Multi-symplectic Runge-Kutta-Nyström Methods for Nonlinear Schrödinger Equations

Jialin Hong†, Xiao-yan Liu‡§ and Chun Li†‡

†State Key Laboratory of Scientific and Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, P.O.Box 2719, Beijing 100080, P. R. China
‡Graduate School of the Chinese Academy of Sciences, Beijing 100080, P. R. China
§Department of Mathematics, Northeast Normal University, Changchun 130024, P.R. China

Abstract

In this paper, we investigate multi-symplectic Runge-Kutta-Nyström (RKN) methods for nonlinear Schrödinger equations. Concatenating symplectic Nyström methods in spatial direction and symplectic Runge-Kutta methods in temporal direction for nonlinear Schrödinger equations leads to multi-symplectic integrators, i.e. to numerical methods which preserve the multi-symplectic conservation law (MSCL), we present the corresponding discrete version of MSCL. We show that the multi-symplectic RKN methods preserve not only the global symplectic structure in time, but also local and global discrete charge conservation laws under periodic boundary conditions. Lower and higher order multi-symplectic RKN methods are utilized in numerical experiments. The errors of numerical solutions, the numerical errors of discrete energy, discrete momentum and discrete charge are exhibited. The precise conservation of discrete charge under the multi-symplectic RKN discretizations is attested numerically. By comparing with non-multi-symplectic methods, some numerical superiorities of the multi-symplectic RKN methods are exhibited.

Keywords: Nonlinear Schrödinger equations, multi-symplectic methods, Runge-Kutta-Nyström methods, charge conservation law.

1 Introduction

The nonlinear Schrödinger equation in its many versions is one of the most important models of mathematical physics, with applications to different fields such as plasma physics, nonlinear optics, water waves, bimolecular dynamics and many other fields. And many numerical methods have been investigated to solve it (see [3, 4, 5, 6, 10, 11, 17] and references therein). In the last two decades, symplectic methods have predominated over non-symplectic schemes for long-time numerical computations and nowadays applied to many fields of science which include celestial mechanics, quantum physics, statistics and so on [4, 9, 18]. The multi-symplectic integrators which preserve the discrete form of the multi-symplectic conservation law have been suggested by Bridges and Reich in [2, 17]. Some results on multi-symplectic methods have been presented in [2, 5, 6, 7, 8, 10, 11, 13, 15, 16, 17] and references therein. Reich in [17] considered Hamiltonian wave equations, and showed that the Gauss-Legendre discretization applied to the scalar wave equation (also to the nonlinear Schrödinger equation) both in temporal and spatial directions, leads to a multi-symplectic integrator (also see [10]). For the general Hamiltonian partial differential equations (HPDEs), some sufficient conditions for multi-symplecticity of partitioned Runge-Kutta (PRK) methods have been presented by Hong et al.[7]. In [7] it has been shown that concatenating symplectic PRK methods in temporal and spatial directions leads to the multi-symplectic integrators. Some conservative properties on charge, energy and momentum for multi-symplectic Gauss-Legendre methods,
multi-symplectic Runge-Kutta methods and multi-symplectic partitioned Runge-Kutta methods have been discussed in [6, 7, 8, 10, 11, 15, 17] and some references therein. One pays much more attention to the special symplectic methods for special kinds of Hamiltonian ordinary differential equations. Nyström methods for the second order differential equation \( y' = g(y) \),

\[
\begin{cases}
  l_i = g(y_0 + c_i h \dot{y}_0 + h^2 \sum_{j=1}^{s} a_{ij} l_j), \\
  y_1 = y_0 + h \dot{y}_0 + h^2 \sum_{j=1}^{s} \beta_j l_i,
\end{cases}
\]

are very useful and important in applications to some practical situations. In [19, 20] (also see [4, 18]), Suris obtained the symplectic condition of Nyström methods as follows

\[
\begin{cases}
  \beta_i = b_i(1 - c_i) \quad \text{for} \quad i = 1, \ldots, s, \\
  b_i(\beta_j - a_{ij}) = b_j(\beta_i - a_{ji}) \quad \text{for} \quad i, j = 1, \ldots, s,
\end{cases}
\]

that is very interesting, and guarantees the conservation of quadratic invariants ([12, 18]).

Because the derivative in Schrödinger equations in spatial direction is of second order, we apply symplectic Nyström Methods in spatial direction and symplectic Runge-Kutta methods in temporal direction. Naturally, one wonders whether such concatenation methods lead to the multi-symplectic integrators, and whether they conserve classical conservation laws, such as the global symplecticity in time and the charge conservation laws and so on. In this paper we give affirmative answers, such numerical methods preserve the multi-symplectic conservation law (thus called multi-symplectic Runge-Kutta-Nyström (RKN) methods), moreover, some important properties, such as the global symplecticity in time and charge conservation law are also conserved. The charge conservation law can be seen as a quadratic invariant which is, in general, not preserved by the symplectic integrators in the case of Hamiltonian ODEs ([12, 18]).

Numerical experiments presented in this paper tell us more about the numerical variations of discrete energy and discrete momentum under lower and higher order multi-symplectic RKN discretizations.

This paper is organized as follows. In section 2, based on the multi-symplectic structure of the nonlinear Schrödinger equations, we present the condition of multi-symplecticity of RKN methods, which are given by concatenating the symplectic Nyström methods in spatial direction and symplectic Runge-Kutta methods in temporal direction for the equations. In order to study the classical conservative properties of multi-symplectic RKN methods, we also discuss some local and global conservation laws, e.g., energy, momentum and charge, for the nonlinear Schrödinger equations. In section 3, we show that the multi-symplectic RKN methods have the global symplectic conservation in time, and prove that they have the local discrete charge conservative property, thus have the global one which is very important in the application to some physical problems. In section 4, in order to illustrate our theoretical results, we make use of lower and higher order multi-symplectic RKN methods to present some numerical experiments, in which the errors of numerical solutions, the collision of solitons, the numerical variations of discrete energy, discrete momentum and discrete charge are observed, the charge conservative properties are validated. The conclusion of this paper is presented in Section 5.

2 Conservation laws

2.1 Multi-symplectic conservation law

We consider the following nonlinear Schrödinger equation (NLSE)

\[
i \partial_t \psi = \partial_{xx} \psi + V'(|\psi|^2) \psi, \quad (x, t) \in U \subset \mathbb{R}^2,
\]

where \( V : \mathbb{R} \to \mathbb{R} \) is a smooth function. Let \( \Psi = q + i p \). Then (2.1) can be written as

\[
\begin{align*}
\partial_t q &= \partial_{xx} p + V'(|q|^2 + p^2) p, \\
\partial_t p &= -\partial_{xx} q - V'(|q|^2 + p^2) q.
\end{align*}
\]

We introduce a pair of conjugate momenta \( v = q_x, \ w = p_x \) and obtain

\[
M \partial_t z + K \partial_z z = \nabla_z S(z),
\]

(2.3)
where \( z = (q, p, v, w)^T \), \( M \) and \( K \) are skew-symmetric matrices,
\[
M = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},
\]
and the smooth function \( S(z) = \frac{1}{2}(v^2 + w^2 + V(q^2 + p^2)) \). (2.3) has a multi-symplectic conservation law (see [1, 2, 5, 6, 10, 11, 12])
\[
\frac{\partial \omega}{\partial t} + \frac{\partial \kappa}{\partial x} = 0,
\]
where \( \omega \) and \( \kappa \) are pre-symplectic forms,
\[
\omega = \frac{1}{2} dz \wedge M dz \quad \text{and} \quad \kappa = \frac{1}{2} dz \wedge K dz.
\]
The corresponding equations for the differential one forms \( da = (dq, dp, dv, dw)^T \) are given by
\[
\begin{align*}
\partial_t dq - \partial_x dw &= V'(q^2 + p^2)dp + (2pqdq + 2p^2 dp)V''(q^2 + p^2), \\
-\partial_t dp - \partial_x dv &= V'(q^2 + p^2) dq + (2pqdp + 2q^2 dp)V''(q^2 + p^2), \\
\partial_x dq &= dv, \\
\partial_x dp &= dw,
\end{align*}
\]
where we use the fact that the exterior derivative operator \( d \) can commute with the partial derivative operators \( \partial_t \) or \( \partial_x \). From (2.6a)-(2.6b) it follows that
\[
\begin{align*}
\partial_t dq \wedge dp - \partial_x dw \wedge dp &= 2qpV''(q^2 + p^2) dq \wedge dp, \\
-\partial_t dp \wedge dq - \partial_x dv \wedge dq &= 2qpV''(q^2 + p^2) dp \wedge dq.
\end{align*}
\]
This leads the multi-symplectic conservation law
\[
\partial_t (dp \wedge dq) + \partial_x (dq \wedge dv + dp \wedge dw) = 0. \quad \text{(MSCL)}
\]
Now we rewrite (2.3) as the following form
\[
\begin{align*}
\partial_x v &= -\partial_t p - V'(q^2 + p^2)q, \\
\partial_x w &= \partial_t q - V'(q^2 + p^2)p, \\
\partial_x q &= v, \\
\partial_x p &= w.
\end{align*}
\]
It has been shown that concatenating two symplectic RK (or PRK) methods in temporal and spatial directions leads a multi-symplectic integrator for HPDEs, the discrete energy and the discrete momentum are preserved by the multi-symplectic integrator for the linear HPDEs [2, 7, 10, 12, 17]. In [8], authors discuss some properties of multi-symplectic Runge-Kutta (MSRK) methods for one-dimensional nonlinear Dirac equations in relativistic quantum physics, in particular, the conservation of energy, momentum and charge under MSRK discretization is investigated by means of numerical experiments and numerical comparisons with non-MSRK methods. A remarkable advantage of MSRK methods applied to the nonlinear Dirac equation is the precise preservation of charge conservation law. Let us consider the multi-symplecticity of concatenating Nystrom methods in spatial direction and Runge-Kutta methods in temporal direction for the nonlinear Schrödinger equations. In order to process the numerical discretization, we introduce a uniform grid [9] \((x_j, t_k) \in \mathbb{R}^2\) with mesh-length \( \Delta t \) in the \( t \)-direction and mesh-length \( \Delta x \) in the \( x \)-direction, and denote the value of the function \( \psi(x,t) \) at the mesh point \((x_j, t_k) \) by \( \psi_j^k \). For (2.8a)-(2.8d), in \( x \)-direction applying an \( s \)-stage Nystrom method, with coefficients \( \{a_{m_j}\}, \{b_m\}, \{\beta_m\} \) and \( \{c_m\} \), and in \( t \)-direction applying an \( r \)-stage Runge-Kutta method with coefficients \( \{\tilde{a}_{k,j}\}, \{\tilde{b}_k\} \) and \( \tilde{a}_k = \sum_{j=1}^s \tilde{a}_{k,j} \), it is concluded that
As a preparation of the further discussion, we present some classical conservation laws. For a mult-

2.2 Some important classical conservation laws

The equation (2.12) is the discrete multi-symplectic conservation law (in short, DMSCL) correspond-

The notations above are in the following sense, $Q_{l,m}^k \approx q((l+c_m)\Delta x, \tilde{d}_k \Delta t)$, $q_{l}^{k} \approx q(l\Delta x, \tilde{d}_k \Delta t)$, $\partial_t Q_{l,m}^k \approx \partial_t q((l+c_m)\Delta x, \tilde{d}_k \Delta t)$, $P_{l,m}^k \approx p((l+c_m)\Delta x, \tilde{d}_k \Delta t)$, $\partial_t P_{l,m}^k \approx \partial_t p((l+c_m)\Delta x, \tilde{d}_k \Delta t)$, $v_{l+1}^j \approx v(l\Delta x, \tilde{d}_k \Delta t)$.

The following result is the characterization of multi-symplectic RKN methods for the nonlinear
Schrödinger equations, it has a similar proof (therefore omitted) to the results in [11, 17].

**Theorem 1.** In the method (2.9a)-(2.9j), if

\[
\beta_m = b_m(1-c_m), \quad b_m(\beta_j - a_{mj}) = b_j(\beta_m - a_{jm}), \quad \text{for} \quad m, j = 1, 2, \ldots, s, \tag{2.10}
\]

and

\[
\tilde{b}_k \tilde{b}_i = \tilde{b}_k \tilde{a}_{ki} + \tilde{b}_i \tilde{a}_{ik}, \quad \text{for} \quad i, k = 1, 2, \ldots, r, \tag{2.11}
\]

then the method (2.9a)-(2.9j) is multi-symplectic with the discrete multi-symplectic conservation law

\[
\Delta t \sum_{k=1}^{r} \tilde{b}_k [dq_{l+1}^k \wedge dv_{l+1}^k - dq_{l}^k \wedge dv_{l}^k + dp_{l+1}^k \wedge dw_{l+1}^k - dp_{l}^k \wedge dw_{l}^k] + \Delta x \sum_{m=1}^{s} b_m[dq_{l,m}^0 \wedge dp_{l,m}^0 - dq_{l,m}^0 \wedge dp_{l,m}^0] = 0. \tag{2.12}
\]

The equation (2.12) is the discrete multi-symplectic conservation law (in short, DMSCL) corresponding to the continuous version (MSCL). More general discrete multi-symplectic conservation laws for multi-symplectic RK (or PRK) methods of HPDEs corresponding to (2.4) can be found in [7].

2.2 Some important classical conservation laws

As a preparation of the further discussion, we present some classical conservation laws. For a multi-
symplectic Hamiltonian system (2.3), it has a local energy conservation law (ECL)

\[
\frac{\partial E}{\partial t} + \frac{\partial F}{\partial x} = 0 \tag{2.13}
\]

\[Q_{l,m}^k = q_{l}^{k} + c_m \Delta x v_{l}^{k} + \Delta x^2 \sum_{j=1}^{s} a_{mj}( - \partial_t P_{l,j}^k - V'((Q_{l,j}^k)^2 + (P_{l,j}^k)^2)Q_{l,j}^k), \tag{2.9a}
\]

\[P_{l,m}^k = p_{l}^{k} + c_m \Delta x w_{l}^{k} + \Delta x^2 \sum_{j=1}^{s} a_{mj} (\partial_t Q_{l,j}^k - V'((Q_{l,j}^k)^2 + (P_{l,j}^k)^2)P_{l,j}^k), \tag{2.9b}
\]

\[v_{l+1}^j = v_{l}^{j} + \Delta x \sum_{m=1}^{s} b_{m} ( - \partial_t P_{l,m}^k - V'((Q_{l,m}^k)^2 + (P_{l,m}^k)^2)Q_{l,m}^k), \tag{2.9c}
\]

\[w_{l+1}^j = w_{l}^{j} + \Delta x \sum_{m=1}^{s} b_{m} (\partial_t Q_{l,m}^k - V'((Q_{l,m}^k)^2 + (P_{l,m}^k)^2)P_{l,m}^k), \tag{2.9d}
\]

\[q_{l+1}^k = q_{l}^{k} + \Delta x v_{l}^{k} + \Delta x^2 \sum_{j=1}^{s} b_{mj} ( - \partial_t P_{l,j}^k - V'((Q_{l,j}^k)^2 + (P_{l,j}^k)^2)Q_{l,j}^k), \tag{2.9e}
\]

\[p_{l+1}^k = p_{l}^{k} + \Delta x w_{l}^{k} + \Delta x^2 \sum_{j=1}^{s} b_{mj} (\partial_t Q_{l,j}^k - V'((Q_{l,j}^k)^2 + (P_{l,j}^k)^2)P_{l,j}^k), \tag{2.9f}
\]

\[Q_{l,m}^k = q_{l}^{0,k} + \Delta t \sum_{i=1}^{r} \tilde{a}_{ki} \partial_t Q_{l,m}^k, \tag{2.9g}
\]

\[P_{l,m}^k = p_{l}^{0,k} + \Delta t \sum_{i=1}^{r} \tilde{a}_{ki} \partial_t P_{l,m}^k, \tag{2.9h}
\]

\[q_{l,m}^k = q_{l}^{0,k} + \Delta t \sum_{k=1}^{r} b_{k} \partial_t Q_{l,m}^k, \tag{2.9i}
\]

\[p_{l,m}^k = p_{l}^{0,k} + \Delta t \sum_{k=1}^{r} b_{k} \partial_t P_{l,m}^k. \tag{2.9j}
\]
with energy density $E = S(z) - \frac{1}{2} z^T K z$ and energy flux $F = \frac{1}{2} z^T K z_t$. For the nonlinear Schrödinger equation here, it is easy to verify that

$$E(z) = \frac{1}{2} \Re(\bar{\psi} \partial_{xx} \psi + V(|\psi|^2))$$

and

$$F(z) = \frac{1}{2} \Re( - \bar{\psi} \partial_t \psi + \partial_x \bar{\psi} \partial_x \psi),$$

where $\Re$ denotes the real part of a complex number. The system has also a local momentum conservation law (MCL)

$$\frac{\partial I}{\partial t} + \frac{\partial G}{\partial x} = 0 \quad (2.14)$$

with momentum density $I = \frac{1}{2} z^T M x$ and momentum flux $G = S(z) - \frac{1}{2} z^T M z_t$. Similarly, we can rewrite $I(z)$ and $G(z)$ as the following compact forms

$$I(z) = \frac{1}{2} \Im(\bar{\psi} \partial_x \psi) \quad \text{and} \quad G(z) = \frac{1}{2} \Im(\partial_x |\psi|^2 + V(|\psi|^2) - \bar{\psi} \partial_x \psi),$$

where $\Im$ denotes the imaginary part of complex number. The calculation process of the conservation laws (2.13) and (2.14) are given in [17] (also see [1, 2]). Now we take a product with (2.3) by $(M z) T$ and notice that $(M z) T \nabla_x S(z)$ vanishes, it follows that $(M z) T M z_t + (M z) T K z = 0$. Since \( \frac{\partial}{\partial t} (M z) T M z = 0 \), the above equation can be written as

$$\partial_t \left( (M z) T M z \right) + \partial_x \left( 2 z^T M^T K z \right) = 0 \quad (2.15)$$

Similarly, (2.15) is equivalent to a compact form $\partial_t(|\psi|^2) + \partial_x \left( i \bar{\psi} \partial_t \psi - i \partial_x \psi \right) = 0$, which is the local charge conservation law. The above three local conservation laws (2.13), (2.14) and (2.15) can lead to the global properties of the system under appropriate assumptions (e.g., suitable boundary conditions).

Throughout this context, we assume that the solution is smooth enough, the spatial interval we consider is $[x_L, x_R]$ ($x_L$ and $x_R$ can be infinite). If $\psi(x, t)$ and $\partial_x \psi(x, t)$ are periodic, that means $\psi(x_L, t) = \psi(x, t)$ and $\partial_x \psi(x_L, t) = \partial_x \psi(x, t)$ (here requires that $\psi(x_L, t)$ and $\partial_x \psi(x, t)$ are finite) for any $t$ where is defined, then we will have three global conservation laws corresponding to the above three local conservation laws respectively,

$$\frac{d}{dt} \mathcal{E}(z)(t) = 0 \quad (2.16)$$

$$\frac{d}{dt} \mathcal{I}(z)(t) = 0 \quad (2.17)$$

and

$$\frac{d}{dt} \mathcal{C}(z)(t) = 0 \quad (2.18)$$

where $\mathcal{E}(z)(t) \triangleq \int_{x_L}^{x_R} E(z(x, t)) dx$ is the total energy, $\mathcal{I}(z)(t) \triangleq \int_{x_L}^{x_R} I(z(x, t)) dx$ is the total momentum, $\mathcal{C}(z)(t) \triangleq \int_{x_L}^{x_R} |\psi(x, t)|^2 dx$ is the charge, which is also called mass or plasmon number (or wave power) in different scientific fields. For simplicity, we omit the proofs of the three global conservation laws here.

Now we take $\tau = \Delta t$ and $h = \Delta x$, we integrate the energy conservation law (2.13) over the local domain $[0, \tau] \times [0, h]$, namely

$$\int_0^h [E(z(x, \tau)) - E(z(x, 0))] dx + \int_0^\tau [F(z(h, t)) - F(z(0, t))] dt = 0 \quad (2.19)$$

Corresponding to the discretization (2.9), we use a discrete form

$$E_{te} \triangleq h \sum_{m=1}^{s} b_m (E(z_m^1) - E(z_0^m)) + \tau \sum_{k=1}^{r} b_k (F(z_k^1) - F(z_0^k)) \quad (2.20)$$

to approximate the left side of (2.13). Similarly, from (2.14) and (2.15) we have

$$\int_0^h [I(z(x, \tau)) - I(z(x, 0))] dx + \int_0^\tau [G(z(h, t)) - G(z(0, t))] dt = 0 \quad (2.21)$$
and
\[\int_0^h \left[C(z(x, \tau)) - C(z(x, 0))\right] dx + \int_0^T \left[J(z(h, t)) - J(z(0, t))\right] dt = 0 \tag{2.22}\]
respectively, where \(C(z) = (Mz)^T Mz\) and \(J(z) = 2z^T M^T Kz\) are the charge density and the charge flow respectively. Thus, we define
\[M_{le} = h \sum_{m=1}^s b_m (I(z_{1m}^k) - I(z_{0m}^k)) + \tau \sum_{k=1}^r \bar{b}_k (G(z_{1k}^k) - G(z_{0k}^k)) \tag{2.23}\]
and
\[C_{le} = h \sum_{m=1}^s b_m (C(z_{1m}^k) - C(z_{0m}^k)) + \tau \sum_{k=1}^r \bar{b}_k (J(z_{1k}^k) - J(z_{0k}^k)) \tag{2.24}\]
as the discrete form of the left side of (2.14) and (2.15) respectively.

Besides the conservation laws of energy, momentum and charge, in our numerical experiments we will investigate numerical behavior of another integral of the nonlinear Schrödinger equations
\[I_5 = \int_{x_L}^{x_R} \left[|\psi_{xx}|^2 + 2|\psi|^6 - 6|\psi_x|^2|\psi|^2 - ((|\psi|^2)_x)^2\right] dx, \tag{2.25}\]
which, after the total energy, is the next-most complicated global conservation law.

3 Total symplecticity and discrete charge conservation law

By using the complex-valued state variable \(z = (\psi, \phi)^T \in \mathbb{C}^2, \partial_x \psi = \phi\), we can rewrite the multi-symplectic formulation of the nonlinear Schrödinger equation in the following equivalent compact form
\[\text{i}\partial_t \psi - \partial_x \phi = V'(|\psi|^2)\psi, \quad \partial_x \psi = \phi.\]

Now we make use of the symplectic Nyström method in \(x\)-direction and the symplectic Runge-Kutta method in \(t\)-direction, a multi-symplectic method reads
\[
\begin{align*}
\Psi_{l,m}^k & = \psi_{l,m}^0 + \Delta t \sum_{i=1}^r \tilde{a}_i \partial_t \Psi_{l,m}^k, \\
\psi_{l,m}^1 & = \psi_{l,m}^0 + \Delta t \sum_{k=1}^r \bar{b}_k \partial_t \Psi_{l,m}^k, \\
\Psi_{l,m}^{k+1} & = \psi_{l,m}^{k+1} + \Delta x^2 \sum_{j=1}^s \alpha_{ij} \partial_{xx} \Psi_{l,m}^k, \\
\phi_{l+1,m}^k & = \phi_{l,m}^0 + \Delta x \sum_{m=1}^s b_m \partial_x \Psi_{l,m}^k, \\
\psi_{l,m}^k & = \psi_{l,m}^0 + \Delta x \sum_{m=1}^s \beta_m \partial_x \Psi_{l,m}^k, \\
\Psi_{l,m}^s & = \psi_{l,m}^0 + \Delta t \sum_{i=1}^r \tilde{a}_i \partial_t \Psi_{l,m}^k, \\
\psi_{l,m}^s & = \psi_{l,m}^0 + \Delta t \sum_{k=1}^r \bar{b}_k \partial_t \Psi_{l,m}^k, \\
i \partial_t \Psi_{l,m}^k & = \partial_{xx} \Psi_{l,m}^k + V'(\Psi_{l,m}^k)^2 \Psi_{l,m}^k. \tag{3.1f}
\end{align*}
\]

The discrete conservation of multi-symplecticity as discussed in section 2 is a local property of the multi-symplectic Hamiltonian systems. The global symplecticity in time and the charge are the important conservation quantities for the nonlinear Schrödinger equations (2.1), and the charge conservation plays an important role in self-focusing of laser in dielectrics, propagation of signals in optical fibers, 1D Heisenberg magnets and so on.
An important question is if the multi-symplectic RKN methods can conserve the discrete global symplecticity in time and the discrete charge under the appropriate boundary conditions.

To answer this question, firstly we aim to obtain the discrete global symplectic conservation. Use the same technique as in [7, 8] under the periodic boundary conditions we integrate the multi-symplectic conservation law (2.4) over the spatial interval $[-L, L]$, which yields the following identity

$$0 = \int_{-L}^{L} \left( \frac{\partial}{\partial t} \omega + \frac{\partial}{\partial x} \kappa \right) dx = \frac{d}{dt} \int_{-L}^{L} \omega dx,$$

namely,

$$\int_{-L}^{L} \omega(x, t) dx = \int_{-L}^{L} \omega(x, 0) dx,$$

which shows the global symplecticity is conserved in time in the continuous case. By summing the discrete symplectic conservation law over all spatial grid points, we have

$$0 = \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m(\omega_{l,m}^1 - \omega_{l,m}^0) + \tau \sum_{l=0}^{N-1} \sum_{k=1}^{r} b_k(\kappa_{l+1,0}^k - \kappa_{l,0}^k) = \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m(\omega_{l,m} - \omega_{l,m}^0),$$

where the last equality comes from the periodic boundary condition (or zero boundary condition) on the spatial domain. This implies the following discrete total symplectic conservation law in time

$$\sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m\omega_{l,m}^1 = \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m\omega_{l,m}^0. \tag{3.3}$$

Comparing (3.2) with (3.3), we find that (3.3) is the discrete approximation of (3.2) and we draw a conclusion that under appropriate boundary conditions, the multi-symplectic RKN methods have the discrete global symplectic conservation law in time, that is, the local symplectic property implies the global one.

Now we show that the discrete (local and global) charge conservation laws are preserved by means of the multi-symplectic RKN methods for NLSEs with appropriate boundary conditions.

**Theorem 2.** In the method (3.1a)-(3.1f), assume that

$$\beta_m = b_m(1 - c_m), \quad b_m(\beta_j - a_{mj}) = b_j(\beta_m - a_{jm}), \quad \text{for } m, j = 1, 2, \ldots, s,$$

and

$$\tilde{b}_i b_i = \tilde{b}_i \tilde{a}_{ki} + \tilde{b}_i \tilde{a}_{ik}, \quad \text{for } i, k = 1, 2, \ldots, r,$$

then the discretization (3.1) has a discrete local charge conservation law

$$\sum_{m=1}^{s} b_m(|\psi_{l,m}^1|^2 - |\psi_{l,m}^0|^2) + i\tau \sum_{k=1}^{r} \tilde{b}_k \left( (\phi_{l+1}^k \overline{\psi}_{l,m}^k - \psi_{l+1}^k \overline{\phi}_{l,m}^k) - (\phi_{l}^k \overline{\psi}_{l,m}^k - \psi_{l}^k \overline{\phi}_{l,m}^k) \right) = 0. \tag{3.4}$$

**Proof.** (3.1a)-(3.1f) imply

$$|\psi_{l,m}^1|^2 - |\psi_{l,m}^0|^2 = \overline{\psi}_{l,m}^1 \psi_{l,m}^1 - \overline{\psi}_{l,m}^0 \psi_{l,m}^0$$

$$= \tau \sum_{k=1}^{r} \tilde{b}_k (\overline{\psi}_{l,m}^1 \partial_t \psi_{l,m}^k + \partial_t \overline{\psi}_{l,m}^1 \psi_{l,m}^k) + \tau^2 \sum_{i, k=1}^{r} \left( \tilde{b}_i \tilde{a}_{ki} - \tilde{b}_i \tilde{a}_{ik} - \tilde{b}_i \tilde{a}_{ik} \right) \partial_t \overline{\psi}_{l,m}^1 \partial_t \psi_{l,m}^k.$$ 

By making use of $\tilde{b}_i \tilde{b}_i = \tilde{b}_i \tilde{a}_{ki} + \tilde{b}_i \tilde{a}_{ik}$, we have

$$\sum_{m=1}^{s} b_m(|\psi_{l,m}^1|^2 - |\psi_{l,m}^0|^2) = \tau \sum_{k=1}^{r} \tilde{b}_k \sum_{m=1}^{s} b_m (\overline{\psi}_{l,m}^1 \partial_t \psi_{l,m}^k + \partial_t \overline{\psi}_{l,m}^1 \psi_{l,m}^k). \tag{3.5}$$
On the other hand, it follows that
\[
(\psi^k_{l+1})^k_k - (\psi^k_l)^k_k = h|\phi_l^k|^2 + h \sum_{m=1}^s b_m(\overline{\psi^k_{l,m}})\partial_{xx}\psi^k_{l,m}
\]
\[+ h^2 \sum_{m=1}^s \beta_m(\partial_{xx}\overline{\psi^k_{l,m}})\phi^k_l + h^2 \sum_{m=1}^s b_m(1 - c_m)\overline{\phi^k_l}\partial_{xx}\psi^k_{l,m}
\]
\[+ h^3 \sum_{m,j=1}^s b_m(\beta_j - a_m)\phi^k_l \partial_{xx}\overline{\psi^k_{l,j}}\partial_{xx}\psi^k_{l,m}.
\]
By using \(\beta_m = b_m(1 - c_m)\), we have
\[
(\psi^k_{l+1})^k_k - (\psi^k_l)^k_k = h|\phi_l^k|^2 + h \sum_{m=1}^s b_m(\overline{\psi^k_{l,m}})\partial_{xx}\psi^k_{l,m} + 2h^2 \sum_{m=1}^s \beta_m\Re((\partial_{xx}\overline{\psi^k_{l,m}})\phi^k_l)
\]
\[+ h^3 \sum_{m,j=1}^s b_m(\beta_j - a_m)\phi^k_l \partial_{xx}\overline{\psi^k_{l,j}}\partial_{xx}\psi^k_{l,m},
\]
where \(\Re(u)\) denotes the real part of the complex \(u\).

Secondly, we can get
\[
(\psi^k_{l+1})^k_k - (\psi^k_l)^k_k = (\psi^k_{l+1})^k_k - (\psi^k_l)^k_k
\]
\[= h|\phi_l^k|^2 + h \sum_{m=1}^s b_m(\overline{\psi^k_{l,m}})\partial_{xx}\psi^k_{l,m} + 2h^2 \sum_{m=1}^s \beta_m\Re((\partial_{xx}\overline{\psi^k_{l,m}})\phi^k_l)
\]
\[+ h^3 \sum_{m,j=1}^s b_m(\beta_j - a_m)\phi^k_l \partial_{xx}\overline{\psi^k_{l,j}}\partial_{xx}\psi^k_{l,m},
\]
Subtracting (3.7) from (3.6) and using the condition \(b_j(\beta_m - a_m) = b_m(\beta_j - a_m)\), we obtain
\[
(\psi^k_{l+1})^k_k - (\psi^k_l)^k_k - (\psi^k_{l+1})^k_k - (\overline{\psi^k_l})^k_k = h \sum_{m=1}^s b_m[(\overline{\psi^k_{l,m}})\partial_{xx}\psi^k_{l,m} - (\partial_{xx}\overline{\psi^k_{l,m}})\psi^k_{l,m}].
\]
It follows from (3.11) that
\[
i\overline{\psi^k_{l,m}}\partial_{xx}\psi^k_{l,m} + i(\partial_{xx}\overline{\psi^k_{l,m}})\psi^k_{l,m} = (\overline{\psi^k_{l,m}})\partial_{xx}\psi^k_{l,m} - (\partial_{xx}\overline{\psi^k_{l,m}})\psi^k_{l,m}.
\]
Combining (3.5), (3.8) and (3.9), we complete the proof.

The above theorem tells us that the multi-symplectic RKN methods preserve the local charge conservation law for the nonlinear Schrödinger equations. As well known, the global charge conservation law plays an important role in quantum physics. A naturally question is: Do the multi-symplectic RKN methods preserve the global charge conservation law? The following result based on Theorem 2 gives an affirmative answer to the question under the appropriate boundary conditions.

**Theorem 3.** Under the assumptions of Theorem 2, if the periodic boundary condition or zero boundary conditions hold for (2.1), i.e. \(\psi^0_N = \psi^0_0\), \(\partial_x\psi^0_N = \partial_x\psi^0_0\), or \(\psi^0_0 = \psi^0_N = 0\), then the method (3.1) satisfies the discrete charge conservation law, that is,
\[
h \sum_{l=0}^{N-1} \sum_{m=1}^s b_m|\psi^0_{l,m}|^2 = \text{constant},
\]
where \(\psi^0_{l,m} = \psi((l + c_m)h, n\tau)\), \(\psi^0_{l,m} = \psi((l + c_m)h, (n + d_k)\tau)\) and so on. When \(n = 0\) we always omit the subscript \(n\) for simplicity, and \(n\) is a nonnegative integer here.
Proof. Due to Theorem 2, taking the sum of the equation (3.4) over the spatial grid points, it follows that

\[ h \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m (|\psi_{l,m}^1|^2 - |\psi_{l,m}^0|^2) = -\tau \sum_{k=1}^{r} b_k [\overline{\psi_N} \phi_N^k - \overline{\psi_0} \phi_0^k - (\overline{\phi_N} \psi_N^k - \overline{\phi_0} \psi_0^k)]. \]

If the boundary conditions satisfy \( \psi_N^k = \psi_0^k \), \( \phi_N^k = \phi_0^k \), or \( \psi_N^k = \psi_0^k = 0 \), then

\[ h \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m (|\psi_{l,m}^1|^2 - |\psi_{l,m}^0|^2) = 0, \]

this completes the proof.

Theorem 2 and Theorem 3 are non-trivial extensions of results on the quadratic invariants of symplectic RKN methods for Hamiltonian ODEs to the multi-symplectic RKN methods for NLSEs. In numerical experiments in the next section, in fact, the charge conservation law of NLSEs will be preserved precisely, in the round-off errors of computer, by means of the multi-symplectic RKN methods.

4 Numerical Experiments

In this section some numerical experiments are presented to illustrate the theoretical results in the previous sections. Some lower and higher multi-symplectic RKN methods are implemented in several scales of temporal and spatial mesh-lengths.

4.1 Experiment A

We consider the initial-value problem

\[ i \psi_t = \psi_{xx} + 2|\psi|^2 \psi, \quad t > 0, \]
\[ \psi|_{t=0} = \frac{1}{\sqrt{2}} \operatorname{sech}(\frac{1}{\sqrt{2}}(x - 25)) \cdot \exp[-i\frac{x}{20}], \]

(4.1)
(4.2)

The exact solution of (4.1)-(4.2) is

\[ \psi(x, t) = \frac{1}{\sqrt{2}} \operatorname{sech}(\frac{1}{\sqrt{2}}(x - \frac{t}{10} - 25)) \cdot \exp[-i(\frac{x}{20} + \frac{199t}{400})]. \]

(4.3)

Since \( \psi(x, t) \) is exponentially small away from \( x = 0 \) for small \( t \), we can use periodic boundary conditions. In our numerical computation, we implement the following periodic condition

\[ \psi|_{x=x_L} = \psi|_{x=x_R}, \]

(4.4)

which are added to the problem (4.1)-(4.2), where \( x_L \) and \( x_R \) are chosen to be large enough, so that the solution of (4.1)-(4.2) with (4.4) approximately agrees with (4.3). Here we take \( x_L = -60 \) and \( x_R = 120 \), the temporal interval \([0, 200]\) in the numerical experiments of this subsection. Now we take two-stage symplectic Nyström methods with coefficients \( c_1 = 0, \quad c_2 = 1, \quad a_{11} = a_{12} = a_{22} = 0, \quad a_{21} = 1/2, \quad \beta_1 = 1/2, \quad \beta_2 = 0, \quad b_1 = b_2 = 1/2 \) in spatial direction and implicit mid-point scheme in temporal direction (in short, denote by MN2).

Now we introduce some discrete variables which will be investigated in numerical experiments of this section. We make use of

\[ (E_{le}^n)_i = \sum_{m=1}^{s} b_m \frac{E(z_{i,m}^{n+1}) - E(z_{i,m}^n)}{\tau} + \sum_{k=1}^{r} b_k \frac{F(z_{i+1,k}^n) - F(z_{i,k}^n)}{h}, \]

to denote the error of the ECL, which is the general form of (2.20) in the rectangle

\( ((x_1, t_n), (x_{l+1}, t_n), (x_{l+1}, t_{n+1}), (x_l, t_{n+1})) \).
\((E_{le})^n\) doesn’t mean the local error at the mesh point \((x_l,t_n)\), since \((E_{le})^n\) is derived from the local integration \(E_{le}\), and the local integration domain is the rectangle. Similarly, the error \((M_{le})^n\) of MCL can be defined.

The relative global error in the discrete charge is defined as \(C_{rg}(n) = (\mathcal{E}_d(n) - \mathcal{E}_d(0))/|\mathcal{E}_d(0)|\), where \(\mathcal{E}_d(n) = h \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m |\psi_{l,m}^n|^2\).

Due to the total energy defined as before, the relative global error in the discrete total energy is defined as \(E_{rg}(n) = (\mathcal{E}_d(n) - \mathcal{E}_d(0))/|\mathcal{E}_d(0)|\), where \(\mathcal{E}_d(n) = \frac{\tau}{2} \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m (R(\psi_{l,m}^n \partial_x \psi_{l,m}^n) + |\psi_{l,m}^n|^2)\), for \(n = 1,2,\ldots,\bar{N} = T/\tau\).

The discrete momentum is defined as \(I_d(n) = \frac{\tau}{2} \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m (\psi_{l,m}^n \partial_x \bar{\psi}_{l,m}^n),\) the relative global error in the discrete total momentum conservation law is given by \(I_{rg}(n) = (\mathcal{I}_d(n) - \mathcal{I}_d(0))/|\mathcal{I}_d(0)|\).

The discrete form of the integral \(I_5\) is

\[
(I_5)_d(n) = h \sum_{l=0}^{N-1} \sum_{m=1}^{s} b_m \left( (\partial_x \psi_{l,m}^n)^2 + 2|\psi_{l,m}^n|^2 - 6|\psi_{l,m}^n|^2 |\psi_{l,m}^n|^2 - \left( \psi_{l,m}^n \overline{\psi_{l,m}^n} + \overline{\psi_{l,m}^n} \psi_{l,m}^n \right)^2 \right).
\]

Similarly, we can define the relative global error of the discrete \(I_5\) as before.

For the purpose of numerical comparisons, we apply an implicit second-order non-multi-symplectic method, the mid-point scheme in time and the trapezoidal scheme in space (in short, denoted by MT2), to the nonlinear Schrödinger equation. Similarly, the above discrete variables can be given for MT2, and they are different from those for MN2. Note that the discretization of conservative properties investigated must be consistent with the numerical method considered.

All numerical comparisons between MM2 and MT2 are processed in the same numerical conditions. The time stepsize and space stepsize are taken as \(h = 0.2\) and \(\tau = 0.02\) respectively, this means that the numerical implementation in temporal direction will be \(10^4\) steps. Because both of schemes are implicit, the fixed point iteration method is utilized to solve the nonlinear algebraic systems generated by the numerical scheme, each iteration will terminate when the maximum absolute error of the adjacent two iterative values is less than \(10^{-14}\). This terminating condition is also utilized in 4.2 and 4.3. With this initial data, we find that the computation cost of the two methods MN2 and MT2 are almost the same.

Figure 1 shows that the absolute errors of the numerical solutions given by two schemes are in reasonable scale (match the 2-order accuracy), the errors curves are oscillating and in increasing trend, the accumulation of errors of MT2 is almost two times of MN2. This reveals that MN2 is superior to MT2 in the errors of numerical solutions, indeed, in the preservation of the phase space structure. Both can present the correct evolution of the soliton in an appropriate time-space domain, our periodic boundary condition complies with the asymptotic behavior of the exact solution (4.3), the wave function, as \(x \to \pm \infty\).

Figure 2 displays the maximum errors of the local energy and momentum conservation laws by the two schemes utilized. For each \(n\), let \(\max_{0 \leq l \leq N} \|E_{le}^n\|\) and \(\max_{0 \leq l \leq N} \|M_{le}^n\|\) denote the maximum errors of the energy conservation law and the momentum conservation law, respectively. Comparing the top two plots, it is observed that the local energy error of MN2 is in the scale of \(10^{-7}\) and the error of MT2 in the scale of \(10^{-4}\), the error of MT2 is almost two times of MN2. This means that MN2 is superior to MT2 in the errors of numerical solutions, indeed, in the preservation of the phase space structure. Both can present the correct evolution of the soliton in an appropriate time-space domain, our periodic boundary condition complies with the asymptotic behavior of the exact solution (4.3), the wave function, as \(x \to \pm \infty\).

The local energy error of some global conservation laws are displayed in Figure 3 by MN2 and MT2. All error curves are in oscillation. As observed in Figure 2, the local energy error by MN2 is better than by MT2, this phenomena happens in the total energy. We find that the relative global error of the discrete total energy by MN2 is of order \(O(10^{-7})\), but the error by MT2 is only in the scale of \(10^{-4}\). It is also observed that the errors in the discrete total momentum and the integral \(I_5\) by the two methods are almost the same. Figure 2 and Figure 3 tell us that the multi-symplectic RKN methods, in general, do not have the discrete conservation of energy and momentum.

Figure 4 shows the relative global errors of the charge conservation law (CCL) produced by both of the two schemes in the time interval \([0,200]\). The top plot in the figure shows that the discrete charge is conserved within roundoff errors of the computer by means of MN2, however, the error produced by using MT2 are in the scale of \(O(10^{-7})\). This shows that MN2 is much better than MT2 in the preservation of discrete charge. In fact, both methods are stable in the sense of discrete charge conservation.
Figure 1: The error of numerical solutions of $\psi(x, t)$ by MN2 (left) and by MT2 (right) respectively.

4.2 Experiment B

In the previous subsection, the symplectic Nyström method applied to the space is only of second order. In this subsection we implement a numerical experiment, which has been studied in [14] elaborately, by two 3-stage 4-order Nyström schemes, one is symplectic and the other is non-symplectic for giving a comparison as that given between MN2 and MT2 in Experiment A. In [14], the initial condition is $\psi(x, 0) = a(1 - 0.1 \cos x) + b \sin x$, where $a = 0.5$ and $b = 0$ or $10^{-8}$; $b = 10^{-8}$ means that a tiny asymmetry is introduced to the initial condition, as the author pointed out, the asymmetry is a little more subtle to deal with in the investigation. Here, in our numerical experiment, the spatial interval is taken as $[0, L]$, where $L = 4\pi$, and we choose $N$ as the number of the spatial grid points, that is, the spatial stepsize is determined by $h = L/N$. In [14] three cases $N = 32$, $N = 64$ and $N = 128$ are considered for not only symmetric and asymmetric initial data, and the method utilized in [14] is that the LF2 scheme (namely, the mid-point scheme in this paper) is applied to the temporal and the pseudo-spectral method to the spatial. Here we consider the case $N = 32$ and $b = 10^{-8}$, and the initial data for $\psi(x, t)$ is taken $\psi(x, 0) = a(1 - 0.1 \cos x) + b \sin x$, the same one as in [14]; for the initial data of $\phi(x, t)$, we adopt $\phi(x, 0) = \frac{d}{dt}\psi(x, 0) = 0.1a \sin(x) + b \cos(x)$. And we apply the implicit mid-point scheme to the temporal direction and the temporal stepsize we take is $\tau = 0.015$. In this experiment, we also implement the following periodic conditions

$$\psi|_0 = \psi|_L, \quad \phi|_0 = \phi|_L$$

and the time interval $[0, 900]$ ($6 \times 10^4$ time steps).

We construct the symplectic and non-symplectic 3-stage 4-order Nyström schemes, which can be formulated as the following Butcher’s tabulars

$$
\begin{array}{c|ccc}
0 & -1/4 & 1/4 & 0 \\
1/2 & 7/48 & -1/48 & 0 \\
1 & 1/6 & 1/3 & 0 \\
\hline
 & 1/6 & 1/3 & 0 \\
 & 1/6 & 2/3 & 1/6 \\
\end{array}
$$

and

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
1/2 & 17/96 & -1/6 & 11/96 \\
1 & 1/24 & 2/3 & -5/24 \\
\hline
 & 1/6 & 1/3 & 0 \\
 & 1/6 & 2/3 & 1/6 \\
\end{array}
$$

respectively. We denote the multisymplectic RKN method, i.e., the implicit mid-point scheme applied to the temporal and the 3-stage 4-order symplectic Neström scheme to the spatial, by MS-MN3 in
short. Simultaneously, the non-multisymplectic one is denoted by nMS-MN3. All numerical comparisons
between MS-MN3 and nMS-MN3 are processed under the same numerical conditions, and the iteration
method for solving the the nonlinear algebraic system and the stop criteria of the iteration are the same as
introduced in Experiment A. Figs.5-8 are given by means of the two methods, MS-MN3 and nMS-MN3.

Figure 5 shows the maximum errors of the discrete local energy and momentum conservation laws
by the two methods in the time interval [0, 900]. All the errors displayed in this figure are in the same
scale of $O(10^{-2})$. Compared with the ones showed in Figure 2, it seems that the higher-order schemes
preserve the local invariants are not as good as the lower-order ones, and we will see the same phenomena
displayed in Figure 6, the contrary result we can see in Figure 7. And, the same point between Figure
5 and Figure 2 is that, the errors are oscillating near 0 even after the so long computations, thus the
high-order schemes are stable with respect to the local conservation laws numerically.

Figure 6 shows the global errors of the two total invariants, the discrete total energy and the integral
$I_5$. As shown in Figure 5, all the errors in this figure are of order $O(10^{-2})$ and it doesn’t produce any drift
in the long computation and this guarantee the numerical stability with respect to the two conservation
laws, the total energy and $I_5$.

The global errors of the discrete total momentum obtained by MS-MN3 and nMS-MN3 are displayed
in Figure 7. It exhibits some interesting phenomena of the evolutions of the errors here, the error by MS-
MN3 is in the scale of $O(10^{-7})$, and it is two orders of magnitude better than the other one. Moreover,
the error by the multisymplectic method doesn’t have any growth, it is in the reasonable oscillation, but
the error by non-multisymplectic one has a linear growth.

Figure 8 exhibits the global errors in the discrete charge conservation law by the two method. Ob-
serving in the two plots, it can be found that the remarkable advantage of the multi-symplectic RKN
methods is the precise preservation of discrete charge conservation law. In the top plot, it shows that
the involution of the global error of the discrete conservation law is conserved in the scale of $O(10^{-12})$,
almost the roundoff error of the computer; compare with the top plot in Figure 4, there is a very small
error but normal accumulation in such long numerical computation. As for nMS-MN3, the error is only of order $O(10^{-6})$, and it is an interesting phenomenon that the shape of this error is similar to that in the discrete total momentum obtained by MS-MN3, i.e. the first plot in Figure 7.

4.3 Experiment C

In order to investigate the collision of solitons, we consider the following form of the nonlinear Schrödinger equation (4.1)

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0. \quad (4.6)$$

As discussed in (2.1)-(2.3), the above equation can be written as the following form

$$\tilde{M}\partial_t z + \tilde{K}\partial_x z = \nabla_z \tilde{S}(z), \quad (4.7)$$

where $z$ is the state vector variable as introduced in §2, $\tilde{M} = M$, $\tilde{K} = -K$ and $\tilde{S}(z) = -\frac{1}{2}(q^2 + p^2)^2 + v^2 + w^2$. The initial condition on two-soliton interaction is given as follows

$$\psi|_{t=0} = \frac{1}{\sqrt{2}} \left[ \text{sech} \left( \frac{x}{\sqrt{2}} \right) \exp \left( \frac{i}{2} \left( x^2 - 25 \right) \right) \right]. \quad (4.8)$$

In this experiment, we apply a high-order scheme, i.e. 3-stage 6-order Gauss-Legendre RK method, to the temporal direction and the symplectic 2-stage 2-order Néström method introduced in Experiment A to the spatial direction, we denote this method by GL3-N2 in short. In the sequel, we make use of GL3-N2 to exhibit the two-soliton interaction, and the space mesh-length $h = 0.2$ and the time mesh-length $\tau = 0.01$. The computation time interval we choose here is $[0, 100]$. The spatial interval is taken as $[-60, 120]$.

Figure 9 shows the real part and imaginary part of numerical result of the two-soliton interaction respectively. The numerical solution depicts two waves where the shape evolution both before and after collision do not change obviously. The figure displays the correct behavior of the two-soliton interaction, and implies the good preservation of the phase space structure.

Figure 10 shows the maximum errors of local conservation laws by GL3-N2 in the time interval $[0, 100]$. The error of the discrete local energy conservation law displayed in this figure is in the same scale of $O(10^{-13})$. However for the local momentum conservation law, the error is of $O(10^{-2})$. Numerical results are very interesting! From the observing, one can find that the errors get to the maximums at a certain time between 20 and 30, namely at the collision time of two waves.

The global errors of the discrete charge and the discrete total energy are exhibited in Figure 11. The error in charge is of order $O(10^{-14})$, it matches the theoretical analysis in §3 very well. The error in energy arrives at the scale of $O(10^{-15})$, it is out of our expectation. And it gets to a local maximum, which look like a local shock, at the collision time, the shock reflects the collision effect.

Figure 12 shows the global errors of the discrete total momentum and the integral $I_5$. The global error of the momentum is in the scale of $O(10^{-9})$ and the error of $I_5$ is only of $O(10^{-1})$, but both of them reach the maximums at the collision time, and this reflects the collision mechanism at some degree numerically.

Generally speaking, the multi-symplectic RKN methods may not preserve the discrete total energy, the discrete total momentum and the integral $I_5$ exactly. In our numerical experiment, the evolutions of the errors of the local momentum, the integral $I_5$ and the total momentum have a similar character, that is, before and after the collision time, the errors vary much more slowly with oscillation.

5 Conclusions

The concatenation of symplectic Runge-Kutta methods in temporal direction and symplectic Nystrom methods in spatial direction for nonlinear Schrödinger equations leads to the multi-symplectic integrators (so called multi-symplectic RKN methods). The conclusions of this paper are listed as follows.
• It is shown theoretically that the discrete total symplecticity (3.3) in temporal direction is preserved precisely by the multi-symplectic RKN methods for nonlinear Schrödinger equations. Numerical results reveal the stability of multi-symplectic RKN methods in the sense of classical conservation laws and the good preservation of phase space structure.

• Theoretical and numerical results show that the remarkable advantage of multi-symplectic RKN methods is the precise preservation of discrete (local and global) charge conservation law for the equations.

• Numerical implementation shows that multi-symplectic methods, in general, do not preserve energy conservation law, the multi-symplectic RKN methods are superior to non-multi-symplectic methods in the energy conservation for nonlinear Schrödinger equations. An interesting observation is that the numerical accuracy of global energy under the multi-symplectic RKN discretization may reach a higher order in contrast to the accuracy of numerical solutions.

• Multi-symplectic RKN schemes of higher order in spatial and temporal directions are implemented in numerical experiments. The two-soliton interaction can be depicted correctly by means of multi-symplectic RKN methods. Some interesting numerical results are exhibited, and they reveal the superiorities of multi-symplectic RKN methods not only in the conservation of multi-symplectic geometric structure, but also in the preservation of some crucial conservative properties in physics.

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References


465-492.


1994.

[19] Y. B. Suris, On the conservation of the symplectic structure in the numerical solution of Hamiltonian
systems (in Russian), In: *Numerical Solution of Ordinary Differential Equations*, ed. S. S. Filippov,

[20] Y. B. Suris, The canonicity of mapping generated by Runge-Kutta type methods when integrating
the systems $\ddot{x} = -\partial U/\partial x$, Zh. Vychisl. Mat. i Mat. Fiz. 29 (1989) 138-144.
Figure 3: The relative global errors of the total conservation laws, the discrete total energy (top), the
discrete total momentum (middle) and the discrete conserved integral $I_5$ (bottom). The left figures are
obtained by using MN2 and the right ones by MT2.
Figure 4: The relative global error of the discrete charge, MN2(top), MT2(bottom).

Figure 5: The maximum errors of the discrete local conservation laws. Top: ECL; bottom: MCL. The left is obtained by using MS-MN3 and the right by nMS-MN3.
Figure 6: The global errors of the discrete energy and $I_5$. Top: the discrete total energy; bottom: $I_5$, MS-MN3(left) and nMS-MN3(right).

Figure 7: The global errors of the discrete total momentum, MS-MN3 (left) and nMS-MN3(right).
Figure 8: The global errors of the discrete charge, the top shows that by MS-MN3 and the bottom by nMS-MN3.

Figure 9: The numerical solutions of $\psi(x, t)$ by GL3-N2, the left one is the real part $q(x, t)$ and the right is the imaginary part $p(x, t)$. 
Figure 10: The maximum errors of the local discrete energy (left) and momentum (right) conservation laws.

Figure 11: The global errors of the discrete charge and the discrete total energy.

Figure 12: The global errors of the discrete conservation laws, the discrete momentum (top) and the discrete conserved integral $I_5$ (bottom).