Symplectic structure-preserving integrators for the two-dimensional Gross–Pitaevskii equation for BEC

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\begin{abstract}
Symplectic integrators have been developed for solving the two-dimensional Gross–Pitaevskii equation. The equation is transformed into a Hamiltonian form with symplectic structure. Then, symplectic integrators, including the midpoint rule, and a splitting symplectic scheme are developed for treating this equation. It is shown that the proposed codes fulfill the discrete charge conservation law. Furthermore, the global error of the numerical solution is theoretically estimated. The theoretical analysis is supported by some numerical simulations.
\end{abstract}

\section{Introduction}

Symplectic integrators have been attracting a lot of attention over the last three decades \cite{1–4}. A lot of methods for designing symplectic integrators have appeared, including the generating function method, the (partitioned) Runge–Kutta method, etc. However, most of the symplectic integrators constructed by these methods are implicit, such as the midpoint rule adopted in the article. It will be necessary to find the solutions for nonlinear algebraic equations if the Hamiltonian system is infinite dimensional \cite{5,6,1,7}. This involves massive computational labor, especially for multi-dimensional problems. To increase the efficiency, the splitting method which splits the original vector field into several simpler ones is combined with a symplectic integrator \cite{8–11}. One can often pick out explicit or semi-explicit symplectic integrators \cite{8,11}.

Nonlinear Schrödinger (NLS) equations concentrate on a variety of mathematical and physical areas. One of the most important classes of NLS equations with a trapped potential, namely the Gross–Pitaevskii (G–P) equations, have attracted a lot of attention recently. The equation which describes the dynamics of a Bose–Einstein condensate at extremely low temperature \cite{12} reads

\[
i\psi_t(x, t) = -\frac{1}{2} \Delta \psi + V_d(x) \psi + \beta_d |\psi|^2 \psi, \quad x \in \mathbb{R}^d, \ t \geq 0,
\] (1.1)

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where $\beta_d$ is a real constant, and the trapped potential $V_d(x)$ usually takes the form

$$V_d(x) = \begin{cases} x^2/2, & d = 1, \\ (x^2 + y^2)/2, & d = 2, \\ (x^2 + y^2 + z^2)/2, & d = 3. \end{cases} \tag{1.2}$$

To make the problem (1.1) well-posed, the following initial and boundary conditions are prescribed:

$$\psi(x, 0) = \psi^0(x), \quad x \in \mathbb{R}^d, \tag{1.3}$$

$$\lim_{|x| \to \infty} \psi(x, t) = 0, \quad t > 0. \tag{1.4}$$

By direct calculation and the Green formula, the initial–boundary value problem (1.1)--(1.4) exactly conserves two invariants:

- The charge is invariant:

$$Q(t) = \int_{\mathbb{R}^d} |\psi(x, t)|^2 \, dx = \int_{\mathbb{R}^d} |\psi(x, 0)|^2 \, dx = Q(0). \tag{1.5}$$

- The energy is independent of the time $t$:

$$E(t) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} \nabla \psi(x, t)^2 + V_d(x) |\psi|^2 + \frac{\beta_d}{2} |\psi|^4 \right] \, dx = E(0). \tag{1.6}$$

The one-dimensional (1D) G–P equation has been studied extensively [13,7,14,15]. Recently, some numerical contributions have aimed to solve multi-dimensional problems of such kinds [16–21], including using the splitting method and symplectic and multisymplectic integrators. However, these methods either conditionally stable or do not preserve symplectic structure. In this article, we investigate symplectic integrators for the 2D G–P equation

$$\begin{cases} i\psi_t = -\frac{1}{2} \Delta \psi + V(x, y) \psi + \beta_2 |\psi|^2 \psi, & (x, y) \in \Omega, \ t > 0, \\
\psi(x, y, 0) = \psi^0(x, y), \\
\psi(x, y, t) = \psi(x + b - a, y, t) = \psi(x, y + d - c, t), \end{cases} \tag{1.7}$$

where $\Omega = [a, b] \times [c, d]$. The midpoint symplectic scheme is developed first. However, it is completely implicit. On the basis of the scheme, we shall propose splitting symplectic integrators for treating this equation which are free of coupled nonlinear algebraic systems and unconditionally stable.

To the purpose, we project the 2D G–P equation (1.7) upon the symplectic framework. Set $\psi = p + iq$, we can put (1.7) into a pair of real-valued equations:

$$\begin{cases} p_t + \frac{1}{2}(q_{xx} + q_{yy}) - V(x, y) q - \beta_2 (p^2 + q^2) q = 0, \\
q_t - \frac{1}{2}(p_{xx} + p_{yy}) + V(x, y) p + \beta_2 (p^2 + q^2) p = 0. \end{cases} \tag{1.8}$$

Let $z = [p, q]^T$; then we get the Hamiltonian formulation of Eq. (1.7):

$$\frac{d}{dt} z = J^{-1} \frac{\delta H(z)}{\delta z}, \tag{1.9}$$

where $J^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$. The Hamiltonian function is

$$H(p, q) = \frac{1}{2} \int_{\Omega} \left[ \frac{1}{2} (\nabla p)^2 + (\nabla q)^2 \right] + V(p^2 + q^2) + \frac{1}{2} \beta_2 (p^2 + q^2)^2 \right] \, d\Omega, \tag{1.10}$$

where $(\nabla p)^2 = (p_x)^2 + (p_y)^2$, $(\nabla q)^2 = (q_x)^2 + (q_y)^2$. The infinite-dimensional Hamiltonian system (1.9) is symplectic structure preserving:

$$\frac{d}{dt} \omega = \frac{d}{dt} \int_{\Omega} (dp \wedge dq) d\Omega = 2 \int_{\Omega} (dp \wedge dq) d\Omega = 0.$$

The rest of the paper is outlined as follows. In Section 2, we propose some symplectic integrators for the two-dimensional G–P equations, including the symplectic midpoint rule and the splitting symplectic integrators. The conservative properties and the error estimation are studied in Section 3. In Section 4, we present some numerical results in order to test our theoretical analysis and the physical phenomena that the G–P equations depicted. Finally, we summarize this paper and discuss future work.
2. Symplectic codes for the G–P equation

In this section, we construct symplectic schemes for the 2D G–P equation (1.7). For conciseness of notation, we take the spatial–temporal domain as \( \Omega \times [0, T] \), and divide it by three families of parallel lines:

\[
x_j = a + j\Delta x, \quad y_k = c + k\Delta y, \quad t^n = n\tau,
\]

where \( N, K, M \in \mathbb{N} \) are mesh numbers in the \( x, y, t \) directions, respectively, and \( \Delta x, \Delta y, \tau \) are mesh sizes in the \( x, y, t \) directions, respectively. The approximation of \( \psi(x, y, t) \) at the node \((x_j, y_k, t^n)\) is denoted by \( \psi^n_{jk} \). We present the notation for the inner product and norm:

\[
(U^n, V^n) = \Delta x\Delta y \sum_{j,k} u^n_{jk}v^n_{jk}, \quad ||U^n|| = \sqrt{(U^n, U^n)}.
\]

The basic idea for designing a symplectic scheme for an infinite-dimensional Hamiltonian system is to convert it into a finite-dimensional one via spatial approximation. And the key to success is the discretization to \( \partial^2/\partial x^2 \) and \( \partial^2/\partial y^2 \). For simplicity, here we use the symmetric and central difference quotient operator which is of second-order accuracy:

\[
\Delta_{2x}v_{j,k} = \frac{v_{j-1,k} - 2v_{j,k} + v_{j+1,k}}{\Delta x^2}, \quad \Delta_{2y}v_{j,k} = \frac{v_{j,k-1} - 2v_{j,k} + v_{j,k+1}}{\Delta y^2}.
\]

Certainly, one can use other discrete methods with this goal; see [7] and references therein. These kinds of approximations lead to a system of Hamiltonian ODEs for them and symplectic time integrators like the midpoint rule can be applied [22].

2.1. The midpoint symplectic integrator

We first consider the 2D linear problem with periodic boundary conditions:

\[
\begin{align*}
p_t &= -\frac{1}{2}(q_{xx} + q_{yy}), \\
q_t &= \frac{1}{2}(p_{xx} + p_{yy}).
\end{align*}
\]

The Hamiltonian function is

\[
H^{(1)}(p, q) = \frac{1}{4} \int_\Omega [(\nabla p)^2 + (\nabla q)^2] \, d\Omega.
\]

The difference quotient operator (2.1) of second-order accuracy is adopted for discretizing in the spatial directions; this then leads to the finite-dimensional Hamiltonian system

\[
\begin{align*}
\frac{dp_{jk}}{dt} &= -\frac{1}{2}(\Delta_{2x}q_{j,k} + \Delta_{2y}q_{j,k}), \\
\frac{dq_{jk}}{dt} &= \frac{1}{2}(\Delta_{2x}p_{j,k} + \Delta_{2y}p_{j,k}),
\end{align*}
\]

(2.4)

Here we have taken \( \Delta x = \Delta y = h, a = c \) and \( b = d \).

Set \( P = [p_{11}, \ldots, p_{N1}, p_{12}, \ldots, p_{NN}], Q = [q_{11}, \ldots, q_{N1}, q_{12}, \ldots, q_{NN}]^T \); the semi-discretization system (2.4) can be transformed into

\[
\frac{d}{dt} \begin{bmatrix} P \\ Q \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & -I_{N^2} \\ I_{N^2} & 0 \end{bmatrix} \begin{bmatrix} M & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} P \\ Q \end{bmatrix},
\]

(2.5)

where \( I_{N^2} \) is an \( N^2 \times N^2 \) identity matrix, and

\[
M = D_{xx} \otimes I_N + I_N \otimes D_{yy},
\]

where \( I_N \) is an \( N \times N \) identity matrix and ‘\( \otimes \)’ denotes the tensor product, with

\[
D_{xx} = D_{yy} = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & \cdots & 1 \\ 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & -2 & 1 \\ 1 & \cdots & 1 & -2 \end{bmatrix}.
\]

The Hamiltonian function is

\[
H(P, Q) = \frac{1}{4} [P^T, Q^T] \begin{bmatrix} M & 0 \\ 0 & M \end{bmatrix} [P \\ Q].
\]
Extending the discretization in spatial directions to the nonlinear problem, we obtain the semi-discretization system for Eq. (1.8):

\[
\frac{d}{dt} \begin{bmatrix} p \\ Q \end{bmatrix} = \begin{bmatrix} 0 & -I_N \\ I_N & 0 \end{bmatrix} \begin{bmatrix} M_1 & 0 \\ 0 & M_1 \end{bmatrix} \begin{bmatrix} p \\ Q \end{bmatrix},
\]

where

\[
M_1 = \frac{M}{2} + \begin{bmatrix} D_1 & D_2 & \cdots & D_N \\ D_1 & D_2 & \cdots & D_N \\ \vdots & \vdots & \ddots & \vdots \\ D_1 & D_2 & \cdots & D_N \end{bmatrix}.
\]

Here \( D_k \) (\( k = 1, 2, \ldots, N \)) are \( N \times N \) diagonal matrices with diagonal entries \( (D_k)_{ij} = -2[V_{jk} + \beta_2(p_{jk}^2 + q_{jk}^2)], \quad j, k = 1, 2, \ldots, N, \)

where \( V_{jk} = V(x_j, y_k) \). Under the symmetry of the matrices \( M, D_k \) (\( k = 1, 2, \ldots, N \)), we know that the system (2.6) is Hamiltonian \( \{22\} \) and its Hamiltonian function is

\[
H(P, Q) = \frac{1}{4} [P^T, Q^T] M [P \\ 0] - \frac{1}{2} \sum_{j,k} (V_{jk} (p_{jk}^2 + q_{jk}^2) + \frac{\beta_2}{2} (p_{jk}^2 + q_{jk}^2)^2).
\]

Applying the midpoint rule \( \{6\} \) to the semi-discretized system (2.6), one obtains a symplectic integrator for the 2D G–P equation (1.7):

\[
\frac{p^{n+1} - p^n}{\tau} + \frac{1}{2} MQ^{n+\frac{1}{2}} - VQ^{n+\frac{1}{2}} - \beta_2 [(P^{n+\frac{1}{2}})^2 + (Q^{n+\frac{1}{2}})^2]Q^{n+\frac{1}{2}} = 0,
\]

\[
\frac{Q^{n+1} - Q^n}{\tau} + \frac{1}{2} MP^{n+\frac{1}{2}} - VP^{n+\frac{1}{2}} + \beta_2 [(P^{n+\frac{1}{2}})^2 + (Q^{n+\frac{1}{2}})^2]P^{n+\frac{1}{2}} = 0,
\]

where \( V = [V_{11}, \ldots, V_{N1}, V_{12}, \ldots, V_{N2}, \ldots, V_{NN}]^T, P^n = [p_{11}, \ldots, p_{N1}, p_{12}, \ldots, p_{N2}, \ldots, p_{NN}]^T. \)

Multiplying Eq. (2.7) with \( i \), then subtracting it from Eq. (2.8), results in

\[
\frac{\psi^{n+1} - \psi^n}{\tau} + \frac{1}{2} MP^{n+\frac{1}{2}} - VP^{n+\frac{1}{2}} + \beta_2 [(P^{n+\frac{1}{2}})^2 + (Q^{n+\frac{1}{2}})^2]P^{n+\frac{1}{2}} = 0.
\]

In practical computation, the symplectic integrator (2.9) is adopted instead of (2.7) and (2.8).

It is easy to see that \( M \) is symmetric and negative semi-definite. According to the Green formula, there exists a matrix \( A \) such that

\[
-M = A^T A.
\]

This will be useful in the next section.

2.2. Splitting symplectic integrators

The symplectic integrator (2.9) is completely implicit. It is required to solve an \( N^2 \)-scale nonlinear algebraic equation at every time step. The computational labor is considerable. To reduce the computational cost, we introduce the splitting idea for the symplectic integrators.

The splitting method was originally designed to improve the speed, accuracy and stability of numerical simulation. Now it is very popular because of its flexibility. On the basis of the fact that the composition of symplectic integrators is symplectic \( \{11\} \), the splitting method has become one of the most important methods for constructing symplectic integrators by decomposing the vector field. In other words, the Hamiltonian system

\[
\frac{dz}{dt} = J \nabla_z H(z) = J \nabla_z (H_1(z) + H_2(z) + \cdots + H_m(z)).
\]

can be split into \( m \) subsystems:

\[
\frac{dz}{dt} = J \nabla_{z_j} H_j(z), \quad j = 1, 2, \ldots, m,
\]

provided that the field vector can be split into

\[
H(z) = H_1(z) + H_2(z) + \cdots + H_m(z).
\]
For example, it is easy to see that the Hamiltonian function (1.10) can be split into the sum of (2.3) and

\[ H^{(2)}(p, q) = \frac{1}{2} \int_{\Omega} \left[ V(p^2 + q^2) + \frac{1}{2} \beta_2 (p^2 + q^2)^2 \right] \, d\Omega. \]  

(2.13)

Then, we simulate the sub-Hamiltonian systems with the Hamiltonian functions \( H^{(1)}(p, q) \) and \( H^{(2)}(p, q) \) in a given sequence.

We split the Hamiltonian system (1.8) into a linear Hamiltonian system (2.2) and a nonlinear infinite-dimensional Hamiltonian system:

\[
\begin{align*}
\dot{p}_i &= V(x, y)q + \beta_2 (p^2 + q^2)q, \\
\dot{q}_i &= -V(x, y)p - \beta_2 (p^2 + q^2)p.
\end{align*}
\]

(2.14)

The linear part (2.2) and the nonlinear subsystem (2.14) can be fully discretized as follows:

\[
\begin{align*}
\frac{p^n_{i+1} - p^n_i}{\tau} &= V_{jk} q^n_{j+\frac{1}{2}} - \beta_2 (p^n_{jk} + \frac{1}{2} p^n_{jk}^2 + (q^n_{jk} + \frac{1}{2} q^n_{jk}^2))^2 - (q^n_{jk} + \frac{1}{2} q^n_{jk}^2)^2 = 0, \\
\frac{q^n_{i+1} - q^n_i}{\tau} &= V_{jk} p^n_{j+\frac{1}{2}} + \beta_2 (p^n_{jk} + \frac{1}{2} p^n_{jk}^2 + (q^n_{jk} + \frac{1}{2} q^n_{jk}^2))^2 - (q^n_{jk} + \frac{1}{2} q^n_{jk}^2)^2 = 0,
\end{align*}
\]

i.e.,

\[
\begin{align*}
\frac{\psi^n_{i+1} - \psi^n_i}{\tau} &= \frac{1}{2} M \psi^{n+\frac{1}{2}} = 0, \\
\frac{\psi^n_{j, k+1} - \psi^n_{j, k}}{\tau} &= -V_{jk} \psi^n_{j+\frac{1}{2}, k} - \beta_2 |\psi^n_{j+\frac{1}{2}, k}|^2 \psi^n_{j, k} = 0.
\end{align*}
\]

(2.15)

where \( \psi^{n+\frac{1}{2}} = \frac{1}{2} (\psi^n + \psi^*) \) and \( \psi^{n+\frac{3}{2}} = \frac{1}{2} (\psi^{n+1} + \psi^*) \), etc.

The program effected in this way is of first order in time, by the Baker–Campbell–Hausdorff formula. To improve the accuracy, it can be coded as follows:

\[
\begin{align*}
\frac{\psi^n_{j, k+1} - \psi^n_{j, k}}{\tau} &= -V_{jk} \psi^n_{j+\frac{1}{2}, k} - \beta_2 |\psi^n_{j+\frac{1}{2}, k}|^2 \psi^n_{j, k} = 0, \\
\frac{\psi^n_{i+1} - \psi^n_i}{\tau} &= \frac{1}{2} M \psi^{n+\frac{1}{2}} = 0, \\
\frac{\psi^n_{j, k+1} - \psi^n_{j, k}}{\tau} &= -V_{jk} \psi^n_{j+\frac{1}{2}, k} - \beta_2 |\psi^n_{j+\frac{1}{2}, k}|^2 \psi^n_{j, k} = 0.
\end{align*}
\]

(2.18)

where \( \psi^{n+\frac{1}{2}} = \frac{1}{2} (\psi^n + \psi^*) \), \( \psi^{n+\frac{3}{2}} = \frac{1}{2} (\psi^{n+1} + \psi^*) \). The symplectic integrator (2.18) is just the Strang splitting [23] which is of second order in time. Moreover, the splitting symplectic integrators (2.17) and (2.18) succeed in avoiding coupled nonlinear algebraic systems. In fact, it is just necessary to solve a linear algebraic system from the second equality of (2.17) or (2.18), and some uncoupled nonlinear algebraic systems from the first and third equalities. This will greatly decrease the computational cost, which will be verified in Section 4.

3. Analysis of the symplectic codes

3.1. Conservation properties

As mentioned previously, the initial–boundary value problem (1.1)–(1.4) satisfies two conservation laws. We analyze the discrete analogues of the invariants for the proposed symplectic codes. For the symplectic integrators (2.9), (2.17) and (2.18), we have the following results.

Theorem 1. All the symplectic integrators (2.9), (2.17) and (2.18) satisfy the discrete charge conservation law

\[ Q^{n+1} = h^2 \sum_{j, k} |\psi^{n+1}_{jk}|^2 = h^2 \sum_{j, k} |\psi^0(x_j, y_k)|^2 = Q^0. \]  

(3.1)
Proof. Taking the inner product of Eq. (2.9) with $\psi^{n+\frac{1}{2}}$ leads to
\begin{equation}
\frac{i}{2\tau} (\psi^{n+1} - \psi^n, \psi^{n+1} + \psi^n) + \frac{1}{2} (M\psi^{n+\frac{1}{2}}, \psi^{n+\frac{1}{2}}) - h^2 \sum_{j,k} (V_{jk} + \beta_2 |\psi_{jk}|^2) \psi_{jk}^{n+\frac{1}{2}} \psi_{jk}^{n+\frac{1}{2}} = 0. \tag{3.2}
\end{equation}
According to Eq. (2.10), the second term of (3.2) is real, and it is obvious that the third term is also real; then the first term of (3.2) is equal to
\begin{equation}
\frac{i}{2\tau} (||\psi^{n+1}||^2 - ||\psi^n||^2) + \frac{i}{2\tau} ((\psi^{n+1}, \psi^n) - (\psi^n, \psi^{n+1})). \tag{3.3}
\end{equation}
The second part in Eq. (3.3) is real. In summary, taking the imaginary part of Eq. (3.2) yields
\begin{equation}
-\frac{i}{2\tau} (||\psi^{n+1}||^2 - ||\psi^n||^2) = 0.
\end{equation}
That is to say, the midpoint rule (2.9) conserves the discrete charge $Q^n$. From the previous proof, we derive that
\begin{equation}
Q^{n+1} = ||\psi^{n+1}||^2 = ||\psi^n||^2 = ||\psi^n||^2 = Q^n.
\end{equation}
As a matter of fact, from the first equality of the symplectic integrator (2.18), one has $||\psi^n||^2 = ||\psi^n||^2$, and $||\psi^n||^2 = ||\psi^n||^2$, $||\psi^n||^2 = ||\psi^n||^2$ follow from the second and third equalities, respectively. This means that the splitting integrators (2.17) and (2.18) leave the charge unchanged throughout, too. \square

Theorem 2. The symplectic scheme (2.9) has the following implicit discrete energy conservation rule:
\begin{equation}
\frac{1}{2} (||A\psi^{n+1}||^2 - ||A\psi^n||^2) + h^2 \sum_{j,k} \left( V_{jk} + \beta_2 |\psi_{jk}|^2 \right) \left( ||\psi_{jk}^{n+1}||^2 - ||\psi_{jk}^n||^2 \right) = 0. \tag{3.4}
\end{equation}
In particular, if $\beta_2 = 0$, it admits the explicit energy conservation law
\begin{equation}
\frac{1}{2} (||A\psi^{n+1}||^2 - ||A\psi^n||^2) + h^2 \sum_{j,k} \left( |\psi_{jk}^{n+1}|^2 - |\psi_{jk}^n|^2 \right) = 0. \tag{3.5}
\end{equation}
Proof. Computing the inner product of Eq. (2.9) with $\psi^{n+1} - \psi^n$ yields
\begin{equation}
\frac{i}{\tau} (\psi^{n+1} - \psi^n, \psi^{n+1} - \psi^n) + \frac{1}{4} (M(\psi^{n+1} + \psi^n), \psi^{n+1} - \psi^n) - \frac{h^2}{2} \sum_{j,k} \left( V_{jk} + \beta_2 |\psi_{jk}|^2 \right) \left( ||\psi_{jk}^{n+1}||^2 - ||\psi_{jk}^n||^2 \right) = 0. \tag{3.6}
\end{equation}
The first term in Eq. (3.6) is equal to
\begin{equation}
\frac{i}{\tau} ||\psi^{n+1} - \psi^n||^2,
\end{equation}
which is a purely imaginary number, and the second term in Eq. (3.6) is
\begin{equation}
\frac{1}{4} (M(\psi^{n+1} + \psi^n), \psi^{n+1} - \psi^n) = \frac{1}{4} (-A^T A(\psi^{n+1} + \psi^n), \psi^{n+1} - \psi^n),
\end{equation}
with the real part
\begin{equation}
-\frac{1}{4} (||A\psi^{n+1}||^2 - ||A\psi^n||^2).
\end{equation}
The third term in Eq. (3.6) reads
\begin{equation}
-\frac{h^2}{2} \sum_{j,k} \left( V_{jk} + \beta_2 |\psi_{jk}|^2 \right) \left( ||\psi_{jk}^{n+1}||^2 - ||\psi_{jk}^n||^2 \right) + \psi_{jk}^{n+1 T} \psi_{jk}^n - \psi_{jk}^{n+1} \psi_{jk}^n, \tag{3.7}
\end{equation}
and the real part in Eq. (3.7) is
\begin{equation}
-\frac{h^2}{2} \sum_{j,k} \left( V_{jk} + \beta_2 |\psi_{jk}|^2 \right) \left( ||\psi_{jk}^{n+1}||^2 - ||\psi_{jk}^n||^2 \right).
\end{equation}
One derives the result by taking the real part in Eq. (3.6). The derivation of the explicit conservation law (3.5) is straightforward. This ends the proof. \square
3.2. Error estimation

In this subsection, the goal is to establish the error estimation for the new symplectic codes (2.9), (2.17) and (2.18). To this end and for convenience, we use the following notation: $\psi^n_j$ denotes the exact solution at $(x_j, y_k, t^n)$, and the pointwise error of the scheme is denoted by $e^n_{jk} = \psi^n_j - \psi^n_k$.

From the conservation law (1.5), (1.6) and Theorem 1, it is well-founded to assume that

$$
\|\psi^n\|^2 \leq Q(u^n(x)), \quad \|\psi^n\|^2 \leq Q(u^n(x)), \quad \|e^n\|^2 \leq 4Q(u^n(x)).
$$

(3.8)

By Taylor expansion, it is observed that the truncation error of the midpoint symplectic code (2.9) is

$$
T^n_j = \frac{1}{2} \psi^{n+1} - \psi^n + \frac{1}{2} M \psi^{n+\frac{1}{2}} - \left( V + \beta_2 |\psi^{n+\frac{1}{2}}|^2 \right) \psi^{n+\frac{1}{2}} = O(\tau^2 + h^2).
$$

(3.9)

**Lemma 1** ([24, Gronwall’s inequality]), Suppose that the mesh functions $w^n$ ($n = 0, 1, 2, \ldots, M$) satisfy the relationship

$$
u^n_j - w^{n-1} \leq \mathcal{A} w_n + B \tau w_{n-1} + \mathcal{C}_n,
$$

where $M = \frac{1}{\tau}, T$ is the length of time, $A, B, C_n$ are non-negative constants, and the sequence $w^n$ satisfies

$$
\|w^n\|_\infty \leq \left( u^0 + \tau \sum_{k=1}^{M} C_k \right) e^{\mathcal{A}(A+B)T},
$$

where $\tau$ is sufficiently small, such that $(A + B) \tau \leq \frac{M-1}{2M}$ ($M > 1$).

In the following context, $C$ is a general non-negative constant which means that it may have different values in different situations.

**Theorem 3.** There exists a positive constant $C$ depending only on the initial value $\psi^0(x, y)$, such that the errors of the symplectic schemes (2.9) satisfy

$$
\|e^n\|^2 \leq \left( \|e_0\|^2 + \tau O(\tau^2 + h^2) \right) e^{4CT} = O(\tau^2 + h^2)^2.
$$

(3.10)

where $\tau$ is sufficiently small such that $2CT \leq \frac{M-1}{2M}$.

**Proof.** Substituting (2.9) from (3.9) leads to

$$
T^n_j = \frac{1}{\tau}(e^{n+1} - e^n) + \frac{1}{2} M e^{n+\frac{1}{2}} - V e^{n+\frac{1}{2}} - \beta_2 |\psi^{n+\frac{1}{2}}|^2 e^{n+\frac{1}{2}} - \beta_2 (|\psi^{n+\frac{1}{2}}|^2 - |\psi^{n+\frac{1}{2}}|^2) \psi^{n+\frac{1}{2}}.
$$

(3.11)

Computing the inner product of (3.11) with $e^{n+\frac{1}{2}}$ yields

$$
\langle T^n, e^{n+\frac{1}{2}} \rangle = \frac{1}{2\tau} (e^{n+1} - e^n, e^{n+1} + e^n) + \frac{1}{2} (M e^{n+\frac{1}{2}}, e^{n+\frac{1}{2}}) - (V e^{n+\frac{1}{2}}, e^{n+\frac{1}{2}})
$$

$$
- \beta_2 (|\psi^{n+\frac{1}{2}}|^2 e^{n+\frac{1}{2}}, e^{n+\frac{1}{2}}) - \beta_2 \left( (|\psi^{n+\frac{1}{2}}|^2 - |\psi^{n+\frac{1}{2}}|^2) \psi^{n+\frac{1}{2}}, e^{n+\frac{1}{2}} \right).
$$

(3.12)

According to Eq. (3.8), there exists a constant $C$ such that

$$
\left| \left( \psi^{n+\frac{1}{2}} - \psi^{n+\frac{1}{2}} \right) \psi^{n+\frac{1}{2}} \right| \leq \left| \left( \psi^{n+\frac{1}{2}} \psi^{n+\frac{1}{2}} - \psi^{n+\frac{1}{2}} \psi^{n+\frac{1}{2}} \right) \psi^{n+\frac{1}{2}} \right|
$$

$$
\leq e^{n+\frac{1}{2}} + \psi^{n+\frac{1}{2}} \psi^{n+\frac{1}{2}} \left| \psi^{n+\frac{1}{2}} \right|
$$

$$
\leq 2 \max_j \left| \psi^{n+\frac{1}{2}} \right| \max_j \left| \psi^{n+\frac{1}{2}} \right| \left| e^{n+\frac{1}{2}} \right|
$$

$$
\leq C |e^{n+\frac{1}{2}}|.
$$

Taking the imaginary part of (3.12), we have

$$
\frac{1}{2\tau} (\|e^{n+1}\|^2 - \|e^n\|^2) = \mathcal{A}(T^n_j, e^{n+\frac{1}{2}}) + 3\beta_2 \left( (|\psi^{n+\frac{1}{2}}|^2 - |\psi^{n+\frac{1}{2}}|^2) \psi^{n+\frac{1}{2}}, e^{n+\frac{1}{2}} \right)
$$

$$
\leq \frac{1}{2} (\|T^n_j\|^2 + \|e^{n+\frac{1}{2}}\|^2) + C \|e^{n+\frac{1}{2}}\|^2
$$

$$
\leq O(\tau^2 + h^2)^2 + C (\|e^{n+1}\|^2 + \|e^n\|^2),
$$
4. Numerical simulation

In this section, we present some numerical studies in order to illustrate and test the proposed symplectic integrators, including the errors and the conservative properties. The following notation is offered to present the error between the exact solution and the numerical solution:

\[ e^2_n = h^2 \sum_{j,k} |\psi_{jk}^n - \psi_{jk}^n|^2, \quad e^\infty_n = \max_{j,k} |\psi_{jk}^n - \psi_{jk}^n|. \]

**Example 1.** We first consider the following linear periodic initial–boundary problem:

\[
\begin{align*}
\frac{\partial \psi}{\partial t} &= -\frac{1}{2} (\psi_{xx} + \psi_{yy}), \\
\psi(x, y, t) &= \psi(x, y + 2\pi, t) = \psi(x + 2\pi, y, t), \\
\psi(x, y, 0) &= e^{-i(x+y)}.
\end{align*}
\]

The theoretical solution of the problem is

\[ \psi(x, y, t) = e^{-i(x+y+t)}. \]

To verify the theoretical analysis, we choose different spatial–temporal step sizes to solve the initial–boundary value problem (4.1) by using the symplectic scheme (2.9). The results for \( t = 10 \) are listed in Table 1. Furthermore, Fig. 1 pictures the residuals of the charge and energy with the division of \( \tau = 0.01 \) and \( h = \frac{\pi}{80} \). And the figure shows that the scheme preserves the charge and the energy exactly, corresponding to the conservation laws (3.1) and (3.5).

**Example 2.** In the example, we consider the following nonlinear initial–boundary value problem with a trapped potential:

\[
\begin{align*}
\frac{\partial \psi(x, y, t)}{\partial t} &= -\frac{1}{2} (\psi_{xx} + \psi_{yy}) + (1 - \sin^2 x \sin^2 y) \psi + |\psi|^2 \psi, \\
\psi(x, y, 0) &= \sin x \sin y, \quad (x, y) \in [0, 2\pi] \times [0, 2\pi].
\end{align*}
\]
Fig. 2. Surface plots and contour plots for the numerical solution $\psi(x, y, 100)$: left for the real part; right for the imaginary part.

Fig. 3. The residuals of charge and energy: left for charge; right for energy.

The exact solution of Eq. (4.2) is

$$\psi(x, y, t) = e^{-2it} \sin x \sin y.$$  

We choose $h = \frac{\pi}{32}$ and different time step lengths to compare the efficiencies of the symplectic integrators (2.9), (2.17) and (2.18). The time length is $T = 100$. The problem is nonlinear, and the symplectic integrators are implicit. The fixed point iteration method is utilized to solve the coupled or uncoupled nonlinear algebraic systems generated by them; each iteration will terminate when the maximum absolute error of two adjacent iterative values is less than $10^{-15}$. Fig. 2 shows the surface plots and contour plots of the numerical solution $\psi(x, y, t)$ at $t = 100$ using the second-order splitting symplectic integrator (2.18), and Fig. 3 presents the residuals of the invariants. Table 2 exhibits the numerical errors in 2-norm and $\infty$-norm of $\psi(x, y, t)$, the residual of conservation quantities at $t = 100$, and the required CPU time as well. From the table, it is observed that the splitting symplectic integrators are more efficient than the general symplectic integrators. All of them leave the charge unaltered.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$\tau$</th>
<th>$\varepsilon_\infty$</th>
<th>$\varepsilon_2$</th>
<th>$\varepsilon_0$</th>
<th>$\varepsilon_1$</th>
<th>CPU (s)</th>
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</thead>
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<tr>
<td>(2.9)</td>
<td>0.05</td>
<td>2.48e−4</td>
<td>5.29e−3</td>
<td>1.78e−14</td>
<td>9.40e−4</td>
<td>6640</td>
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<tr>
<td></td>
<td>0.025</td>
<td>7.44e−5</td>
<td>2.77e−3</td>
<td>2.68e−13</td>
<td>2.56e−4</td>
<td>10456</td>
</tr>
<tr>
<td></td>
<td>0.0125</td>
<td>2.64e−5</td>
<td>1.64e−3</td>
<td>6.57e−14</td>
<td>8.69e−5</td>
<td>18987</td>
</tr>
<tr>
<td>(2.17)</td>
<td>0.05</td>
<td>3.29e−3</td>
<td>4.73e−2</td>
<td>9.59e−11</td>
<td>4.81e−2</td>
<td>626</td>
</tr>
<tr>
<td></td>
<td>0.025</td>
<td>1.47e−3</td>
<td>1.85e−2</td>
<td>9.23e−14</td>
<td>1.14e−2</td>
<td>1237</td>
</tr>
<tr>
<td></td>
<td>0.0125</td>
<td>1.34e−4</td>
<td>4.33e−3</td>
<td>2.72e−12</td>
<td>6.18e−3</td>
<td>2103</td>
</tr>
<tr>
<td>(2.18)</td>
<td>0.05</td>
<td>9.82e−5</td>
<td>2.97e−3</td>
<td>8.88e−14</td>
<td>1.33e−4</td>
<td>675</td>
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<tr>
<td></td>
<td>0.025</td>
<td>8.19e−5</td>
<td>4.36e−3</td>
<td>2.73e−12</td>
<td>6.30e−4</td>
<td>1181</td>
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<td>1.07e−14</td>
<td>1.71e−4</td>
<td>2341</td>
</tr>
</tbody>
</table>
Example 3. Lastly, we consider the defocusing condensate on \([-8, 8] \times [-8, 8]\). The parameters present here are \(\beta_2 = 2\) in (1.1) and \(\gamma_y = 1\) in (1.2). The initial value is taken as

\[
\psi(x, y, 0) = \frac{1}{\sqrt{\pi}} \exp\left(-\frac{x^2 + y^2}{2}\right).
\]

We simulate the problem by using the symplectic integrators (2.9), (2.17) and (2.18). The time span investigated is \(T = 200\) and the mesh step size is \(h = \frac{16}{20}, r = 0.1\). The surface plot at \(t = 200\) and the contour plots at \(t = 0, 100, 200\) are shown in Fig. 4. Since the plots are similar for all three symplectic integrators, we only present the surface plot obtained by using integrator (2.9) and the contour plots obtained by using (2.18). Fig. 5 pictures the residuals of charge and energy obtained by using the three symplectic integrators (2.9), (2.17) and (2.18). It is observed that all three symplectic integrators retain the charge unaltered throughout and the residual of energy takes on quasi-periodic oscillation. This also suggests that all three symplectic integrators can simulate the BEC problem without an exact solution well over the long term.

5. Conclusion

In this work, we investigate the symplectic integrators for the two-dimensional G–P equations for BEC, including the unconditionally stable midpoint rule, and the first-order and second-order splitting symplectic integrators. The sub-Hamiltonians of the splitting symplectic integrators are approximated by the midpoint rule in time, too. It is suggested that all the proposed symplectic integrators conserve the charge. The residual of the energy takes on quasi-periodic fluctuation in a small range over the long term. To avoid solving a coupled nonlinear algebraic system, we propose two split symplectic integrators. They are more efficient than the midpoint rule and have almost all the advantages of the midpoint rule. We will discuss other split-step symplectic and multisymplectic integrators for the G–P equations in other papers, including three-dimensional ones.

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Fig. 5. The residuals of charge and energy: left for charge; right for energy. (a) Scheme (2.18), (b) scheme (2.17), (c) scheme (2.9).

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References