High-order compact splitting multisymplectic method for the coupled nonlinear Schrödinger equations

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\begin{abstract}
In this paper, we develop a new kind of multisymplectic integrator for the coupled nonlinear Schrödinger (CNLS) equations. The CNLS equations are cast into multisymplectic formulation. Then it is split into a linear multisymplectic formulation and a nonlinear Hamiltonian system. The space of the linear subproblem is approximated by a high-order compact (HOC) method which is new in multisymplectic context. The nonlinear subproblem is integrated exactly. For splitting and approximation, we utilize an HOC–SMS integrator. Its stability and conservation laws are investigated in theory. Numerical results are presented to demonstrate the accuracy, conservation laws, and to simulate various solitons as well, for the HOC–SMS integrator. They are consistent with our theoretical analysis.
\end{abstract}

1. Introduction

Schrödinger equations describe a wide range of physical phenomena, such as hydrodynamics, plasma physics, nonlinear optics, self-focusing in laser pulses, propagation of heat pulses in crystals, and the dynamics of Bose–Einstein condensate at extremely low temperature. They play essential roles in the mathematical and physical contexts, and more and more focus has been concentrated on their numerical solvers in recent decades. In this paper, we are concerned with a high-order compact–splitting multisymplectic (HOC–SMS) algorithm for the coupled nonlinear Schrödinger (CNLS) equations

\begin{align}
&i u_t + i \alpha u_x + \frac{1}{2} u_{xx} + (|u|^2 + \beta |v|^2) u = 0, \\
&i v_t - i \alpha v_x + \frac{1}{2} v_{xx} + (|v|^2 + \beta |u|^2) v = 0,
\end{align}

with the initial condition

\begin{align}
u(x, 0) &= u_0(x), \quad v(x, 0) = v_0(x), \quad x \in \mathbb{R},
\end{align}

where $i^2 = -1$, $\mathbb{R}$ marks the spatial domain, $u$ and $v$ are the complex amplitudes or envelopes of two wave packets, $u_0(x)$ and $v_0(x)$ are known functions.

\textbf{Proposition 1.} Under the homogeneous boundary condition, Eq. (1) satisfies the following conservation laws:
• The energy is invariant
\[ \mathcal{E}(t) = \int_{\mathbb{R}} \left[ 2i\alpha (\bar{v}x - u\bar{u}_{x}) + |u|^{4} + |v|^{4} - |u_{x}|^{2} - |v_{x}|^{2} + 2\beta |u|^{2}|v|^{2} \right] dx = \mathcal{E}(0). \] (3)

• The momentum is independent of \( t \)
\[ \mathcal{M}(t) = \int_{\mathbb{R}} [u(x, t)\bar{u}_{x}(x, t) + v(x, t)\bar{v}_{x}(x, t)] dx = \mathcal{M}(0). \] (4)

Numerical contributions for various nonlinear Schrödinger equations are hot topics during the past decades [1–11]. High-order compact (HOC) technique is popular due to its high resolution, compactness and economy in scientific computation [2,12–14]. Splitting method is widely adopted in many nonlinear problems for the sake of its efficiency in aspects of saving CPU time and computer memory [15–19]. Therefore, the two kinds of numerical methods are often unitedly used in many nonlinear problems, which are referred to as HOC splitting methods [20]. It gathers various advantages that exist in HOC method and splitting skill, such as small stencil, high accuracy, low computational cost.

At the end of the last century, symplectic integrators which were systematically studied by Feng et al. [21,22] were generalized from Hamiltonian ODEs (HODEs) to Hamiltonian PDEs (HPDEs), which are called multisymplectic integrators [23]. Many scientific computing researchers are enjoyed themselves in its incommensurable advantages over other numerical methods in structure-preserving [24–26], including local conservation laws and long-term simulation [3]. It has been used to investigate Hamiltonian dynamics, such as Klein–Gordon–Schrödinger equation [27], KdV equation [28,23,29], Dirac equation [30]. Yet most of the multisymplectic integrators are completely implicit, which will greatly suppress the efficiency. To overcome the drawbacks of general multisymplectic integrators, the conception of splitting multisymplectic (SMS) integrator was offered recently. In 2007, Ryland and McIachlan [31] proposed the conception of SMS method which combines the advantages of the splitting method with multisymplectic approach, but there is no concrete numerical scheme or numerical illustration. Hong & Kong investigated the SMS integrators for nonlinear Schrödinger equations and three-dimensional Maxwell equations lately [32,33] from different aspects.

As for the numerical approaches for the CNLS equations, Bandrauk developed a high-order split-step Fourier pseudo-spectral method [20]. Later, Ismail and Alamri designed an implicit finite difference method [13], which is unconditionally stable. Then, Sun & Qin considered the multisymplecticity [34]. Three multisymplectic integrators were proposed by Wang and Li [35]. Chen et al. proposed an SMS approach coupled with pseudo-spectral method [1].

The basic idea of SMS technique for the CNLS equations, is to split the original system into a linear multisymplectic subsystem and a nonlinear subsystem [1]. The splitting brings an unexpected pleasure for investigators that the linear problem is uncoupling, relatively easy to solve, and the nonlinear subsystem can be transformed into HODEs by parameterizing the spatial independent argument \( x \). Furthermore, the HODEs can be solved exactly due to their point-wise conservation law. Chen seized the pseudo-spectral method on the spatial discretization for a linear subproblem, which is extremely accurate, while, is expensive in computer memory and is just limited to periodic or homogeneous boundary conditions only. In this paper, we apply the HOC technique to the spatial approximation of the linear subproblem. It can not only deal with non-periodic and non-homogeneous problems with high accuracy, but also occupy less computer resource. Deliberating on the stability, we choose the implicit temporal discretization as well. Then, for the nonlinear subproblem, it is noticed that it meets the point-wise conservation law
\[ |u(x, t_{n+1})|^{2} = |u(x, t_{n})|^{2} = \cdots = |u_{0}(x)|^{2}, \]
\[ |v(x, t_{n+1})|^{2} = |v(x, t_{n})|^{2} = \cdots = |v_{0}(x)|^{2}, \quad \forall x \in \mathbb{R}, \] (5)
which leads the solution to explicit and exact. Therefore, an HOC–SMS scheme is designed for the CNLS equations which concentrates on various advantages, such as spectral-like resolution, less memory, unconditional stability, long-term simulation, preservation of discrete conservation laws.

The current paper is arranged as follows. In Section 2, we describe the detailed multisymplectic framework for the CNLS equations, including multisymplectic method and splitting multisymplectic method. We present an HOC–SMS scheme for the CNLS equations in Section 3. The stability and discrete conservation laws are investigated in Section 4. In Section 5, various examples with detailed numerical results are listed to verify the theoretical analysis. Some conclusions are given to end the work.

2. Multisymplectic framework for the CNLS equations

In the present section, we briefly review the multisymplectic structure for the CNLS equations and the basic idea of SMS technique.
2.1. Multisymplectic structure for the CNLS equations

Supposing \( u = p + iq \) and \( v = \phi + i\psi \), Eq. (1) can be written as a series of real-valued equations

\[
\begin{align*}
q_t + \alpha q_x - \frac{1}{2} \frac{\partial^2 q}{\partial x^2} &= [(p^2 + q^2) + \beta (\phi^2 + \psi^2)]p, \\
p_t + \alpha p_x + \frac{1}{2} \frac{\partial^2 p}{\partial x^2} &= -[(p^2 + q^2) + \beta (\phi^2 + \psi^2)]q, \\
\psi_t - \alpha \psi_x - \frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} &= [(\phi^2 + \psi^2) + \beta (p^2 + q^2)]\phi, \\
\phi_t - \alpha \phi_x + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} &= -[(\phi^2 + \psi^2) + \beta (p^2 + q^2)]\psi.
\end{align*}
\]

(6)

Next, by introducing new canonical variables \( \gamma, f, g, \eta \), Eq. (6) can be noted as

\[
\begin{align*}
q_t + \alpha q_x - \gamma_x &= [(p^2 + q^2) + \beta (\phi^2 + \psi^2)]p, \\
-p_t - \alpha p_x - \eta_x &= [(p^2 + q^2) + \beta (\phi^2 + \psi^2)]q, \\
\psi_t - \alpha \psi_x - f_x &= [(\phi^2 + \psi^2) + \beta (p^2 + q^2)]\phi, \\
-\phi_t + \alpha \phi_x - g_x &= [(\phi^2 + \psi^2) + \beta (p^2 + q^2)]\psi.
\end{align*}
\]

(7)

Letting \( z = (p, q, \phi, \psi, \eta, f, g)^T \), we can cast Eq. (7) into multisymplectic framework

\[
M_z + K_z = \nabla_z S(z),
\]

(8)

where \( \nabla \) is the gradient operator and the skew-symmetric matrices \( M, K \) are as follows:

\[
M = \begin{bmatrix} J & 0_4 \\ 0_4 & 0_4 \end{bmatrix}, \quad K = \begin{bmatrix} \alpha J & -I_4 \\ I_4 & \alpha 0_4 \end{bmatrix},
\]

where \( J = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}, 0_4 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, I_4 \) is a \( 4 \times 4 \) identity matrix. The Hamiltonian function is

\[
S(z) = \frac{1}{4} (p^2 + q^2)^2 + \frac{1}{4} (\phi^2 + \psi^2)^2 + \frac{\beta}{2} (p^2 + q^2)(\phi^2 + \psi^2) + \gamma^2 + \eta^2 + f^2 + g^2.
\]

In terms of the multisymplectic theory, system (8) satisfies local conservation laws as follows:

- Multisymplectic conservation law:
  \[
  \frac{\partial}{\partial t} \omega + \frac{\partial}{\partial x} \kappa = 0,
  \]
  (9)

  where \( \omega \) and \( \kappa \) are pre-symplectic 2-forms
  \[
  \omega = dq \wedge dp + d\psi \wedge df, \\
  \kappa = \alpha (dq \wedge dp + d\phi \wedge d\psi) + dp \wedge d\gamma + dq \wedge d\eta + d\phi \wedge df + d\psi \wedge dg.
  \]

- Local energy conservation law:
  \[
  \frac{\partial}{\partial t} E(z) + \frac{\partial}{\partial x} F(z) = 0,
  \]
  (10)

  where the energy density \( E(z) \) and the energy flux \( F(z) \) are
  \[
  E(z) = S(z) - \alpha (pq_t - q\psi_f - \phi g) - (\gamma^2 + \eta^2 + f^2 + g^2) + \frac{1}{2} (p\gamma_s + q\eta_s + \phi f_x + \psi g_x),
  \]
  \[
  F(z) = \frac{\alpha}{2} (pq_t - q\psi_f - \phi g) - \frac{1}{2} (p\gamma_s + q\eta_s + \phi f_x + \psi g_x).
  \]

- Local momentum conservation law:
  \[
  \frac{\partial}{\partial t} I(z) + \frac{\partial}{\partial x} G(z) = 0,
  \]
  (11)

  where the momentum density \( I(z) \) and the momentum flux \( G(z) \) are
  \[
  G(z) = S(z) - \frac{1}{2} (pq_t - q\psi_f - \phi g), \quad I(z) = q\gamma - p\eta + \psi_f - \phi g.
  \]

The local conservation laws imply that the density can be different from time to time, however, the increment of the density in time is just offset by the deficit of the flux in space. Under the periodic or homogeneous circumstance, the global
conservation laws can be inferred as follows:
\[
\bar{\omega}(t) = \int_{\mathbb{R}} \omega(x, t) dx = C_1,
\]
\[
\mathcal{E}(t) = \int_{\mathbb{R}} E(x, t) dx = C_2,
\]
\[
\mathcal{I}(t) = \int_{\mathbb{R}} I(x, t) dx = C_3,
\]
where \( C_1, C_2 \) and \( C_3 \) are irrespective of time.

2.2. Splitting multisymplectic technique for the CNLS equations

In this subsection, we give an outline of the popular splitting method for a nonlinear equation
\[
w_t = (\mathcal{L}(t) + \mathcal{N}(t, w))w,
\]
where \( \mathcal{L} \) and \( \mathcal{N} \) are linear and nonlinear operators, respectively. We decompose the nonlinear problem into the following subproblems
\[
w_t = \mathcal{L}(t)w, \quad \text{(13)}
\]
\[
w_t = \mathcal{N}(t, w)w. \quad \text{(14)}
\]

To solve Eq. (12) over \( t \in [t_n, t_{n+1}] \), we employ the standard Strang splitting technique [36] to solve (13), (14) and have
\[
\begin{aligned}
& w^* = \exp \left[ \frac{1}{2} \int_{t_n}^{t_{n+1}} \mathcal{N}(t, w(t_n)) dt \right] w(t_n), \\
& w^{**} = \exp \left[ \int_{t_n}^{t_{n+1}} \mathcal{L}(t) dt \right] w^*, \\
& w(t_{n+1}) = \exp \left[ \frac{1}{2} \int_{t_n}^{t_{n+1}} \mathcal{N}(t, w^{**}) dt \right] w^{**}.
\end{aligned}
\]

As is well known, the temporal splitting accuracy of the Strang splitting is of second order.

Now, we apply the splitting technique to the multisymplectic system (8). Eq. (1) can be split into such two subproblems:
\[
\mathcal{L} : \begin{cases}
  iu_t + \alpha u_x + \frac{1}{2} u_{xx} = 0, \\
  iv_t - \alpha v_x + \frac{1}{2} v_{xx} = 0,
\end{cases} \quad \text{(16)}
\]
and
\[
\mathcal{N} : \begin{cases}
  iu_t + (|u|^2 + \beta |v|^2) u = 0, \\
  iv_t + (|v|^2 + \beta |u|^2) v = 0.
\end{cases} \quad \text{(17)}
\]

It is noticed that the nonlinear subproblem (17) satisfies the point-wise conservation law (5).

It is obvious that the linear subproblem (16) is an uncoupled problem and can be tackled in the manner of single Schrödinger equation which is simpler than the coupled ones. For the nonlinear part (17), the point-wise conservation law (5) makes its solver explicit and exact in that it becomes linear and variable separable ODEs.

The linear subproblem can be rewritten as
\[
\begin{aligned}
& q_t + \alpha q_x - \gamma_s = 0, \\
& p_t - \alpha p_x - \eta_s = 0, \\
& \psi_t - \alpha \psi_x - f_x = 0, \\
& \phi_t + \alpha \phi_x - g = 0, \\
& p_x = 2\gamma, \quad q_x = 2\eta, \\
& \phi_x = 2f, \quad \psi_x = 2g.
\end{aligned}
\]

In the multisymplectic context, it reads
\[
\begin{aligned}
Mz_t + Kz_x = \nabla_z S_1(z),
\end{aligned}
\]
where \( S_1(z) = \gamma^2 + \eta^2 + f^2 + g^2 \).
We can derive the multisymplectic conservation law
\[
\frac{\partial}{\partial t} \omega + \frac{\partial}{\partial x} \kappa_1 = 0, \quad \omega = \frac{1}{2} \text{d}z \wedge M \text{d}z, \quad \kappa_1 = \frac{1}{2} \text{d}z \wedge K \text{d}z.
\] (19)

Then, the nonlinear subproblem (17) will be reduced to HODEs by parameterizing the spatial independent argument \( x \)
\[
\begin{align*}
\frac{dq(x, t)}{dt} &= [(p^2 + q^2) + \beta (\phi^2 + \psi^2)]p, \\
\frac{dp(x, t)}{dt} &= [(p^2 + q^2) + \beta (\phi^2 + \psi^2)]q, \\
\frac{d\psi(x, t)}{dt} &= [(\phi^2 + \psi^2) + \beta (p^2 + q^2)]\phi, \\
\frac{d\phi(x, t)}{dt} &= [(\phi^2 + \psi^2) + \beta (p^2 + q^2)]\psi,
\end{align*}
\] (20)

for any \( x \in R \), with the framework
\[
\frac{d}{dt} z_2 = J^{-1} \nabla_2 S_2(z_2),
\]
where \( z_2 = [p, q, \phi, \psi]^T \). The Hamiltonian functional is
\[
S_2(z_2) = \frac{1}{4} (p^2 + q^2)^2 + \frac{1}{4} (\phi^2 + \psi^2)^2 + \frac{\beta}{2} (p^2 + q^2)(\phi^2 + \psi^2).
\]

Similarly, for the nonlinear subproblem, the symplectic conservation law is available
\[
\frac{d}{dt} \omega(x, t) = 0, \quad \forall x \in R, \quad \omega = \frac{1}{2} \text{d}z_2 \wedge J \text{d}z_2 = \frac{1}{2} \text{d}z \wedge M \text{d}z.
\] (21)

3. HOC–SMS discretization for the CNLS equations

We might firstly retrospect the basic thought of HOC method as well. It approximates to derivatives with fewer nodes and of higher accuracy. The derivatives can be implicitly evaluated by solving a tri-diagonal or a pent-diagonal linear algebraic system. It is confirmed that the HOC method features high accuracy with smaller dispersive error [14].

3.1. Discretization for the linear subproblem

We consider the linear subproblem with boundary condition
\[
u(a, t) = u(b, t), \quad v(a, t) = v(b, t), \quad t \in [0, T].
\]

Firstly, we discretize the temporal–spatial region \( R \times [0, T] = [a, b] \times [0, T] \) with coordinates \( x_j = a + jh, j = 0, 1, \ldots, J \) and \( t_k = \tau k, k = 0, 1, \ldots, K \), where \( h = \frac{b-a}{J} \) and \( \tau = \frac{T}{K} \) are spatial step size and temporal step length, respectively.

Considering the discretization of the first-order derivative \( f'_j = \frac{d}{dx} f(x) |_{x=x_j} \), we have the formula [14]:
\[
\alpha f'_{j-1} + f'_j + \alpha f'_{j+1} = b_1 f_{j-1} - f_{j-2} + a_1 \frac{f_{j+1} - f_{j-1}}{2h},
\] (22)

where \( a_1, b_1 \) and \( \alpha \) are undetermined parameters which depend on the order condition constraints
\[
\begin{align*}
& a_1 + b_1 = 1 + 2\alpha, \quad \text{second order}, \\
& a_1 + 2^2 b_1 = 6\alpha, \quad \text{fourth order}, \\
& a_1 + 2^4 b_1 = 10\alpha, \quad \text{sixth order}.
\end{align*}
\] (23)

In accordance with the above equations, choosing a free parameter, such as \( \alpha \), it derives a family of fourth-order schemes
\[
a_1 = \frac{2}{3} (\alpha + 2), \quad b_1 = \frac{1}{3} (4\alpha - 1).
\]

The leading term of the truncation error is \( \frac{4}{5} (3\alpha - 1) f^{(5)} h^4 \). In particular, \( \alpha = \frac{1}{3} \) is taken into account in this paper. Now it yields a sixth-order approximation with \( \alpha = \frac{1}{3}, a_1 = \frac{14}{21}, b_1 = \frac{1}{3} \). The dominant part of the truncation error is \( \frac{4}{7} f^{(7)} h^6 \).

Under the periodic or homogeneous boundary condition, the approximation to \( f \) can be written in the matrix form
\[
Af_x = Bf \Rightarrow f_x = Df,
\] (24)
where \( D = A^{-1}B \), and

\[
A = \frac{1}{3} \begin{bmatrix}
3 & 1 & 1 & 1 \\
1 & 3 & 1 & 1 \\
& & & \\
& & & \\
& & & \\
& & & \\
1 & 1 & 3 & 1
\end{bmatrix},
\]

\[
B = \frac{1}{36h} \begin{bmatrix}
0 & 28 & 1 & -1 & -28 \\
-28 & 0 & 28 & 1 & -1 \\
& & & & \\
& & & & \\
& & & & \\
1 & -1 & -28 & 0 & 28 \\
28 & 1 & -1 & -28 & 0
\end{bmatrix}.
\]

**Remark 1.** It is obvious that matrix \( A \) is symmetric, while, \( B \) is skew-symmetric. Moreover, \( D \) is skew-symmetric, whereas \( D^2 \) is symmetric. They are all real.

**Remark 2.** From the form of matrices \( A \) and \( B \), they are tri-diagonal or pentagon-diagonal. Nevertheless, to obtain a symmetric six-order numerical approximation to \( \frac{d}{dx} f(x) \), seven nodes are covered at every point by general method. This will make the bandwidth of the matrix seven which is wider than the former.

Now, we discretize Eq. (18) in the spatial direction with the sixth-order compact scheme

\[
\begin{align*}
q_{t} - D\gamma + \alpha Dq &= 0, \\
-p_{t} - D\eta - \alpha Dp &= 0, \\
\psi_{t} - Df - \alpha D\psi &= 0, \\
-\phi_{t} - Dg + \alpha D\phi &= 0, \\
Dp &= 2\gamma, \\
Dq &= 2\eta, \\
D\phi &= 2f, \\
D\psi &= 2g. (25)
\end{align*}
\]

where \( p = [p_1, p_2, \ldots, p_j], \ q = [q_1, q_2, \ldots, q_l], \ \phi = [\phi_1, \phi_2, \ldots, \phi_j], \ \psi = [\psi_1, \psi_2, \ldots, \psi_j] \). Eliminating the variables \( \gamma, f, g, \eta, \) it results in

\[
\begin{align*}
p_{t} &= -\frac{1}{2}D^2q - \alpha Dp, \\
q_{t} &= \frac{1}{2}D^2p - \alpha Dq, \\
\phi_{t} &= -\frac{1}{2}D^2\phi + \alpha D\phi, \\
\psi_{t} &= \frac{1}{2}D^2\psi + \alpha D\psi. \\
(26)
\end{align*}
\]

Then, we discretize Eq. (26) in time by the symplectic implicit midpoint rule and have

\[
\begin{align*}
(p^{k+1} - p^{k})/\tau &= -\frac{1}{4}D^2(q^{k+1} + q^{k}) - \frac{\alpha}{2}D(p^{k+1} + p^{k}), \\
(q^{k+1} - q^{k})/\tau &= \frac{1}{4}D^2(p^{k+1} + p^{k}) - \frac{\alpha}{2}D(q^{k+1} + q^{k}), \\
(\phi^{k+1} - \phi^{k})/\tau &= -\frac{1}{4}D^2(\psi^{k+1} + \psi^{k}) + \frac{\alpha}{2}D(\phi^{k+1} + \phi^{k}), \\
(\psi^{k+1} - \psi^{k})/\tau &= \frac{1}{4}D^2(\phi^{k+1} + \phi^{k}) + \frac{\alpha}{2}D(\psi^{k+1} + \psi^{k}). \\
(27)
\end{align*}
\]

The matrix form of the approximation (27) is

\[
\begin{bmatrix}
1 + \frac{\alpha\tau}{2}D & \frac{\tau}{4}D^2 \\
-\frac{\tau}{4}D^2 & 1 + \frac{\alpha\tau}{2}D
\end{bmatrix}
\begin{bmatrix}
p^{k+1} \\
q^{k+1}
\end{bmatrix}
= \begin{bmatrix}
1 - \frac{\alpha\tau}{2}D & -\frac{\tau}{4}D^2 \\
\frac{\tau}{4}D^2 & 1 - \frac{\alpha\tau}{2}D
\end{bmatrix}
\begin{bmatrix}
p^{k} \\
q^{k}
\end{bmatrix},
\]

\[
\begin{bmatrix}
1 - \frac{\alpha\tau}{2}D & \frac{\tau}{4}D^2 \\
-\frac{\tau}{4}D^2 & 1 - \frac{\alpha\tau}{2}D
\end{bmatrix}
\begin{bmatrix}
\phi^{k+1} \\
\psi^{k+1}
\end{bmatrix}
= \begin{bmatrix}
1 + \frac{\alpha\tau}{2}D & -\frac{\tau}{4}D^2 \\
\frac{\tau}{4}D^2 & 1 + \frac{\alpha\tau}{2}D
\end{bmatrix}
\begin{bmatrix}
\phi^{k} \\
\psi^{k}
\end{bmatrix}. (28)
\]
3.2. Discretization for the nonlinear subproblem

In this subsection, we discuss the symplectic approach to the nonlinear subproblem (20). It can be computed exactly as

\[
\begin{align*}
\begin{bmatrix}
p_j^{k+1} \\
q_j^{k+1} \\
\phi_j^{k+1} \\
\psi_j^{k+1}
\end{bmatrix}
&= 
\begin{bmatrix}
\cos \theta_j & - \sin \theta_j \\
\sin \theta_j & \cos \theta_j \\
\cos \sigma_j & - \sin \sigma_j \\
\sin \sigma_j & \cos \sigma_j
\end{bmatrix}
\begin{bmatrix}
p_j^k \\
q_j^k \\
\phi_j^k \\
\psi_j^k
\end{bmatrix}, \quad j = 0, 1, 2, \ldots, J,
\end{align*}
\]

(29)

where \( \theta_j = \tau((p_j^k)^2 + (q_j^k)^2) + \beta((\phi_j^k)^2 + (\psi_j^k)^2) \) = \( \tau(|u_j|^2) + \beta(|v_j|^2) \).

\( \sigma_j = \tau((p_j^k)^2 + (q_j^k)^2) + \beta((\phi_j^k)^2 + (\psi_j^k)^2) \) = \( \tau(|\alpha_j|^2) + \beta(|\beta_j|^2) \).

It is clear that the solver is explicit and exact because of the point-wise conservation law (5). By direct calculation, the numerical solver preserves the symplectic structures

\[
\begin{align*}
dp_j^{k+1} \wedge dq_j^{k+1} &= dp_j^k \wedge dq_j^k, \\
d\phi_j^{k+1} \wedge d\psi_j^{k+1} &= d\phi_j^k \wedge d\psi_j^k, \quad j = 0, 1, \ldots, J.
\end{align*}
\]

(30)

Consequently, solver (29) is symplectic for the nonlinear subproblem (17).

3.3. HOC–SMS scheme for the CNLS equations

We combine the linear discretization (28) with the nonlinear approximate (29) and implement the standard Strang splitting technique [36] on CNLS equations. The numerical algorithm is completed from \( t_k \) to \( t_{k+1} \) as follows:

**Step 1:**

\[
\begin{align*}
\begin{bmatrix}
p_j^k \\
q_j^k \\
\phi_j^k \\
\psi_j^k
\end{bmatrix}
&= 
\begin{bmatrix}
\cos \theta_j & - \sin \theta_j \\
\sin \theta_j & \cos \theta_j \\
\cos \sigma_j & - \sin \sigma_j \\
\sin \sigma_j & \cos \sigma_j
\end{bmatrix}
\begin{bmatrix}
p_j^{k} \\
q_j^{k} \\
\phi_j^{k} \\
\psi_j^{k}
\end{bmatrix}, \quad j = 0, 1, \ldots, J.
\end{align*}
\]

(31)

**Step 2:**

\[
\begin{align*}
\begin{bmatrix}
p_j^{**} \\
q_j^{**} \\
\phi_j^{**} \\
\psi_j^{**}
\end{bmatrix}
&= 
\begin{bmatrix}
I - \frac{\alpha \tau}{2} D & \frac{\tau}{4} D^2 & - \frac{\alpha \tau}{2} D & - \frac{\tau}{4} D^2 \\
- \frac{\tau}{4} D^2 & I + \frac{\alpha \tau}{2} D & \frac{\tau}{4} D^2 & \frac{\alpha \tau}{2} D \\
\frac{\alpha \tau}{2} D & - \frac{\tau}{4} D^2 & I - \frac{\alpha \tau}{2} D & \frac{\tau}{4} D^2 \\
- \frac{\tau}{4} D^2 & - \frac{\alpha \tau}{2} D & \frac{\tau}{4} D^2 & I + \frac{\alpha \tau}{2} D
\end{bmatrix}
\begin{bmatrix}
p_j^k \\
q_j^k \\
\phi_j^k \\
\psi_j^k
\end{bmatrix}, \quad j = 0, 1, \ldots, J.
\end{align*}
\]

(32)

**Step 3:**

\[
\begin{align*}
\begin{bmatrix}
p_j^{k+1} \\
q_j^{k+1} \\
\phi_j^{k+1} \\
\psi_j^{k+1}
\end{bmatrix}
&= 
\begin{bmatrix}
\cos \theta_j & - \sin \theta_j \\
\sin \theta_j & \cos \theta_j \\
\cos \sigma_j & - \sin \sigma_j \\
\sin \sigma_j & \cos \sigma_j
\end{bmatrix}
\begin{bmatrix}
p_j^{**} \\
q_j^{**} \\
\phi_j^{**} \\
\psi_j^{**}
\end{bmatrix}, \quad j = 0, 1, \ldots, J.
\end{align*}
\]

(33)

The numerical method is of second order in time and of sixth order in space.

4. Theoretical analysis

4.1. Stability analysis

In current subsection, we analyze the stability of the numerical integrators (31)-(33). As is stated previously, the discretization of Eq. (1) is split into two parts. Since the numerical solver (29) is exact for the nonlinear subproblem (20), the global stability is bound up with that of the linear subproblem.
For the linear subproblem Eq. (26), by noting \( u = p + iq \) and \( v = \phi + i\psi \), we can formulate Eq. (27) into the matrix form
\[
\begin{align*}
(I + \alpha \tau D - i \frac{\tau}{4} D^2) u^* &= (I - \alpha \tau D + i \frac{\tau}{4} D^2) v^*, \\
(I - \alpha \tau D - i \frac{\tau}{4} D^2) v^* &= (I + \alpha \tau D + i \frac{\tau}{4} D^2) u^*,
\end{align*}
\]
which is equal to
\[
\begin{align*}
&\begin{cases}
\begin{aligned}
I + \alpha \tau D - i \frac{\tau}{4} D^2 &
\quad \text{for } u = p + iq, \\
I - \alpha \tau D - i \frac{\tau}{4} D^2 &
\quad \text{for } v = \phi + i\psi,
\end{aligned}
\end{cases}
\end{align*}
\]

Let \( \lambda_j(D) \) be the jth eigenvalue of the matrix \( D \). Then, reminding the skew-symmetry of \( D \) and the symmetry of \( D^2 \), we deduce that \( \lambda_j(D) \) is purely imaginary or zero, nevertheless, \( \lambda_j(D^2) \) is real. The eigenvalues of the amplification matrices are
\[
\begin{align*}
\lambda_j(H_u) &= \frac{1 - \alpha \frac{\tau}{2} \lambda_j(D) + i \frac{\tau}{2} \lambda_j(D^2)}{1 + \alpha \frac{\tau}{2} \lambda_j(D) - i \frac{\tau}{2} \lambda_j(D^2)}, \\
\lambda_j(H_v) &= \frac{1 + \alpha \frac{\tau}{2} \lambda_j(D) + i \frac{\tau}{2} \lambda_j(D^2)}{1 - \alpha \frac{\tau}{2} \lambda_j(D) - i \frac{\tau}{2} \lambda_j(D^2)}.
\end{align*}
\]

Furthermore, it is derived that the spectral radii of \( H_u \) and \( H_v \) are
\[
\rho(H_u) = \max_j |\lambda_j(H_u)| = 1, \quad \rho(H_v) = \max_j |\lambda_j(H_v)| = 1.
\]

**Theorem 1.** The HOC–SMS method for the CNLS Eq. (1) is unconditionally stable. Furthermore, it is non-dissipative.

**4.2. Discrete conservation laws**

In this part, we discuss the conservation laws of the numerical integrator, including the discrete multisymplectic, charge, energy and momentum conservation laws.

Firstly, it can be analyzed that (31) and (33) are exact time \( \tau \) flow maps which satisfy the relation
\[
\omega_j^k = \omega_j^{k+1} = \omega_j^*, \quad j = 0, 1, \ldots, J,
\]
where \( \omega_j^k = \frac{1}{\tau} \text{d}z^k \wedge M \text{d}z^k \). That is, the map \( \varphi : (p^k, q^k) \rightarrow (p^*, q^*) \) is symplectic at any spatial point.

Next, we rewrite Eq. (25) as the discrete multisymplectic Hamiltonian form
\[
\begin{align*}
M(z_{j+1}^* - z_j^*) / \tau + K(Dz_j + 1^2) &= \nabla_z S_{12} \left( z_j^{*+\frac{1}{2}} \right),
\end{align*}
\]
where \( M, K \) are the same as previously stated, and \( z_j^{*+\frac{1}{2}} = \frac{1}{2} (z_j^{*+} + z_j^{*}) \). The variational equation for Eq. (38) reads
\[
M(dz_j^{*+} - dz_j^*) / \tau + K(Dd z_j + 1^2) = S_{122} \left( z_j^{*+\frac{1}{2}} \right) dz_j^{*+\frac{1}{2}}.
\]

Taking the wedge product with \( dz_j^{*+\frac{1}{2}} \), we can obtain
\[
S_{122} \left( z_j^{*+\frac{1}{2}} \right) dz_j^{*+\frac{1}{2}} \wedge dz_j^{*+\frac{1}{2}} = 0.
\]

It engenders
\[
\frac{\omega_j^{*+\frac{1}{2}} - \omega_j^*}{\tau} + \frac{1}{2} [D(\kappa^{*+} + \kappa^*)] |_{j} = 0.
\]

Consequently, one obtains the following theorem:

**Theorem 2.** The Strang splitting HOC–SMS integrator (31)–(33) for the CNLS Eq. (1) meets the discrete approximation to the multisymplectic conservation law (9)
\[
\frac{\omega_j^{*+\frac{1}{2}} - \omega_j^*}{\tau} + \frac{1}{2} [D(\kappa^{*+} + \kappa^*)] |_{j} = 0.
\]

**Furthermore, it is totally symplectic. In other words**
\[
\sum_j \omega_j^{k+1} = \sum_j \omega_j^k = \cdots = \sum_j \omega_j^0.
\]
Next, we are interested in the discrete charge conservation law for the CNLS Eq. (1). It is obviously revealed that the solver for the nonlinear subproblem is exact. For (31) and (33), we have

\[
\begin{align*}
\|u^k\|_2 = |u|^k, & \quad \|v^k\|_2 = |v|^k, \\
\|u^{k+1}\|_2 = |u|^{k+1}, & \quad \|v^{k+1}\|_2 = |v|^{k+1},
\end{align*}
\tag{41}
\]

where \(\|u\|_2 = \left(\sum_j |u^j|^2\right)^{1/2}\). Then, for the linear subproblem, one has

\[
\begin{align*}
\|u^{**}\|_2 & \leq \|H_u\|_2 \|u^*\|_2, & \quad \|v^{**}\|_2 & \leq \|H_v\|_2 \|v^*\|_2,
\end{align*}
\tag{42}
\]

where \(\|H_u\|_2 = \sqrt{\rho(H^2_u H_u)}\) and \(\|H_v\|_2 = \sqrt{\rho(H^2_v H_v)}\).

We can analyze that \(\|H_u\|_2 = 1\) and \(\|H_v\|_2 = 1\) because of the conclusion (36). Thus,

\[
\begin{align*}
\|u^{**}\|_2 & \leq \|u\|_2, & \quad \|v^{**}\|_2 & \leq \|v\|_2.
\end{align*}
\]

Similarly, we have

\[
\begin{align*}
\|u^*\|_2 & \leq \|u^{**}\|_2, & \quad \|v^*\|_2 & \leq \|v^{**}\|_2.
\end{align*}
\]

In summary, the following is true

\[
\begin{align*}
\|u^{**}\|_2 = \|u^*\|_2, & \quad \|v^{**}\|_2 = \|v^*\|_2.
\end{align*}
\tag{43}
\]

Then, associating Eq. (41) with Eq. (43), it is accessible to

\[
\begin{align*}
\|u^{k+1}\|_2 = \|u^k\|_2, & \quad \|v^{k+1}\|_2 = \|v^k\|_2.
\end{align*}
\tag{44}
\]

Therefore, it results in the following theorem:

**Theorem 3.** The Strang splitting HOC–SMS integrator (31)–(33) for the CNLS Eq. (1) grants the discrete charge conservation law

\[
\|u^{k+1}\|_2 + \|v^{k+1}\|_2 = \|u^k\|_2 + \|v^k\|_2.
\tag{45}
\]

**Theorem 3** on the discrete charge conservation law is robust under any cases. But things are different from the discrete energy and momentum invariants, and they are sensitive except for certain conditions.

**Theorem 4.** *If the solution functions* \(u\) and \(v\) *for the CNLS Eq. (1) are separable, i.e.*

\[
\begin{align*}
u(x, t) = X_u(x)T_u(t), & \quad \psi(x, t) = X_v(x)T_v(t),
\end{align*}
\]

*then, for the Strang splitting HOC–SMS (31)–(33), we gain the discrete conservation laws*

\[
\begin{align*}
\varepsilon^{n+1} = \varepsilon^n = \cdots = \varepsilon^0, & \quad \mathcal{M}^{n+1} = \mathcal{M}^n = \cdots = \mathcal{M}^0,
\end{align*}
\]

*which are corresponding to the energy conservation law and momentum conservation law, respectively. Here*

\[
\begin{align*}
\varepsilon^n = h \sum_j [2|u|^{n+1} - |u|^n] + |v|^n - |v|^{n+1} - |(D u)^n| - |v^{n+1}|^2 - 2|v^n|^2 |v^{n+1}|^2,
\end{align*}
\]

\[
\mathcal{M}^n = h \sum_j [u_j^n (D u_j^n) + v_j^n (D v_j^n)].
\]

*For simplicity, we only demonstrate the proof of the discrete momentum conservation law in detail.*

**Proof.** According to the assumption and (44), one has

\[
\begin{align*}
|T_u^{n+1}|^2 = |T_u^n|^2, & \quad |T_v^{n+1}|^2 = |T_v^n|^2.
\end{align*}
\]

*Then, we have the derivation*

\[
\begin{align*}
h \sum_j (u_j^{n+1} (D u_j^n) + v_j^{n+1} (D v_j^n)) = h |T_u^{n+1}|^2 \sum_j (X_u)_j (D X_u)_j + h |T_v^{n+1}|^2 \sum_j (X_v)_j (D X_v)_j
\end{align*}
\]

\[
\begin{align*}
= h |T_u^n|^2 \sum_j (X_u)_j (D X_u)_j + h |T_v^n|^2 \sum_j (X_v)_j (D X_v)_j
\end{align*}
\]

\[
\begin{align*}
= h \sum_j (u_j^n (D u_j^n) + v_j^n (D v_j^n)).
\end{align*}
\]

*On the analogy of the above method, we have the similar proof for the discrete energy conservation law likewise. The proof is completed. \(\square\)
Table 1
Temporal convergent rate of \( u \) and \( v \) with \( h = \frac{\pi}{50} \).

<table>
<thead>
<tr>
<th>( \tau )</th>
<th>( 1/20 )</th>
<th>( 1/40 )</th>
<th>( 1/80 )</th>
<th>( 1/160 )</th>
<th>( 1/320 )</th>
<th>( 1/640 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( |e_u|_\infty )</td>
<td>7.0254e−4</td>
<td>1.7575e−4</td>
<td>4.3947e−5</td>
<td>1.0990e−5</td>
<td>2.7503e−6</td>
<td>6.9040e−7</td>
</tr>
<tr>
<td>Order</td>
<td>-</td>
<td>1.9999</td>
<td>1.9999</td>
<td>1.9996</td>
<td>1.9985</td>
<td>1.9841</td>
</tr>
<tr>
<td>( |e_u|_2 )</td>
<td>5.0000e−3</td>
<td>1.2000e−3</td>
<td>3.1075e−4</td>
<td>7.7711e−5</td>
<td>1.9448e−5</td>
<td>4.8819e−6</td>
</tr>
<tr>
<td>Order</td>
<td>-</td>
<td>2.0589</td>
<td>1.9492</td>
<td>1.9996</td>
<td>1.9985</td>
<td>1.9941</td>
</tr>
<tr>
<td>( |e_u|_\infty )</td>
<td>2.6039e−5</td>
<td>6.5103e−6</td>
<td>1.6276e−6</td>
<td>4.0690e−7</td>
<td>1.0173e−7</td>
<td>2.5431e−8</td>
</tr>
<tr>
<td>Order</td>
<td>-</td>
<td>1.9999</td>
<td>2.0000</td>
<td>2.0000</td>
<td>1.9999</td>
<td>2.0001</td>
</tr>
<tr>
<td>( |e_u|_2 )</td>
<td>1.8413e−4</td>
<td>4.6035e−5</td>
<td>1.1509e−5</td>
<td>2.8772e−6</td>
<td>7.1931e−7</td>
<td>1.7982e−7</td>
</tr>
<tr>
<td>Order</td>
<td>-</td>
<td>1.9999</td>
<td>2.0000</td>
<td>2.0000</td>
<td>2.0000</td>
<td>2.0001</td>
</tr>
</tbody>
</table>

5. Numerical examples

In this section, we conduct some typical numerical experiments for the HOC–SMS integrators (31)–(33) to verify the theoretical conclusions, including the accuracy, conservation laws, efficiency and various physical phenomena described by CNLS equations.

5.1. Example 1: accuracy test

The objective of the present example is to numerically observe the following two aspects for the HOC–SMS integrators (31)–(33): (i) It is of second order convergence rate in time and sixth order in space; (ii) It is more efficient than Fourier spectral method. We investigate Eq. (1) with the periodic initial values

\[
\begin{align*}
    u(x, 0) &= \exp(\ii x), & v(x, 0) &= \exp(\ii x), & x \in [0, 2\pi].
\end{align*}
\]

The parameters are fixed by \( \alpha = 1, \beta = 1 \) and \( T = 1 \). The exact solution is in the separable form

\[
\begin{align*}
    u(x, t) &= \exp[\ii(x + t/2)], & v(x, t) &= \exp[\ii(x + 5t/2)].
\end{align*}
\]

(46)

To this end, we design a series of numerical experiments performed by the HOC–SMS integrator (31)–(33). Firstly, we exhibit in Table 1 the \( L_{\infty}, L_2 \) numerical errors of \( u \) and \( v \), and the convergent rate order in time with the fixed spatial step length \( h = \frac{\pi}{50} \). The table suggests that the numerical solution perfectly converges to the exact solution with second order in time.

Then, we perform some numerical experiments with various spatial steps and fixed temporal size \( \tau = 0.0001 \), to test whether the HOC–SMS integrators (31)–(33) are of sixth order in space. The numerical results are presented in Table 2. As is expected, the convergent rate is consistent with our academic analysis of \( O(h^6) \).

We have stated that the HOC strategy is much more economical in occupying computer resource than the spectral method in that its stencil is much smaller than that of the latter. We compare the CPU time consumed by the HOC–SMS scheme with which occupies by the SMS spectral method in [1] for the above problem. To this end, we fixed the time step \( \tau = 1/100 \), and \( N \) denotes the mesh grid number of the spatial interval. The error of the numerical solution with respect to the exact solution is very close, which is showed in the left hand of Fig. 1, while, the consumed CPU time by them is charted in the right hand of Fig. 1. It implies that the spectral method is much more accurate than the HOC method when the mesh numbers are small. However, the advantage is annihilated if the mesh number is larger than a certain extent, and the increment of CPU time consumed by the latter is much less than the former. Therefore, the new proposed HOC–SMS integrator is very efficient with spectral-like resolution.
5.2. Example 2: single soliton

We apply the HOC–SMS integrator (31)–(33) to simulate a single soliton problem with the homogeneous boundary conditions over $[-10, 60]$. The initial values are given by

$$
\begin{align*}
    u_0(x) &= \sum_{j=1}^{2} \frac{2a_i}{1 + \beta} \text{sech}[\sqrt{2a_i}(x - x_i)] \exp[i(c_i - \alpha)(x - x_i)], \\
    v_0(x) &= \sum_{j=1}^{2} \frac{2a_i}{1 + \beta} \text{sech}[\sqrt{2a_i}(x - x_i)] \exp[i(c_i + \alpha)(x - x_i)],
\end{align*}
$$

with the parameters $\alpha = 0.2$, $\beta = 2/3$, $x_0 = 0$, $a_1 = 1$ and $c_1 = 1$. The profiles of $|u|$ and $|v|$ are illustrated in Fig. 2 with the mesh step size $h = 0.14$ and $\tau = 0.1$. From the figure, we can view a good approximation to the original soliton.

Now, we turn to verify the discrete conservation laws in Theorems 3 and 4 by testing the numerical errors of charge, energy and momentum. The hypothesis of the theorems hints that the discrete energy and momentum invariants are sensitive to the function type of the solution, while the charge not. From the exact solution (46) and the initial data (47), one can extrapolate that the wave function of Example 1 is separable which meets the requirement of Theorem 4, while Example 2 is not eligible. We examine the conservation laws of the HOC–SMS integrators (31)–(33) via Example 1 and Example 2. We simulate both of the examples with the mesh division $\tau = 0.01$ and $h = 2\pi/50$ for Example 1, $h = 0.14$ for Example 2. The numerical results are shown in Fig. 3. One can obtain the desired conclusion from the graphs. Moreover, we can find that the energy is more sensitive to the function type of the solution than the momentum.

5.3. Example 3: double solitons

We consider the collision of two solitons. The initial data are chosen as

$$
\begin{align*}
    u_0(x) &= \sum_{j=1}^{2} \frac{2a_i}{1 + \beta} \text{sech}[\sqrt{2a_i}(x - x_i)] \exp[i(c_i - \alpha)(x - x_i)], \\
    v_0(x) &= \sum_{j=1}^{2} \frac{2a_i}{1 + \beta} \text{sech}[\sqrt{2a_i}(x - x_i)] \exp[i(c_i + \alpha)(x - x_i)],
\end{align*}
$$

where $\alpha = 0.5$, $\beta = 2/3$, $x_1 = 0$, $x_2 = 25$, $a_1 = 1$, $a_2 = 0.5$, $c_1 = 1$ and $c_2 = 0.1$. The numerical experiment is conducted under the mesh step $h = 0.2$ and $\tau = 0.01$. Fig. 4 shows the wave shape of $|u|$ and $|v|$ at different times. From the graphs,
one can discover that the solitons advance in their own speeds and their wave shapes remain unchanged after collision. Fig. 5 shows the evolution of $Q(t)$ and $M(t)$ against time $t$. The figure suggests that the charge keeps the same exception for the roundoff error and the residual of momentum is relatively small.

5.4. Example 4: collision of triple solitons

In this example, we simulate the collision behavior among three solitons described by the CNLS equations (1). The initial values are taken as

$$u_0(x) = \sum_{j=1}^{3} \sqrt{\frac{2a_j}{1 + \beta}} \text{sech}[\sqrt{2a_j}(x - x_j)] \exp[i(c_j - \alpha)(x - x_j)],$$

$$v_0(x) = \sum_{j=1}^{3} \sqrt{\frac{2a_j}{1 + \beta}} \text{sech}[\sqrt{2a_j}(x - x_j)] \exp[i(c_j + \omega)(x - x_j)],$$

where $\alpha = 0.5$, $\beta = 2/3$, $T = 1$, $x_1 = 0$, $x_2 = 25$, $x_3 = 50$, $a_1 = 1$, $a_2 = 0.72$, $a_3 = 0.36$, $c_1 = 1$, $c_2 = 0.1$ and $c_3 = -1$. The problem is numerically computed by the HOC–SMS integrators (31)–(33) with the mesh step $h = 0.14$ and $\tau = 0.1$. 

![Fig. 3. Numerical residuals of invariants.](image-url)
The absolute values of the wave functions $u$ and $v$ at different moments are displayed in Fig. 6. Fig. 7 exhibits the evolution of the residuals of charge and momentum against time $t$. The similar numerical behavior to the double solitons is taken on.

6. Conclusion and remark

In this paper, we investigate the splitting multisymplectic integrator for the CNLS equations. Most multisymplectic approximations for Hamiltonian system in space are either inaccurate or time-consuming. To bridge over the difficulties,
we import the high-order compact thought into the multisymplectic framework which is new to our knowledge. In order to avoid solving nonlinear algebraic equations, we introduce the splitting idea into the multisymplectic context. The proposed HOC–SMS integrator is very efficient and accurate which can be inferred in theory and in experiments. Certainly, the splitting and high-order compact thoughts can be extended to other multisymplectic Hamiltonian systems, such as Dirac system, Klein–Gordon system. In addition, they can be generalized to multidimensional system. These are our future works.
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