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Novel Multi-Symplectic Integrators for Nonlinear Fourth-Order Schrödinger Equation with Trapped Term

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Abstract. The multi-symplectic Runge-Kutta (MSRK) methods and multi-symplectic Fourier spectral (MSFS) methods will be employed to solve the fourth-order Schrödinger equations with trapped term. Using the idea of split-step numerical method and the MSRK methods, we devise a new kind of multi-symplectic integrators, which is called split-step multi-symplectic (SSMS) methods. The numerical experiments show that the proposed SSMS methods are more efficient than the conventional multi-symplectic integrators with respect to the the numerical accuracy and conservation perserving properties.

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Key words: Schrödinger equation with trapped term, multi-symplectic scheme, Fourier spectral method, conservation law, split-step method.

1 Introduction

Considering the effect of small fourth-order dispersion term in the propagation of intense laser beams in a bulk medium with Kerr nonlinearity, Karpman and Shagalov established the fourth-order Schrödinger equations [1–3]

$$iu_t+u_{xxxx}+\hbar'(|u|^2)u=0,\quad i=\sqrt{-1}. \tag{1.1}$$

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If an external trap potential is considered, the equation becomes the fourth-order nonlinear Schrödinger equation with a trapped term (FNSETT). In this work, we investigate the multi-symplectic integrators of the FNSETT in the form

$$iu_t+u_{xxxx}+6|u|^2u-150(\sin^2 x)u=0,\quad (x,t)\in(0,L)\times(0,T], \tag{1.2}$$

$$u(x,0)=u_0(x),\quad x\in[0,L], \tag{1.3}$$

$$u(x,t)=u(x+L,t),\quad t\in[0,T], \tag{1.4}$$

where $u_0(x)$ is a prescribed complex-valued function. The equation focuses on the most important physical effects, including dispersion, nonlinearity, and effective potential, and in the physical context, issues like Bose-Einstein condensate, nonlinear optics. The potential term $g(x)=-150\sin^2 x$ is to localize the wave around the origin. This model is a special case of the non-self-adjoint nonlinear high-order Schrödinger equation with trapped term [4–7]

$$i\frac{\partial u}{\partial t}+(-1)^m\alpha\frac{\partial^{2m}u}{\partial x^{2m}}+\frac{\partial\hbar(|u|^2)}{\partial|u|^2}u+g(x)u=0, \tag{1.5}$$

with $m=2$, $\alpha=1$, $g(x)=-150\sin^2 x$, $\hbar(|u|^2)=|u|^4$.

For the initial-boundary value problem (1.2)-(1.4), we have the following proposition.

Proposition 1.1. *The solution of the initial-boundary value problem* (1.2)-(1.4) *has at least two conserved quantities:*

1. *Charge conservation law*

$$\mathcal{Q}(t)=\int_0^L|u(x,t)|^2dx=\int_0^L|u_0(x)|^2dx=\mathcal{Q}(0); \tag{1.6}$$

2. *Energy conservation law*

$$\mathcal{E}(t)=\int_0^L[|u_{xx}|^2+3|u|^4-150(\sin^2 x)|u|^2]dx=\mathcal{E}(0). \tag{1.7}$$

Symplectic integrators have received much attention over the last decade, see, e.g., [8–12]. Recently, symplectic integrators had been generalized from Hamiltonian ODEs to Hamiltonian PDEs (HPDEs), see, e.g., [13–15]. We call this kind of numerical method multi-symplectic integrators. Many researchers are attracted by the methods for its incommensurable advantages over others for HPDEs in structure-preserving, such as in local conservation properties and in long-term numerical simulation. The method has been applied to many important physical and mathematical models, such as Schrödinger equations [16, 17], wave equations [18], Dirac equations [20], etc. It is suggested that concatenating a pair of symplectic Runge-Kutta (SRK) methods both in space and time, or concatenating an SRK method in time and Fourier spectral method in space lead to

multi-symplectic integrators, see, e.g., [14, 15, 20]. However, multi-symplectic schemes constructed by these techniques are completely implicit for non-separable HPDEs, and demand substantial computational cost. Moreover, the non-quadratic conserved quantities of the original system are not exactly preserved though their residuals are very small. To overcome the drawbacks, we introduce the split-step technique into the multi-symplectic integrator. We first split the original multi-symplectic system into several subsystems which are multi-symplectic, then construct multi-symplectic integrators for the subsystems. We call such schemes SSMS schemes, which do not require to solve nonlinear algebraic systems and are very economic. We only need to solve one or so linear algebraic system and some uncoupled algebraic equations by iteration. Moreover, the conserved quantities are preserved very well by the SSMS schemes.

We will consider multi-symplectic integrators for the FNSETT (1.2) in the work, including MSRK method, MSFS method and SSMS method.

In the rest of the section, we describe the multi-symplectic structure and local conservation laws for the FNSETT (1.2). To rewrite the complex equation (1.2) as real equations, suppose $u(x,t)=p(x,t)+iq(x,t)$, where $p(x,t),q(x,t)$ are real-valued functions, we have

$$-q_t+p_{xxxx}-150(\sin^2 x)p+6(p^2+q^2))p=0, \tag{1.8a}$$

$$p_t+q_{xxxx}-150(\sin^2 x)q+6(p^2+q^2))q=0. \tag{1.8b}$$

By introducing the Legendre transformation

$$\begin{aligned} &p_x(x,t)=\varphi(x,t), \quad q_x(x,t)=\alpha(x,t), \quad \varphi_x(x,t)=\psi(x,t),\\ &\alpha_x(x,t)=\beta(x,t), \quad \psi_x(x,t)=\eta(x,t), \quad \beta_x(x,t)=\gamma(x,t), \end{aligned}$$

one casts FNSETT (1.2) into the multi-symplectic framework

$$Mz_t+Kz_x=\nabla_z S(z), \tag{1.9}$$

where $z=(p,q,\varphi,\alpha,\psi,\beta,\eta,\gamma)^T$, ∇ is the gradient operator. The Hamiltonian functional is given by

$$S(z)=-\frac{3}{2}(p^2+q^2)^2+75(\sin^2 x)(p^2+q^2)+\frac{1}{2}(\psi^2+\beta^2)-\varphi\eta-\alpha\gamma,$$

and the skew-symmetric matrices M,K are

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

According to the multi-symplectic theories, the multi-symplectic system (1.9) satisfies the following local conservation laws:

- Multi-symplectic conservation law (MSCL):

$$\frac{\partial}{\partial t}\omega+\frac{\partial}{\partial x}\kappa=0, \tag{1.10}$$

where ω and κ are pre-symplectic 2-forms

$$\omega=dp\wedge dq,\quad \kappa=dp\wedge d\eta+dq\wedge d\gamma-d\varphi\wedge d\psi-d\alpha\wedge d\beta.$$

- Local energy conservation law (LECL):

$$\frac{\partial}{\partial t}E(z)+\frac{\partial}{\partial x}F(z)=0, \tag{1.11}$$

where the energy density $E(z)$ and the energy flux $F(z)$ are

$$E(z)=(150\sin^2 x-3(p^2+q^2))(p^2+q^2)-(\varphi\eta+\alpha\gamma+p\eta_x+q\gamma_x),$$
$$F(z)=p\eta_t+q\gamma_t-\varphi\psi_t-\alpha\beta_t+\psi\varphi_t+\beta\alpha_t-\eta p_t-\gamma q_t.$$

- Local momentum conservation law (LMCL):

$$\frac{\partial}{\partial t}I(z)+\frac{\partial}{\partial x}G(z)=0, \tag{1.12}$$

where the momentum density $I(z)$ and the momentum flux $G(z)$ are

$$I(z)=\varphi q-\alpha p,$$
$$G(z)=-3(p^2+q^2)^2+150(\sin^2 x)(p^2+q^2)\psi^2+\beta^2+pq_t-qp_t-2(\varphi\eta+\alpha\gamma).$$

The local conservation laws imply that the density can be varied from time to time; however, the variation of density in time is just offset by that of flux in space. Under appropriate circumstance, the local conservation laws imply total conservation laws

$$\overline{\omega}(t)=\int_0^L \omega(x,t)dx=C_1, \tag{1.13}$$

$$\mathcal{E}(t)=\int_0^L E(x,t)dx=C_2, \tag{1.14}$$

$$\mathcal{I}(t)=\int_0^L I(x,t)dx=C_3, \tag{1.15}$$

where C_1,C_2 and C_3 are constants independent of t.

The arrangement of this paper is as follows. In Section 2, we discuss the conventional multi-symplectic integrators for the FNSETT (1.2), including MSRK method and MSFS method. In Section 3, we sink the split-step technique into the multi-symplectic integrator and propose an SSMS method for the FNSETT. Numerical experiments are presented in Section 4 which mainly check the convergence and conservation properties of the schemes. We conclude the paper in Section 5.

2 Conventional multi-symplectic integrators for FNSETT

In this section, we present two contentional methods for constructing the multi-symplectic integrators for the HPDEs and then apply them to the FNSETT.

As usual, we introduce some notations: $x_j=jh$, $t_n=n\tau$, $j=0,1,2,\cdots,N$; $n=0,1,2,\cdots$, where $h=L/N$, τ are spatial length and temporal step span. The approximation of the value of the function $u(x,t)$ at the node (x_j,t_n) is denoted by u_j^n. $||u^n||=(h\sum_{j=1}^N|u_j^n|^2)^{\frac{1}{2}}$.

2.1 Multi-symplectic Runge-Kutta integrator

It has been proved that concatenating a pair of SRK methods both in time and space directions results in multi-symplectic scheme [13, 14]. The most frequently employed MSRK method for the multi-symplectic formulation (1.9) is the central box scheme

$$M\frac{z_{j+\frac{1}{2}}^{n+1}-z_{j+\frac{1}{2}}^{n}}{\tau}+K\frac{z_{j+1}^{n+\frac{1}{2}}-z_{j}^{n+\frac{1}{2}}}{h}=\nabla_z S\left(z_{j+\frac{1}{2}}^{n+\frac{1}{2}}\right), \tag{2.1}$$

where

$$z_{j+\frac{1}{2}}^{n+\frac{1}{2}}=\frac{1}{2}\left(z_{j+\frac{1}{2}}^{n+1}+z_{j+\frac{1}{2}}^{n}\right)=\frac{1}{2}\left(z_{j+1}^{n+\frac{1}{2}}+z_{j}^{n+\frac{1}{2}}\right)=\frac{1}{4}\left(z_{j+1}^{n+1}+z_{j+1}^{n}+z_{j}^{n+1}+z_{j}^{n}\right).$$

This scheme is of second-order in both time and space directions. For the FNSETT (1.2), the component formulation is

$$-\delta_t q_{j+\frac{1}{2}}^{n+\frac{1}{2}}+\frac{1}{h}\left(\eta_{j+1}^{n+\frac{1}{2}}-\eta_{j}^{n+\frac{1}{2}}\right)=-6|u_{j+\frac{1}{2}}^{n+\frac{1}{2}}|^2p_{j+\frac{1}{2}}^{n+\frac{1}{2}}+150(\sin^2x_{j+\frac{1}{2}})p_{j+\frac{1}{2}}^{n+\frac{1}{2}}, \tag{2.2a}$$

$$\delta_t p_{j+\frac{1}{2}}^{n+\frac{1}{2}}+\frac{1}{h}\left(\gamma_{j+1}^{n+\frac{1}{2}}-\gamma_{j}^{n+\frac{1}{2}}\right)=-6|u_{j+\frac{1}{2}}^{n+\frac{1}{2}}|^2q_{j+\frac{1}{2}}^{n+\frac{1}{2}}+150(\sin^2x_{j+\frac{1}{2}})q_{j+\frac{1}{2}}^{n+\frac{1}{2}}, \tag{2.2b}$$

$$\frac{1}{h}\left(\psi_{j+1}^{n+\frac{1}{2}}-\psi_{j}^{n+\frac{1}{2}}\right)=\eta_{j+\frac{1}{2}}^{n+\frac{1}{2}},\quad \frac{1}{h}\left(\beta_{j+1}^{n+\frac{1}{2}}-\beta_{j}^{n+\frac{1}{2}}\right)=\gamma_{j+\frac{1}{2}}^{n+\frac{1}{2}}, \tag{2.2c}$$

$$\frac{1}{h}\left(\varphi_{j+1}^{n+\frac{1}{2}}-\varphi_{j}^{n+\frac{1}{2}}\right)=\psi_{j+\frac{1}{2}}^{n+\frac{1}{2}},\quad \frac{1}{h}\left(\alpha_{j+1}^{n+\frac{1}{2}}-\alpha_{j}^{n+\frac{1}{2}}\right)=\beta_{j+\frac{1}{2}}^{n+\frac{1}{2}}, \tag{2.2d}$$

$$\frac{1}{h}\left(p_{j+1}^{n+\frac{1}{2}}-p_{j}^{n+\frac{1}{2}}\right)=\varphi_{j+\frac{1}{2}}^{n+\frac{1}{2}},\quad \frac{1}{h}\left(q_{j+1}^{n+\frac{1}{2}}-q_{j}^{n+\frac{1}{2}}\right)=\alpha_{j+\frac{1}{2}}^{n+\frac{1}{2}}, \tag{2.2e}$$

with difference quotient operator $\delta_t u_j^n=(u_j^{n+1}-u_j^n)/\tau$.

The coding for the multi-symplectic central box scheme (2.2) is quite complicated and not convenient with the prescribed initial and boundary conditions. An ideal alternative is to produce a numerical integrator which only depends on original variables u. The purpose can be attained by removing the discretization of the canonical momenta $\alpha,\beta,\eta,\gamma,\varphi,\psi$ at nodes, by using some standard algebraic procedures. The objective scheme reads

$$\begin{aligned}&\frac{i}{16}\left(\delta_t u_{j-2}^n+4\delta_t u_{j-1}^n+6\delta_t u_j^n+4\delta_t u_{j+1}^n+\delta_t u_{j+2}^n\right)+\delta_x^4 u_j^{n+\frac{1}{2}}\\ =&-\frac{3}{4}\left(\left|u_{j-\frac{3}{2}}^{n+\frac{1}{2}}\right|^2 u_{j-\frac{3}{2}}^{n+\frac{1}{2}}+3\left|u_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right|^2 u_{j-\frac{1}{2}}^{n+\frac{1}{2}}+3\left|u_{j+\frac{1}{2}}^{n+\frac{1}{2}}\right|^2 u_{j+\frac{1}{2}}^{n+\frac{1}{2}}+\left|u_{j+\frac{3}{2}}^{n+\frac{1}{2}}\right|^2 u_{j+\frac{3}{2}}^{n+\frac{1}{2}}\right)\\ &+\frac{75}{4}\left(\sin^2 x_{j-\frac{3}{2}} u_{j-\frac{3}{2}}^{n+\frac{1}{2}}+3\sin^2 x_{j-\frac{1}{2}} u_{j-\frac{1}{2}}^{n+\frac{1}{2}}+3\sin^2 x_{j+\frac{1}{2}} u_{j+\frac{1}{2}}^{n+\frac{1}{2}}+\sin^2 x_{j+\frac{3}{2}} u_{j+\frac{3}{2}}^{n+\frac{1}{2}}\right),\end{aligned}\tag{2.3}$$

with the difference quotient operator

$$\delta_x^4 u_j^n=\frac{u_{j-2}^n-4u_{j-1}^n+6u_j^n-4u_{j+1}^n+u_{j+2}^n}{h^4}.$$

This scheme is a second-order multi-symplectic integrator since the discrete version of MSCL is held.

2.2 Multi-symplectic Fourier spectral integrator

It has been verified that an appropriate Fourier discretization in space for the abstract multi-symplectic formulation (1.9) leaves the multi-symplectic character unchanged. In other words, the resulting semi-discrete system fulfills semi-discrete MSCL [15]. Therefore, we can discretize the multi-symplectic system (1.9) first via the Fourier spectral method in space direction, and then apply a standard SRK method to the time direction.

It is noticed that the first-order partial differential operator ∂_x yields the Fourier spectral differential matrix D_1, in case that the space direction is discretized by a Fourier spectral method. Here D_1 is a skew-symmetric matrix, whose entry is

$$(D_1)_{j,l}=\begin{cases}\frac{1}{2}(-1)^{j+l}\mu\cot\left(\mu\frac{x_j-x_l}{2}\right), & j\neq l,\\ 0, & j=l,\end{cases}\quad \text{for } j,l=1,2,\cdots,N,\tag{2.4}$$

where $\mu=2\pi/L$. For more details, see [15] and references therein. Applying the Fourier spectral method to Eq. (1.9) in the spatial direction, one obtains

$$-\frac{d}{dt}q_j+(D_1\eta)_j=-6|u_j|^2p_j+150(\sin^2 x_j)p_j,\tag{2.5a}$$

$$\frac{d}{dt}p_j+(D_1\gamma)_j=-6|u_j|^2q_j+150(\sin^2 x_j)q_j,\tag{2.5b}$$

$$(D_1\psi)_j=\eta_j,\quad (D_1\beta)_j=\gamma_j, \tag{2.5c}$$
$$(D_1\varphi)_j=\psi_j,\quad (D_1\alpha)_j=\beta_j, \tag{2.5d}$$
$$(D_1p)_j=\varphi_j,\quad (D_1q)_j=\alpha_j, \tag{2.5e}$$

where $p=(p_1,p_2,\cdots,p_N)^T$, $q=(q_1,q_2,\cdots,q_N)^T$, etc. The semi-discrete system (2.5) possesses the following N semi-discrete MSCLs

$$\frac{d}{dt}\omega_j+\sum_{l=1}^{N}D_{1jl}\kappa_{jl}=0,\quad l=1,2,\cdots,N, \tag{2.6}$$

where $\omega_j=dp_j\wedge dq_j$, and

$$\begin{aligned}\kappa_j=&dp_j\wedge d\eta_k+dp_k\wedge d\eta_j+dq_j\wedge d\gamma_k+dq_k\wedge d\gamma_j+d\psi_j\wedge d\varphi_k\\&+d\psi_k\wedge d\varphi_j+d\beta_j\wedge d\alpha_k+d\beta_k\wedge d\alpha_j.\end{aligned} \tag{2.7}$$

According to the symmetry of κ_{jl} and skew-symmetry of D_1, we can find that the conservation property of total symplecticity by summing over the spatial index in (2.6)

$$\frac{d}{dt}\sum_j\omega_j=0. \tag{2.8}$$

It can be verified that the semi-discrete system preserves the following N local energy conservation laws

$$\begin{aligned}&\frac{d}{dt}\Big[\big(150\sin^2x_j-3(p_j^2+q_j^2)\big)(p_j^2+q_j^2)-\big(\varphi_j\eta_j+\alpha_j\gamma_j+p_j(D_1\eta)_j+q_j(D_1\gamma)_j\big)\Big]\\&+\Big(D_1(p\eta_t+q\gamma_t-\varphi\psi_t-\alpha\beta_t+\psi\varphi_t+\beta\alpha_t-\eta p_t-\gamma q_t)\Big)_j=0,\quad j=1,2,\cdots,N.\end{aligned} \tag{2.9}$$

Applying the Euler midpoint scheme

$$\frac{z^{n+1}-z^n}{\tau}=J\nabla_zH(z^{n+\frac{1}{2}}), \tag{2.10}$$

to the semi-discretization (2.5), we have

$$-\frac{q^{n+1}-q^n}{\tau}+D_1\eta^{n+1/2}=-6|u^{n+1/2}|^2p^{n+1/2}+150(\sin^2\mathbf{x})p^{n+1/2}, \tag{2.11a}$$
$$\frac{p^{n+1}-p^n}{\tau}+D_1\gamma^{n+1/2}=-6|u^{n+1/2}|^2q^{n+1/2}+150(\sin^2\mathbf{x})q^{n+1/2}, \tag{2.11b}$$
$$D_1\psi^{n+1/2}=\eta^{n+1/2},\quad D_1\beta^{n+1/2}=\gamma^{n+1/2}, \tag{2.11c}$$
$$D_1\varphi^{n+1/2}=\psi^{n+1/2},\quad D_1\alpha^{n+1/2}=\beta^{n+1/2}, \tag{2.11d}$$
$$D_1p^{n+1/2}=\varphi^{n+1/2},\quad D_1q^{n+1/2}=\alpha^{n+1/2}, \tag{2.11e}$$

with $\mathbf{x}=(x_1,x_2,\cdots,x_N)^T$.

Proposition 2.1. *The scheme* (2.11) *is multi-symplectic. In other words, it satisfies N discrete MSCLs*

$$\frac{\omega_j^{n+1}-\omega_j^n}{\tau}+\sum_{l=1}^{N}D_{1jl}\kappa_{jl}^{n+1/2}=0,\quad j=1,2,\cdots,N, \tag{2.12}$$

where $\omega_j^n=dz_j^n\wedge Mdz_j^n=dp_j^n\wedge dq_j^n$ *and* $\kappa_j^{n+1/2}$ *is defined by* (2.7) *with a superscript* $n+1/2$ *on the right-hand side.*

Eliminating the intermediate variables $\alpha,\beta,\eta,\gamma,\varphi,\psi$, it gives rise to

$$i\frac{u^{n+1}-u^n}{\tau}+D_1^4u^{n+1/2}-150(\sin^2\mathbf{x})u^{n+1/2}+6|u^{n+1/2}|^2u^{n+1/2}=0, \tag{2.13}$$

where $u^n=(u_1^n,u_2^n,\cdots,u_N^n)^T$.

Theorem 2.1. *The multi-symplectic Fourier spectral scheme maintains the charge* (1.6) *unchanged, that is to say*

$$\mathcal{Q}^n=\|u^n\|^2=\cdots=\mathcal{Q}^0. \tag{2.14}$$

Proof. Multiplying the MSFS scheme (2.13) with $\overline{u^{n+1/2}}$, we have

$$\begin{aligned}&\frac{i}{2\tau}(u^{n+1}-u^n,u^{n+1}+u^n)+(D_1^4u^{n+1/2},u^{n+1/2})\\&\quad+(6|u^{n+1/2}|^2u^{n+1/2}-150(\sin^2\mathbf{x})u^{n+1/2},u^{n+1/2})=0.\end{aligned} \tag{2.15}$$

The second term of the above equality is real since D_1^4 is symmetric, and the third part is also real. The first term reads

$$\frac{i}{2\tau}(u^{n+1}-u^n,u^{n+1}+u^n)=\frac{i}{2\tau}\left(\|u^{n+1}\|^2-\|u^n\|^2\right)+\frac{i}{2\tau}\left[(u^{n+1},u^n)-(u^n,u^{n+1})\right], \tag{2.16}$$

On the RHS of Eq. (2.16), the last term is real, and the first part is purely imaginary. The conclusion (2.14) is derived from the above facts by induce. The proof is finished. □

3 Split-step multi-symplectic method for the FNSETT

In this section, we consider split-step multi-symplectic methods for the FNSETT (1.2) which penetrate the split-step idea into the multi-symplectic integrators. Splitting technique was originally used for multi-dimensional parabolic equations by Douglas et al. [22, 23]. It was generalized to nonlinear wave equations by Tappert [24], and now is widely employed for solving nonlinear PDEs for its simplicity and flexibility, see, e.g., [26, 27]. The method has also been successfully applied to symplectic geometric integrators [8, 9, 21]. However, the combination of multi-symplectic integrators with splitting

is very limited. The only work was done by Ryland in [19], which mentioned the splitting multi-symplectic concept. The basic idea of splitting is to decompose the original problem into subproblems which are easier to solve than the original one. Then the subproblems are approximated in a given order.

In what follows, we discuss the splitting multi-symplectic integrator for multi-symplectic formulation (1.9) through FNSETT.

Decompose the spatial symplectic structure matrix into $K=K_1+K_2$ and the Hamiltonian function into $S(z)=S^1(z)+S^2(z)$. The multi-symplectic formulation (1.9) splits into sub-multi-symplectic systems

$$Mz_t+K_iz_x=\nabla_z S^i(z),\quad i=1,2. \tag{3.1}$$

We can prove that the subsystems (3.1) satisfy MSCLs similar to (1.10):

$$\omega_t+\kappa_{ix}=0,\quad i=1,2, \tag{3.2}$$

where the new 2-forms are $\kappa_i=dz\wedge K_i dz$, $i=1,2$. It is quite clear that $\kappa_1+\kappa_2=\kappa$. In fact,

$$\kappa=dz\wedge Kdz=dz\wedge(K_1+K_2)dz=dz\wedge K_1dz+dz\wedge K_2dz=\kappa_1+\kappa_2.$$

Moreover, both of the subsystems (3.1) conserve the same total symplecticity ω. Thus, the total symplecticity (1.13) is conserved by the new subsystems. Similarly, we also have the total energy conservation law (1.14) and total momentum conservation law (1.15) for the new subsystems. Certainly, we can split the original system (1.9) into more than two subsystems. The number of subsystems depends entirely on the problem concerned. Next, we can approximate the sub-multi-symplectic systems (3.1) by multi-symplectic integrators, such as MSRK, MSFS, etc. Since both schemes for the subsystems conserve the symplecticity, one expects the total symplecticity to be preserved. We take the FNSETT (1.2) as a concrete example to describe the process.

We adopt linear-nonlinear splitting for the FNSETT (1.2) in the context. Let us first rewrite Eq. (1.2) in the form

$$iu_t=(\mathcal{L}+\mathcal{N})u, \tag{3.3}$$

where the linear and nonlinear operators are

$$\mathcal{L}=-\frac{\partial^4}{\partial x^4},\quad \mathcal{N}=150\sin^2 x-6|u|^2,$$

respectively. We then split Eq. (3.3) into the linear subproblem and nonlinear subproblem:

$$iu_t=\mathcal{L}u=-u_{xxxx}, \tag{3.4}$$

$$iu_t=\mathcal{N}u=150(\sin^2 x)u-6|u|^2u. \tag{3.5}$$

The result of subsystems (3.4) and (3.5) is an approximation of the original system (3.3) because of the incommutability between $\mathcal{L}$ and $\mathcal{N}$. The accuracy is based on the composition of the operators $\mathcal{L}$ and $\mathcal{N}$.

The linear subproblem (3.4) and nonlinear subproblem (3.5) are both multi-symplectic systems. The linear subproblem (3.4) can be rewritten as multi-symplectic formulation (1.9) with the same symplectic structure matrices M,K, and the Hamiltonian function is the quadratic part of $S(z)$, i.e.,

$$S^1(z)=\frac{1}{2}(\psi^2+\beta^2)-\varphi\eta-\alpha\gamma.$$

The nonlinear subproblem (3.5) is also multi-symplectic with zero symplectic structure in space, and the Hamiltonian function is the remainder of $S(z)$

$$S^2(z)=75(\sin^2 x)(p^2+q^2)-\frac{3}{2}(p^2+q^2)^2.$$

Thus, the symplectic structure matrix is $K_1=K$ and $K_2=\mathbf{0}$.

In fact, the nonlinear multi-symplectic system (3.5) reduces to an infinite dimensional Hamiltonian system

$$p_t=(150\sin^2 x-6(p^2+q^2))q, \tag{3.6a}$$
$$q_t=-(150\sin^2 x-6(p^2+q^2))p, \tag{3.6b}$$

with Hamiltonian function

$$H(\hat{z})=\int_0^L\left(75(\sin^2 x)(p^2+q^2)-\frac{3}{2}(p^2+q^2)^2\right)dx.$$

The linear subproblem (3.4) and nonlinear subproblem (3.5) can be approximated by multi-symplectic integrators. We adopt central box scheme (2.1) to discrete linear subproblem (3.4). As for the nonlinear subproblem (3.5), we first discretized it in space and get a finite dimensional Hamiltonian system,

$$\frac{dp_j}{dt}=(150\sin^2 x_j-6(p_j^2+q_j^2))q_j,\quad j=1,2,\cdots,N, \tag{3.7a}$$
$$\frac{dq_j}{dt}=-(150\sin^2 x_j-6(p_j^2+q_j^2))p_j,\quad j=1,2,\cdots,N. \tag{3.7b}$$

For the finite-dimensional Hamiltonian system (3.7), the Euler midpoint scheme (2.10) is employed which is symplectic.

In the split-step method, the solution of one subproblem is employed as the initial value of another. The general techniques of split-step method to solve the problem are

$$u(x,t+\tau)=\exp(-i\tau\mathcal{N})\exp(-i\tau\mathcal{L})u(x,t), \tag{3.8}$$
$$u(x,t+\tau)=\exp(-i\tau\mathcal{N}/2)\exp(-i\tau\mathcal{L})\exp(-i\tau\mathcal{N}/2)u(x,t). \tag{3.9}$$

By the Baker-Campbell-Hausdorf (BCH) formula [24], the first version (3.8) is of first-order and can be realized as follows:

1. Compute u^* from $u(x,t)$ by solving (3.4).
2. Compute $u(x,t+\tau)$ from u^* by solving (3.5).

The second version (3.9) is of second-order which is said to be the standard Strang splitting [25]. It can be carried out in the following procedure:

1. Compute u^* from $u(x,t)$ by solving (3.5) with half time step length.
2. Compute u^{**} from u^* by solving (3.4) with a full time step length.
3. Compute $u(x,t+\tau)$ from u^{**} by solving (3.5) with another half time step length.

There is almost no more computational cost required for the second-order scheme (3.9) than the first-order scheme (3.8). As a matter of fact, scheme (3.9) can be written as

$$\begin{aligned} u(x,t+\tau) &= e^{-\frac{i}{2}\tau\mathcal{N}}e^{-i\tau\mathcal{L}}e^{-\frac{i}{2}\tau\mathcal{N}}u(x,t) \\ &= e^{-\frac{i}{2}\tau\mathcal{N}}e^{-i\tau\mathcal{L}}e^{-i\tau\mathcal{N}}e^{-i\tau\mathcal{L}}e^{-\frac{i}{2}\tau\mathcal{N}}u(x,t-\tau). \end{aligned} \tag{3.10}$$

In summary, for the second-order Strang splitting method, it can be programmed in the following flow-chart:

$$u_j^n \Rightarrow u_j^*, \qquad i\frac{u_j^*-u_j^n}{\tau/2} = \frac{1}{2}\left(150\sin^2 x_j - 1.5|u_j^n+u_j^*|^2\right)\left(u_j^n+u_j^*\right), \tag{3.11a}$$

$$u_j^* \Rightarrow u_j^{**}, \qquad \frac{i}{16}\left(\delta_t\hat{u}_{j-2}+4\delta_t\hat{u}_{j-1}+6\delta_t\hat{u}_j+4\delta_t\hat{u}_{j+1}+\delta_t\hat{u}_{j+2}\right)+\delta_x^4\hat{u}_j=0, \tag{3.11b}$$

$$u_j^{**} \Rightarrow u_j^{n+1}, \quad i\frac{u_j^{n+1}-u_j^{**}}{\tau/2} = \frac{1}{2}\left(150\sin^2 x_j - 1.5|u_j^{n+1}+u_j^{**}|^2\right)\left(u_j^{n+1}+u_j^{**}\right), \tag{3.11c}$$

for $j=0,1,2,\cdots,N$, where

$$\hat{u}_j = \frac{1}{2}(u_j^*+u_j^{**}), \quad \delta_t\hat{u}_j = \frac{u_j^{**}-u_j^*}{\tau}.$$

This algorithm is of second-order in both time and space directions and is very simple. There is no additional memory needed to save the intermediate variables u^* and u^{**}.

4 Numerical experiments

In this section, we present some numerical results to test the multi-symplectic approximations (2.3), (2.13) and (3.11). We mainly focus on the issues of accuracy and conservation properties.

In each time step, the completely implicit schemes (2.3) and (2.13) can be written as

$$A(\tau,h)U^{n+1}=B(\tau,h)U^n+\tau F(U^{n+1},U^n),\quad n=1,2,\cdots,$$

where $A(\tau,h)$ and $B(\tau,h)$ are invertible matrices, and $F(U^{n+1},U^n)$ is the nonlinear term in the nonlinear system. We apply the fixed point iterative method to solve the algebraic system, namely,

$$A(\tau,h)U^{n+1,(k+1)}=B(\tau,h)U^n+\tau F(U^{n+1,(k)},U^n),\quad n=1,2,\cdots, \tag{4.1}$$

$k=0,1,2,\cdots$, is the iterative steps, and

$$U^{n+1,(0)}=U^n.$$

The iteration is terminated when

$$\max_j\left|u_j^{n+1,(k+1)}-u_j^{n+1,(k)}\right|<10^{-13},$$

or

$$\max_j\left|\left[A(\tau,h)U^{n+1,(k+1)}-B(\tau,h)U^n-\tau F(U^{n+1,(k)},U^n)\right]_j\right|<10^{-13}.$$

In the computation, the error for numerical solutions is scaled as follows:

$$\|e^n\|_2^2=h\sum_j\Big(|u_j^n|-|u(x_j,t_n)|\Big)^2,\quad \|e^n\|_\infty=\max_j\Big||u_j^n|-|u(x_j,t_n)|\Big|,$$

and the error for the charge and energy are measured by

$$Error_c^n=\mathcal{Q}^n-\mathcal{Q}^0,\quad Error_e^n=\mathcal{E}^n-\mathcal{E}^0,$$

respectively, where

$$\mathcal{Q}^n=h\sum_j|u_j^n|^2,\quad \mathcal{E}^n=h\sum_j\left(\left|\frac{u_{j-1}^n-2u_j^n+u_{j+1}^n}{h^2}\right|^2-3|u_j^n|^4+150(\sin^2x_j)|u_j^n|^2\right).$$

In what follows, we study the following 2π-periodic initial value problem

$$iu_t+u_{xxxx}-150(\sin^2x)u+6|u|^2u=0, \tag{4.2a}$$

$$u(x,0)=\frac{5}{\sqrt{2}}(1+i)\sin x, \tag{4.2b}$$

$$u(x,t)=u(x+2\pi,t)=0, \tag{4.2c}$$

$$u_{xx}(x,t)=u_{xx}(x+2\pi,t)=0. \tag{4.2d}$$

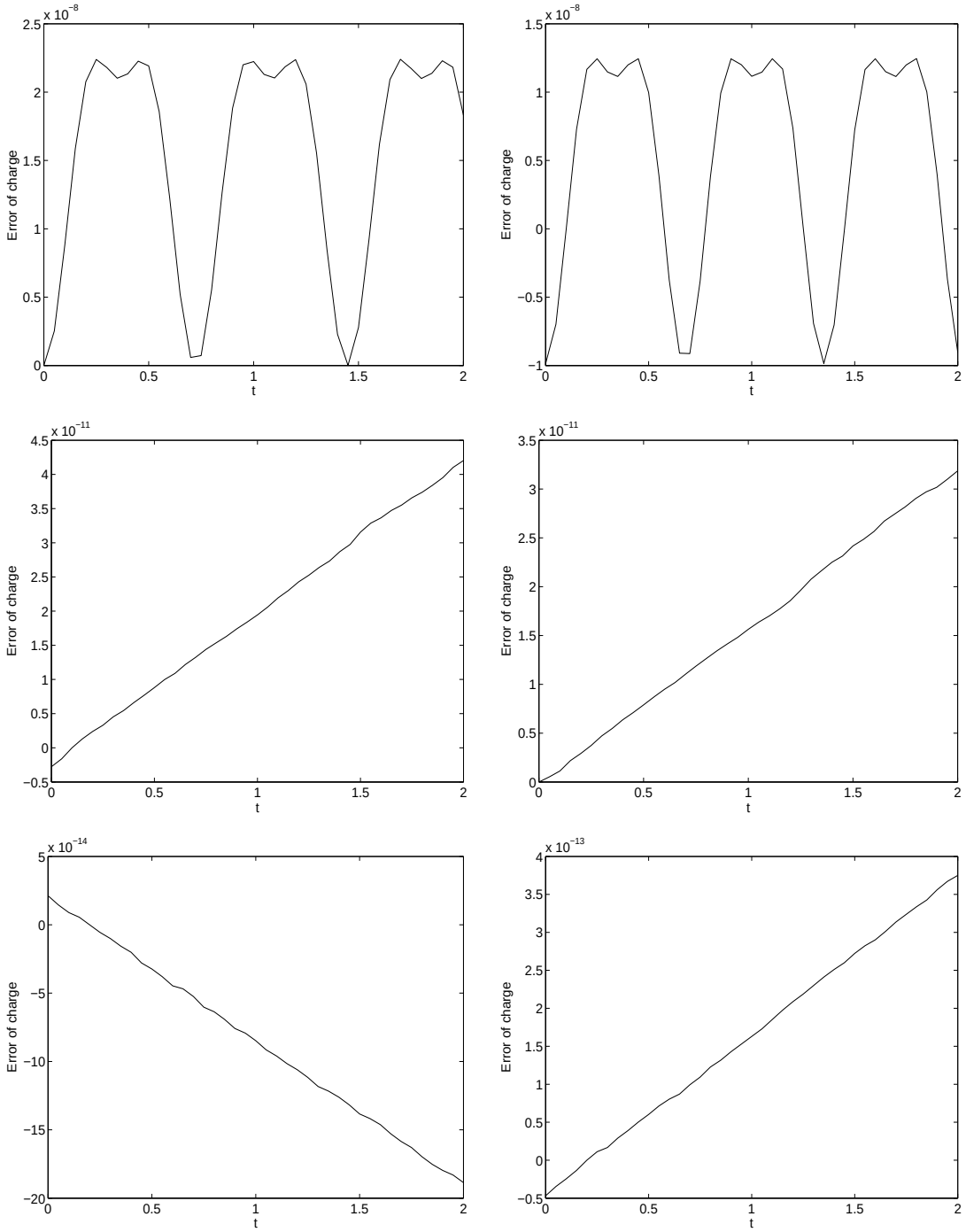

Figure 1: The errors of charge by different mesh division. The top two is by MSRK, the middle two by MSFS, the bottom two by SSMS. Left: $\tau = 0.002$, Right: $\tau = 0.001$.

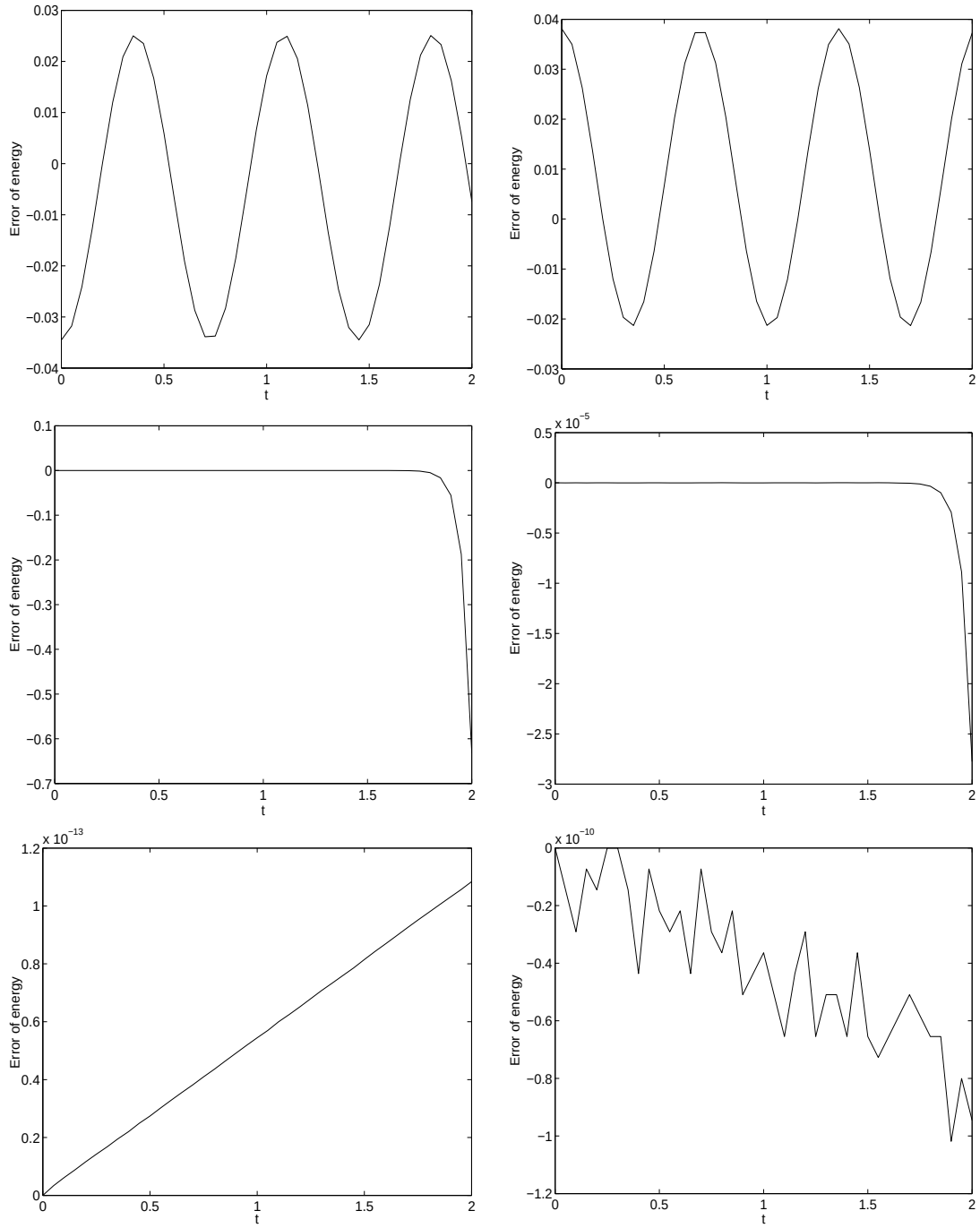

Figure 2: The errors of energy by different mesh division. The top two is by MSRK, the middle two by MSFS, the bottom two by SSMS. Left: $\tau = 0.002$; Right: $\tau = 0.001$.

Table 1: Numerical results for multi-symplectic integrators.

$\tau\backslash h$	scheme	$\|e^n\|_2$	$\|e^n\|_\infty$	CPU(sec)
$\tau=0.001$	MSRK	5.552×10^{-3}	8.255×10^{-3}	14
$h=\frac{\pi}{20}$	MSFS	3.235×10^{-6}	2.690×10^{-3}	16
	SSMS	9.903×10^{-14}	3.250×10^{-13}	2.8
$\tau=0.002$	MSRK	5.922×10^{-4}	1.252×10^{-3}	41
$h=\frac{\pi}{40}$	MSFS	6.693×10^{-6}	2.312×10^{-3}	48
	SSMS	1.084×10^{-13}	6.004×10^{-13}	3
$\tau=0.001$	MSRK	1.845×10^{-5}	3.826×10^{-5}	58
$h=\frac{\pi}{40}$	MSFS	5.645×10^{-6}	2.550×10^{-4}	64
	SSMS	3.973×10^{-13}	1.375×10^{-12}	5

Problem (4.2) admits an exact solution

$$u(x,t)=5\exp\left(i(t+\frac{\pi}{4})\right)\sin x. \tag{4.3}$$

We consider the problem on the time interval $[0,2]$, and simulate it by the multi-symplectic integrators (2.3), (2.13) and (3.11). Data given in Table 1 show the numerical error in L_2 and L_∞ norm and the consumed CPU time with different mesh partitions. Figs. 1 and 2 show the error of charge and energy against time. From the table, it can be seen that all of the schemes simulate the problem well. The numerical result obtained by SSMS method is surprisingly excellent. The numerical solution is almost equal to the exact solution. Moreover, the CPU time consumed by the SSMS method is greatly less than that by the other two schemes. The SSMS method is more efficient and accurate than conventional multi-symplectic methods. Figs. 1 and 2 reveal that the charge is exactly preserved by the MSFS method (2.13) and the SSMS method (3.11). However, for the preservation of charge, the MSRK method is worse than other two. The energy is accurately preserved from the beginning to the end by scheme (3.11), which is seen better than the other two. For conservative cases, the error brought up by coarse mesh is smaller than that by the refined meshes. The results are in contrary with the non-conservative cases. Mesh refinement implies increasing computational cost and larger roundoff errors for conservative situations.

Next, we simulate the problem in a longer time interval $[0,20]$. We again use multi-symplectic integrators (2.3), (2.13) and (3.11) to solve the problem. The mesh step sizes are $h=\pi/40$, $\tau=0.01$. It is observed that we can not obtain satisfactory numerical results by the MSRK method (2.3) and the MSFS method (2.13), and we will not show them here. On the other hand, accurate numerical results can be obtained by using the SSMS method (3.11). The real part and imaginary part of the solitary wave are depicted in Fig. 3, and the errors of charge and energy are presented in Fig. 4. It is observed from Fig. 3 that the solitary wave is perfectly periodic all along. The variations of charge and energy are within the roundoff error of the machine.

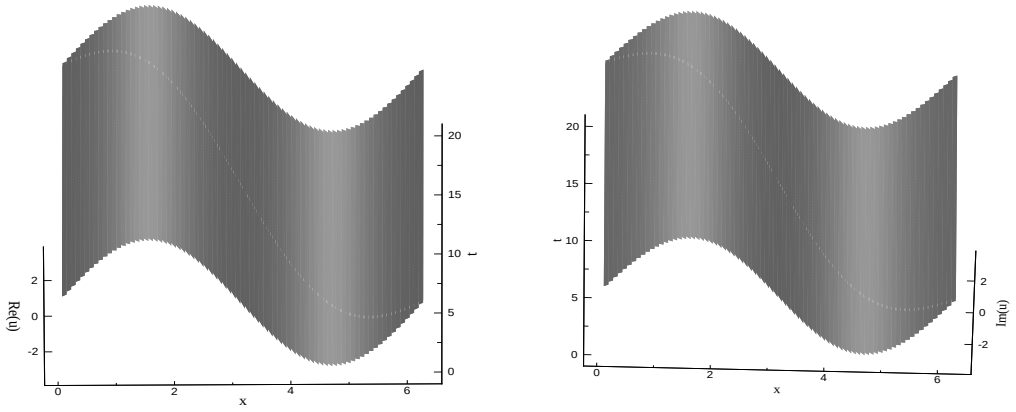

Figure 3: The real and imaginary parts of the solitary wave. Left: real part; Right: imaginary part.

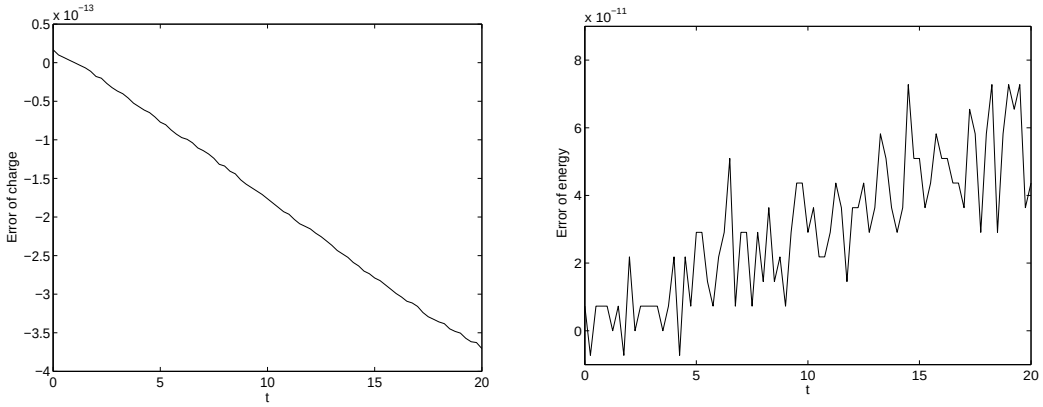

Figure 4: The errors of charge and energy. Left: charge; Right: energy, obtained by the SSMS method.

5 Summary

In this work, we propose some multi-symplectic integrators for the fourth-order nonlinear Schrödinger equation with a trapped term (FNSETT). First, we apply the central box scheme to the equation and obtain an MSRK method. This scheme is completely implicit. A pentagonal nonlinear algebraic system needs to be solved by iteration. The MSFS method is also implicit and charge-preserved. To overcome the drawbacks of completely implicit schemes and avoid solving coupled nonlinear algebraic equations, the split-step idea is introduced to the multi-symplectic integrators. We then can construct a new kind of split-step multi-symplectic method. The method is significantly more efficient than the MSRK method and the MSFS method. In terms of the conservative property and long-term behavior, it is also superior to the conventional multi-symplectic schemes.

The suggested SSMS method for the FNSETT can be naturally generalized to any multi-symplectic formulation in the form (1.9). Furthermore, they can be applied to

multi-dimensional circumstance. In multi-dimensional case, local one-dimensional splitting, alternative direction splitting, fractional step splitting are frequently used. We will discuss it in other papers [28]. For the discretization of subproblems, more types of methods for the concatenation, including symplectic partitioned Runge-Kutta methods, symplectic Runge-Kutta-Nyström methods, SRK-Fourier spectral method, can also be used. This will be investigated in future works.

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