combining (4.10) and (4.11) gives

$$\begin{aligned}&\delta_t^+ S(\mathbf{z}_j^n) - (\delta_t^+ \mathbf{z}_j^n, \nabla_z S(\mu_t \mathbf{z}_j^n))\\ &= \delta_t^+[(\mathbf{K}_+ \mathbf{z}_j^n, (D_N \mathbf{z}^n)_j) + S(\mathbf{z}_j^n)] - (\mathbf{K}_+ \mu_t \mathbf{z}_j^n, (D_N \delta_t^+ \mathbf{z}^n)_j)\\ &-(\delta_t^+ \mathbf{z}_j^n, \mathbf{K}_+ (D_N \mu_t \mathbf{z}^n)_j).\end{aligned} \tag{4.12}$$

It is easy to show that

$$\begin{aligned}&(\mathbf{K}_+ \mu_t \mathbf{z}_j^n, (D_N \delta_t^+ \mathbf{z}^n)_j) + (\delta_t^+ \mathbf{z}_j^n, \mathbf{K}_+ (D_N \mu_t \mathbf{z}^n)_j)\\ &= -[D_N(\delta_t^+ \mathbf{z}_j^n, \mathbf{K}_+ \mu_t \mathbf{z}_j^n)]_j\\ &= -(D_N F^{n+1/2})_j.\end{aligned} \tag{4.13}$$

It follows from (4.12) and (4.13) that

$$(R_E)_j^{n+1/2} = \delta_t^+ S(\mathbf{z}_j^n) - (\delta_t^+ \mathbf{z}_j^n, \nabla S(\mu_t \mathbf{z}_j^n)).$$

The proof of this lemma is complete.

By using similar technique proposed by Hong and Li [10], we obtain the error estimates for the LECL and discrete energy.

Theorem 4.2. *Assume Δt is sufficiently small, and the solution $\mathbf{z}$ of (3.16) and $\partial_t \mathbf{z}$ are bounded in the considering (x,t) domain. Then there exists a constant C_1 independent of Δt and h, such that the residual $(R_E)_j^{n+1/2}$ of discrete LECL satisfies*

$$\left|(R_E)_j^{n+1/2}\right| \le C_1 \Delta t^2. \tag{4.14}$$

Proof. Let $\mathbf{z} = \frac{1}{2}(\mathbf{x}+\mathbf{y})$ and $\mathbf{v} = \mathbf{y} - \mathbf{x}$. Using Taylor's expansion gives

$$\begin{aligned}S(\mathbf{y}) &= S(\mathbf{z}) + \frac{1}{2} DS(\mathbf{z}) \cdot \mathbf{v} + \frac{1}{2! \times 4} D^2 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v})\\ &\quad + \frac{1}{3! \times 8} D^3 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v}, \mathbf{v}) + \frac{1}{4! \times 16} D^4 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v}, \mathbf{v}, \mathbf{v}) + O(\|\mathbf{v}\|^5),\\ S(\mathbf{x}) &= S(\mathbf{z}) - \frac{1}{2} DS(\mathbf{z}) \cdot \mathbf{v} + \frac{1}{2! \times 4} D^2 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v})\\ &\quad - \frac{1}{3! \times 8} D^3 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v}, \mathbf{v}) + \frac{1}{4! \times 16} D^4 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v}, \mathbf{v}, \mathbf{v}) + O(\|\mathbf{v}\|^5),\end{aligned}$$

which gives

$$S(\mathbf{y}) - S(\mathbf{x}) - DS(\mathbf{z}) \cdot \mathbf{v} = \frac{1}{3! \times 4} D^3 S(\mathbf{z}) \cdot (\mathbf{v}, \mathbf{v}, \mathbf{v}) + O(\|\mathbf{v}\|^5), \tag{4.15}$$

where the operator D is the first order derivative with respect to $\mathbf{z}$ (i.e. the gradient ∇_z), D^2 is the second derivative matrix ∇_{zz} and so on.

Let $\mathbf{v} = \alpha \mathbf{w}$, where $\alpha > 0$, and $\mathbf{w} \in R^d$ is a unit vector. Take $\mathbf{y} = \mathbf{z}_j^{n+1}$, $\mathbf{x} = \mathbf{z}_j^n$. Then the expression (4.15) can be written as

$$\begin{aligned}S(\mathbf{z}_j^{n+1}) - S(\mathbf{z}_j^n) &- (\nabla_z S(\mu_t \mathbf{z}_j^n), \mathbf{z}_j^{n+1} - \mathbf{z}_j^n)\\ &= \frac{1}{24} \alpha^3 D^3 S(\mu_t \mathbf{z}_j^n) \cdot (\mathbf{w}, \mathbf{w}, \mathbf{w}) + O(\alpha^5),\end{aligned}$$

or

$$(R_E)_j^{n+1/2} = \frac{1}{24 \Delta t} \alpha^3 D^3 S(\mu_t \mathbf{z}_j^n) \cdot (\mathbf{w}, \mathbf{w}, \mathbf{w}) + \frac{O(\alpha^5)}{\Delta t}. \tag{4.16}$$

Notice that $\frac{\alpha}{\Delta t} = \|\delta_t^+ \mathbf{z}_j^n\|$. Then the boundedness of $\mathbf{z}$ and $\partial_t \mathbf{z}$ imply

$$\frac{\alpha}{\Delta t} = \|\delta_t^+ \mathbf{z}_j^n\| \le C.$$

Thus, we have

$$\left|(R_E)_j^{n+1/2}\right| \le C_1\Delta t^2.$$

This complete the proof of this theorem.

Theorem 4.3. *Under the assumptions of Theorem* 4.2*, the local error of the energy* $\mathcal{E}^n$ *satisfies*

$$\left|\mathcal{E}^{n+1} - \mathcal{E}^n\right| \le C_2\Delta t^3, \tag{4.17}$$

where C_2 *is independent of* Δt *and* h*.*

Proof. By Theorem 4.2 and notice that $h\sum_{j=0}^{N-1}(D_N F^{n+1/2})_j = 0$, we have

$$\begin{aligned}\left|\mathcal{E}^{n+1} - \mathcal{E}^n\right| &= \Delta th\sum_{j=0}^{N-1}(R_E)_j^{n+1/2}\\ &\le \Delta th\sum_{j=0}^{N-1} C_1\Delta t^2 = LC_1\Delta t^3 \le C_2\Delta t^3.\end{aligned}$$

The proof is finished.

Corollary 4.1. *Under the assumptions of Theorem* 4.2*, the global error of the energy* $\mathcal{E}^n$ *satisfies*

$$\left|\mathcal{E}^n - \mathcal{E}^0\right| \le C_3\Delta t^2, \tag{4.18}$$

where C_3 *is independent of* Δt *and* h*.*

Now if

$$S(\mathbf{z}) = \frac{1}{2}\mathbf{z}^T\mathbf{A}\mathbf{z} + \mathbf{b}^T\mathbf{z}, \tag{4.19}$$

where $\mathbf{A}$ is an arbitrary symmetric matrix with the size in terms of $\mathbf{z}$, and $\mathbf{b}$ is any vector with the same size of $\mathbf{z}$, we have

$$D^k(\mathbf{z}) \equiv 0, \quad \text{for } k \ge 3.$$

According to (4.16), we find that

$$(R_E)_j^{n+1/2} \equiv 0.$$

In this situation, from Theorem 4.2 and Theorem 4.3, we can get that

Corollary 4.2. *For the multisymplectic Hamiltonian system* (2.1)*, if the Hamiltonian* $S(\mathbf{z})$ *has the form of* (4.19)*, then the multisymplectic Fourier pseudospectral method conserves the LECL and energy conservation law, i.e.*

$$(R_E)_j^{n+1/2} = 0, \quad \mathcal{E}^n - \mathcal{E}^0 = 0, \quad \textit{for } n \ge 1. \tag{4.20}$$

5. Numerical Experiments

To illustrate our results presented in previous sections, we present the numerical simulation results of the NSEW with periodic initial boundary conditions by using the multisymplectic Fourier pseudospectral method.

The complex vector notation of the multisymplectic Fourier pseudospectral method of (4.1) reads

$$\begin{cases} A_1\psi^{n+1} = A_2\psi^n + 2\Delta t\phi^n - \Delta t^2 g(\left|\psi^{n+1/2}\right|^2)\circ\psi^{n+1/2},\\ \phi^{n+1} = \frac{2}{\Delta t}(\psi^{n+1} - \psi^n) - \phi^n, \end{cases} \tag{5.1}$$

where $A_1 = (2 + i\Delta t)E_N - \frac{1}{2}\Delta t^2 D_N^2$, $A_2 = (2 + i\Delta t)E_N + \frac{1}{2}\Delta t^2 D_N^2$ and E_N is the identity matrix.

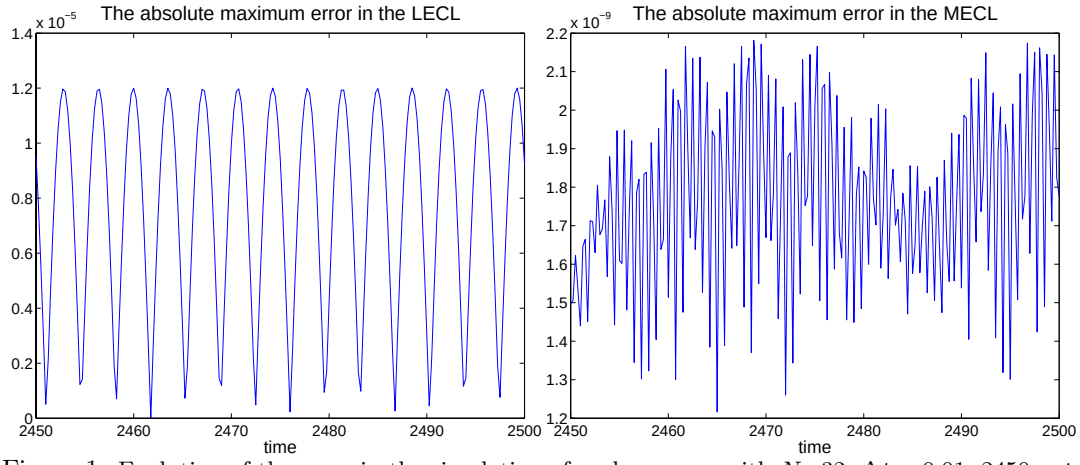

Figure 1: Evolution of the error in the simulation of a plane wave with N=32, $\Delta t = 0.01$, $2450 < t < 2500$. Left: maximum error in the LECL, right: maximum error in the LMCL.

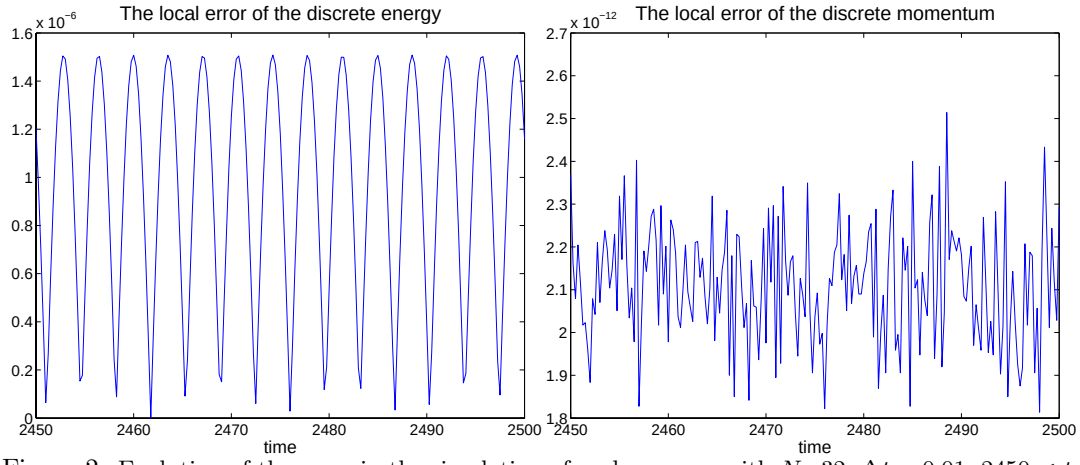

Figure 2: Evolution of the error in the simulation of a plane wave with N=32, $\Delta t = 0.01$, $2450 < t < 2500$. Left: maximum local error of the energy, right: maximum local error of the momentum.

The implementation of the first equation of (5.1) requires the solutions of a nonlinear system at each time step. We propose the following Predictor-Corrector algorithm which is much easier to implement and much more efficient in computations.
Predictor:

$$A_1\psi^{n+1,[0]} = A_2\psi^n + 2\Delta t\phi^n - \Delta t^2 g(|\psi^n|^2)\circ\psi^n \tag{5.2}$$

Corrector:

$$A_1\psi^{n+1,[l+1]} = A_2\psi^n + 2\Delta t\phi^n - \Delta t^2 g(\left|\frac{\psi^n+\psi^{n+1,[l]}}{2}\right|^2)\circ\frac{\psi^n+\psi^{n+1,[l]}}{2} \tag{5.3}$$
$$l = 0, 1, 2, \cdots$$

In our calculation, the iterations to solve system (5.3) on each time step were judged to be convergent if the maximum absolute error of two successive iterative values was less than approximately 1.0×10^{-15}.

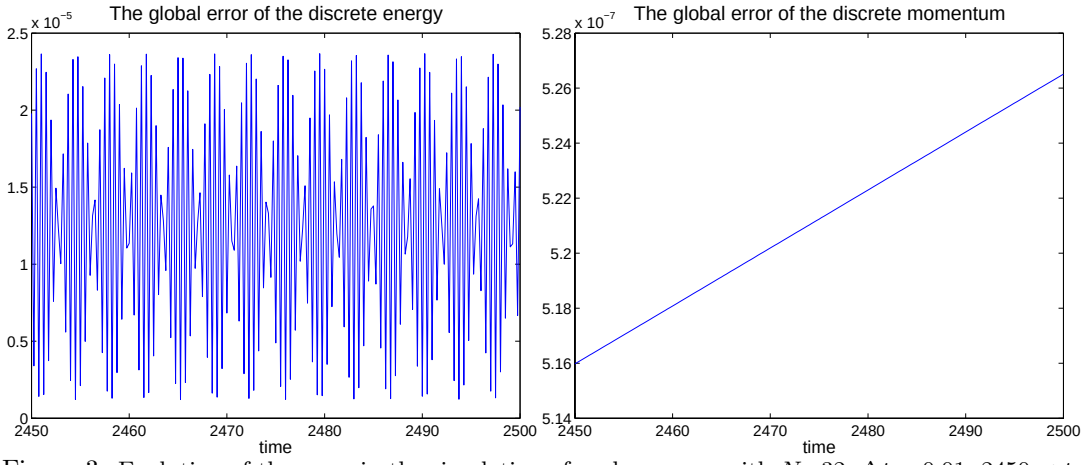

Figure 3: Evolution of the error in the simulation of a plane wave with N=32, $\Delta t = 0.01$, $2450 < t < 2500$. Left: maximum global error of the energy, right: maximum global error of the momentum.

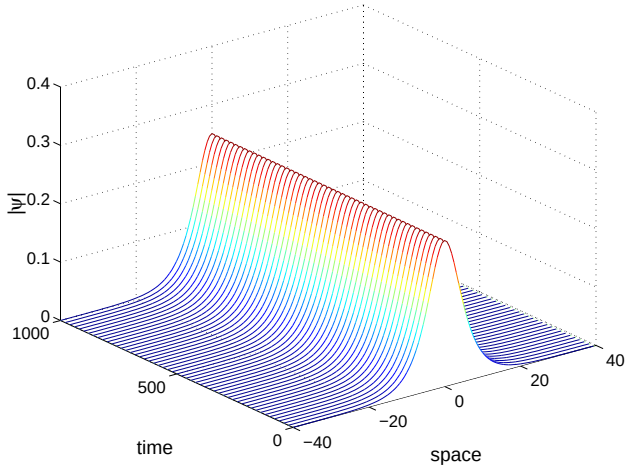

Figure 4: The modulus of the numerical solution of a solitary wave.

Let $\Delta\mathcal{E}^n = \mathcal{E}^n - \mathcal{E}$ and $\Delta\mathcal{P}^n = \mathcal{P}^n - \mathcal{P}$ be the global errors of discrete energy and momentum, $\Delta_l\mathcal{E}^n = \mathcal{E}^n - \mathcal{E}^{n-1}$ and $\Delta_l\mathcal{P}^n = \mathcal{P}^n - \mathcal{P}^{n-1}$ be the local errors of discrete energy and momentum at $t = n\Delta t$, respectively. Let

$$R_E = max|(R_E)_j^{n+1/2}|, \quad R_M = max|(R_M)_j^{n+1/2}|,$$
$$\Delta_l\mathcal{E} = \max|\Delta_l\mathcal{E}^n|, \quad \Delta_l\mathcal{P} = \max|\Delta_l\mathcal{P}^n|,$$
$$\Delta\mathcal{E} = \max|\Delta\mathcal{E}^n|, \quad \Delta\mathcal{P} = \max|\Delta\mathcal{P}^n|.$$

The purpose of the present numerical experiments is to verify numerically for the proposed schemes (i) the error in the energy conservation laws depends only on the temporal step Δt; (ii) the error in LECL and the global error of energy are second-order accurate in time while the local error of energy is of third-order accuracy; and (iii) the discrete momentum is conserved exactly since it is quadratic invariant.

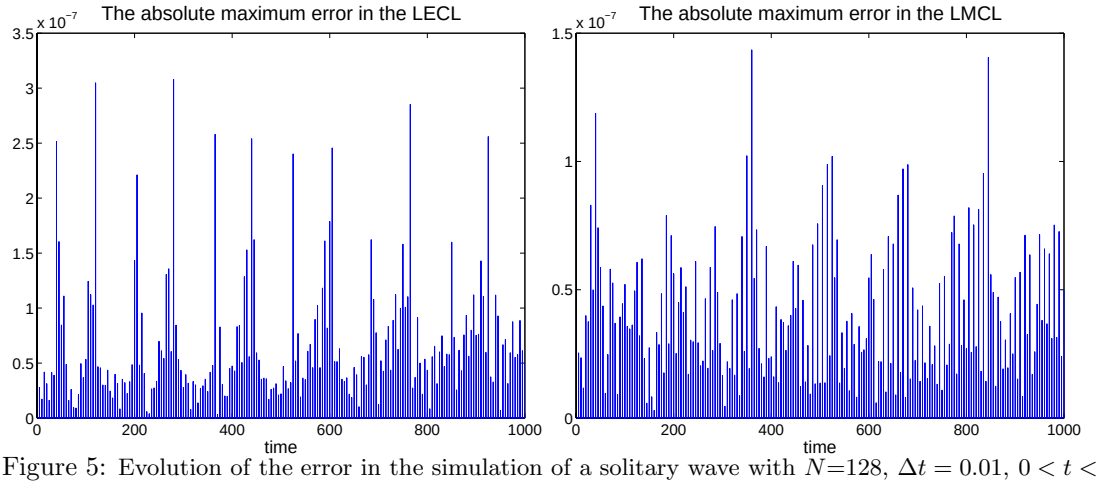

Figure 5: Evolution of the error in the simulation of a solitary wave with N=128, $\Delta t = 0.01$, $0 < t < 1000$. Left: maximum error in the LECL, right: maximum error in the LMCL.

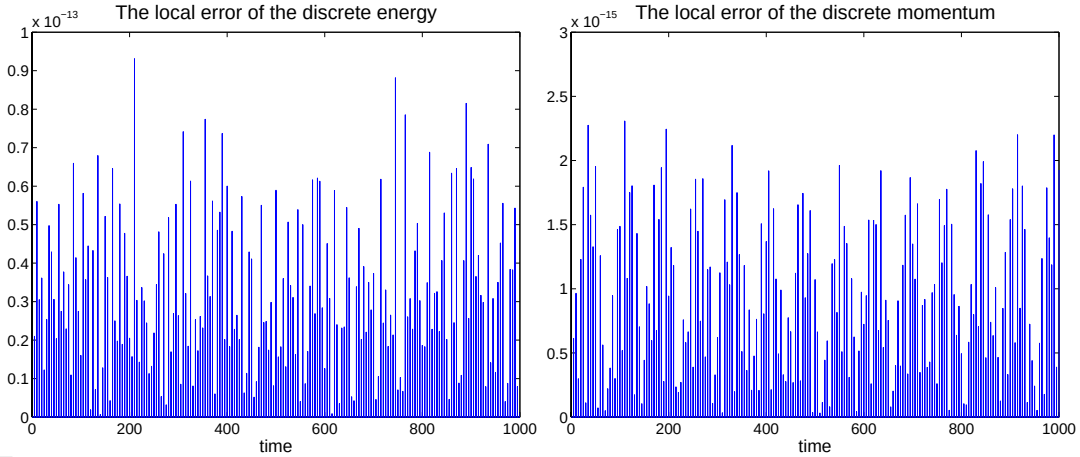

Figure 6: Evolution of the error in the simulation of a solitary wave with N=128, $\Delta t = 0.01$, $0 < t < 1000$. Left: maximum local error of the energy, right: maximum local error of the momentum.

Example 1. In the first example, we choose $g(s) = 2s$. The problem is solved with periodic boundary conditions on the space domain $[0, 2\pi]$, and the initial conditions

$$\psi_0 = (1 + 0.1 * i\cos(x)); \quad \psi_1 = i\sin(x),$$

for times up to $T = 100$.

Table 1 lists the numerical errors in the LECL and LMCL, and in the local and global errors of energy and momentum with various collocation points and temporal steps. It is observed from Table 1 that the errors in the LECL and the discrete energy are numerically independent of the number of collocation points, which are second order in time both in the LECL and in the global error of energy, third order in local error of energy. This is consistent with the theoretical results of Theorem 4.2 , Theorem 4.3 and Corollary 4.1.

Example 2. Plane wave solution. The NSEW (1.1) has a plane wave solution of the form

$$\psi(x,t) = Ae^{i(Kx-\Omega t)}. \tag{5.4}$$

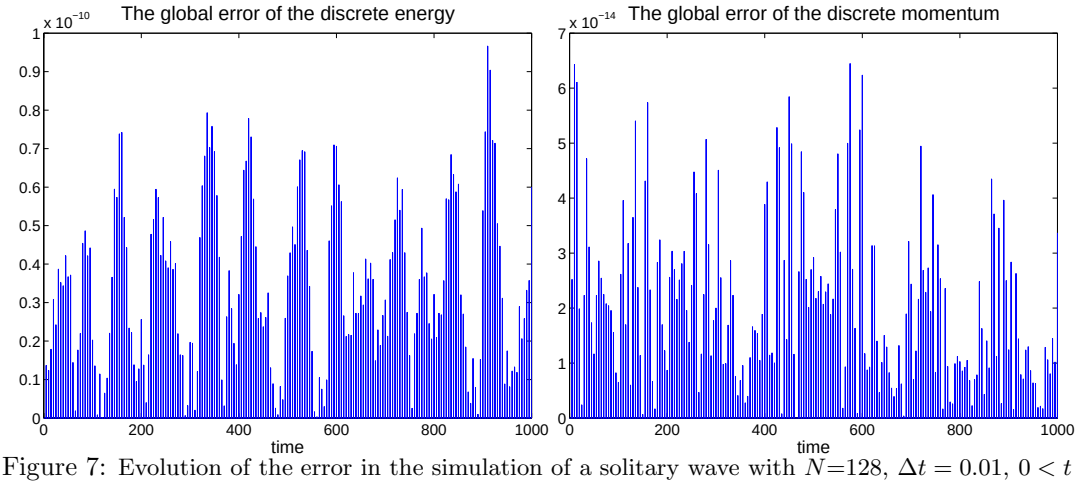

Figure 7: Evolution of the error in the simulation of a solitary wave with N=128, $\Delta t = 0.01$, $0 < t < 1000$. Left: maximum global error of the energy, right: maximum global error of the momentum.

Table 1: The errors in the LECL and LMCL, and the local and global errors of the discrete energy and momentum, with T=100.

N	32	32	32	64	64	64
Δt	0.05	0.01	0.005	0.05	0.01	0.005
R_E	3.95E-03	1.58E-04	4.06E-05	3.98E-03	1.59E-04	3.98E-05
R_M	8.52E-06	1.41E-05	1.39E-05	2.92E-07	4.58E-10	5.52E-11
$\Delta_l\mathcal{E}$	7.61E-04	6.13E-06	7.70E-07	7.61E-04	6.13E-06	7.67E-07
$\Delta_l\mathcal{P}$	1.69E-12	8.71E-13	7.36E-14	1.69E-12	8.70E-13	7.14E-14
$\Delta\mathcal{E}$	5.51E-03	2.21E-04	5.53E-05	5.51E-03	2.21E-04	5.53E-05
$\Delta\mathcal{P}$	2.84E-10	1.99E-10	4.34E-10	1.63E-10	1.80E-10	4.34E-10

where A is the amplitude, K is the wave-number and Ω is the frequency, which satisfy

$$\Omega^2 - \Omega - g(A^2) - K^2 = 0.$$

In this experiment, we choose $g(s) = 2s$, $A = \sqrt{3}$, $K = 6, \Omega = 7$. The problem is solved with periodic boundary conditions on the space domain $[0, 2\pi]$, and the initial conditions

$$\psi_0 = \sqrt{3}e^{i6x}, \quad \psi_1 = -7\sqrt{3}ie^{i6x},$$

for times up to $T = 2500$. It follows from (2.13) that the exact values of the energy $\mathcal{E}$ and the momentum $\mathcal{P}$ for this problem are $\mathcal{E} = 528\pi, \mathcal{P} = 234\pi$, respectively.

The local and global invariants obtained by using the multisymplectic Fourier pseudospectral schemes are very well preserved for long time computations. For example, the maximum errors in the LECL and LMCL for $2450 < t < 2500$ are $\mathcal{O}(10^{-5})$ and $\mathcal{O}(10^{-9})$ (see Figure 1), while the local errors of the discrete energy and momentum are $\mathcal{O}(10^{-6})$ and $\mathcal{O}(10^{-12})$ (see Figure 2), respectively. Moreover, Figure 1-3 show that the errors in the global invariants and the local conservation laws do not exhibit any growth for the duration of the simulation except for the global error of momentum.

Example 3. Solitary wave solution. We consider the following problem

$$\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} + i\frac{\partial\psi}{\partial t} - 2\left|\psi\right|^2\psi = 0, \tag{5.5}$$

with the boundary condition $\psi \to 0$ as $|x| \to +\infty$. The analytic expression of the solitary solution of the equation (5.5) is

$$\psi(x,t) = A\text{sech}(Kx)e^{i\Omega t},$$

where the amplitude A of the wave and Ω are relate to K through the relation

$$A = |K|, \qquad \Omega = \frac{1}{2}(-1 \pm \sqrt{1-4K^2}).$$

It is expected that the solitary solution will also be valid for sufficiently large (finite) region. Thus, we imposed the periodic boundary conditions on spatial domain that was sufficiently large so that the solitary waves were not affected by the boundaries.

We choose $K = \frac{1}{4}$ and $\Omega = -\frac{1}{2} - \frac{\sqrt{3}}{4}$. Using the numerical scheme presented in the previous section, we solve the equation (5.5) together with the initial condition

$$\psi_0 = \frac{1}{4}\text{sech}(Kx), \quad \psi_1 = -\frac{\Omega i}{4}\text{sech}(Kx), \tag{5.6}$$

on the interval $-40 \le x \le 40$ for times up to $T = 1000$. The modulus of the numerical solution obtained using spatial grid points $N = 128$ and a time step of $\Delta t = 0.01$ is presented in Figure 4, which shows that the solitary wave is stable in the sense that it does not leave dispersive oscillations. The evolution of the maximum errors in the LECL and LMCL are plotted in Figure 5 which shows that the errors are up to $\mathcal{O}(10^{-7})$. In Figure 6 and Figure 7, we present the local and global errors of the discrete energy and momentum, respectively. Clearly, we can see from Figure 6 and Figure 7 that the multisymplectic Fourier pseudospectral method preserves each of the conserved quantities very well (up to $\mathcal{O}(10^{-10})$ for energy and up to $\mathcal{O}(10^{-14})$ for momentum). This behavior provides a valuable check on our numerical results.

6. Conclusions

In this paper we have developed the multisymplectic Fourier pseudospectral method for the nonlinear Schrödinger equations with wave operator. The main issues are spatial energy conservation laws and the error estimates in the LECL and in the discrete energy. We have proved that the multisymplectic Fourier pseudospectral method proposed in this work admits the spatial energy conservation. Moreover, we demonstrated that the error in the LECL and the global error in discrete energy are second order in time, while the local error in the discrete energy is of third order. Numerical solutions are in good agreement with our theoretical results.

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