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Dynamic properties of the cubic nonlinear Schrödinger equation by symplectic method*

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The dynamic properties of a cubic nonlinear Schrödinger equation are investigated numerically by using the symplectic method with different space approximations. The behaviours of the cubic nonlinear Schrödinger equation are discussed with different cubic nonlinear parameters in the harmonically modulated initial condition. We show that the conserved quantities will be preserved for long-time computation but the system will exhibit different dynamic behaviours in space difference approximation for the strong cubic nonlinearity.

Keywords: dynamic property, conserved quantity, symplectic method
PACC: 0200, 8220W

1. Introduction

Recently, symplectic methods have been developed to solve the Hamiltonian system. They are superior to the nonsymplectic ones, especially for long-time computation.[1−4] To date, the symplectic method has been applied to many fields: for example, it can be extended to the time-evolution of a quantum system,[5−8] the evolution of vortices in a rotating Bose–Einstein condensate,[9] molecular dynamics,[10] plasma physics, [11] and so on. It is well known that the nonlinear Schrödinger equation (NSE) has been used to describe physical processes in many fields, such as nonlinear optics, plasma physics and fluid dynamics. Many methods have been proposed to solve the NSE analytically and numerically; for example, Chang *et al*[12] presented a new linearized Crank–Nicolson-type scheme by applying an extrapolation technique to the real coefficient of the nonlinear term. The correspondence between quantum chaos of an N-body system and the dynamic chaos of mean-field approximations was discussed and a system of NSEs describing the boson condensate in the mean-field approximation was numerically solved with a modified Crank–Nicholson scheme.[13] Li and Shen[14] studied the pattern formation in nonlinear dynamic systems. Lu[15] considered the stationary state NSE and obtained the exact solutions of the equation in phase space.

In recent years, attention has been focused on analysing the dynamic behaviours of the NSE, and many interesting phenomena have been revealed. Moon[16] illustrated the correlations between a homoclinic orbit (HMO) and coherent patterns in the NSE, and showed that an irregular HMO crossing can be observed corresponding to the chaotic oscillation if adding a perturbed term in the NSE. He and Zhou[17] illustrated the integrability of the cubic–quintic NSE numerically, and showed that the quintic nonlinear term will lead to a spatiotemporal complexity of wave fields. Tan and Mao[18] studied the mechanism of pattern competition of the cubic–quintic NSE and achieved the pattern selection and pattern competition by applying artificial disturbances in the numerical simulation and showed that the drifting of the solution pattern is a common phenomenon in NSE; the pattern drifting was also observed in the cubic–quintic NSE.[19]

The nonlinear Schrödinger equation can be transformed into a Hamiltonian system, thus the symplectic scheme is the natural and effective way to numeri-

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cally solve the NSE.[20] The multi-symplectic method is also improved to solve the Hamiltonian system[21] and can be used to numerically solve the NSE. For example, Hong and Liu[22] considered a novel conservation law called multi-symplecticity, which is essential and intrinsic, for a class of varying coefficient NSEs and presented a multi-symplectic scheme for the NSE with varying coefficient in a large domain of independent variables. Chen *et al*[23] presented symplectic and multi-symplectic integrators based on the Hamiltonian and multi-symplectic formulations of NSE and demonstrated the local conserved properties with the local energy conservation law. In our previous work,[24] we have discussed the dynamic behaviours of a cubic NSE by using the symplectic scheme with varying cubic nonlinear parameter and observed an interesting phenomenon; we have shown that the system will exhibit the regular recurrence, which is elliptic trajectories, for weakly nonlinearity, and illustrated that the strong nonlinearity will lead to various dynamic behaviours which may be regular HMO crossing, irregular HMO crossing, quasi-recurrence or pseudo-recurrence.

In this paper, we demonstrate the basic dynamic properties of the NSE by using the symplectic method with varying nonlinear parameters in space difference approximation. We illustrate that the low-order space difference approximation may numerically induce irregular phase trajectories with strong cubic nonlinearity, but the high-order space difference approximation may give the correct phase trajectories and thereby correct our previous results.[24]

In Section 2, the symplectic method is extended to the calculations of the cubic NSE. First, the finite dimensional canonical equation of the NSE is obtained by substituting the second-order space difference approximation and fourth-order space difference approximation for second-order partial derivative. Then the canonical equations are computed using the symplectic scheme. In Section 3, the evolutions of the three conserved quantities of the cubic NSE with time (the quasi-particle number, the total momentum and the total energy) are illustrated by using the symplectic method. In Section 4, the basic dynamic properties of the NSE with the varying cubic nonlinear parameter q in space difference approximation are illustrated. Discussions are given in Section 5.

2. Symplectic discretization of the cubic nonlinear Schrödinger equation

The NSE is one of the basic evolution models for nonlinear waves in various branches of physics. It is well known that the cubic NSE reads

$$\mathrm{i}\frac{\partial E}{\partial t}+\frac{\partial^2 E}{\partial x^2}+q|E|^2E=0, \tag{1}$$

which has been used to describe many physical processes. Here $E(x,t)$ is a complex function denoting the wavefunction, and q is the cubic nonlinear parameter.

Let us consider the cubic NSE (1) under the following periodic boundary condition:

$$E(x+L)=E(x), \tag{2}$$

where L is the periodic length. If we divide the complex variable $E(x,t)$ of Eq.(1) into real and imaginary parts

$$E(x,t)=u(x,t)+\mathrm{i}v(x,t), \tag{3}$$

and substitute the second-order symmetry difference quotient for the second-order partial derivative

$$\text{Method I}:\begin{cases}\dfrac{\partial^2 u_j}{\partial x^2}\approx\dfrac{1}{h^2}(u_{j-1}-2u_j+u_{j+1}),\\[2mm] \dfrac{\partial^2 v_j}{\partial x^2}\approx\dfrac{1}{h^2}(v_{j-1}-2v_j+v_{j+1}),\end{cases} \tag{4}$$

the cubic NSE (1) can be discretized into the following finite dimensional Hamiltonian canonical equations:

$$\begin{aligned}\frac{\mathrm{d}z}{\mathrm{d}t}=&J^{-1}\frac{\partial H}{\partial z}\\ =&J^{-1}\left(\frac{\partial H}{\partial u},\frac{\partial H}{\partial v}\right)^{\mathrm{T}}=J^{-1}\nabla H=f(z),\end{aligned} \tag{5}$$

where $h=L/N$ is the space step, N is a sufficiently large positive integer; $z=(u,v)^{\mathrm{T}}$, u and v being two column vectors formed with values of different space nodes. The matrix J is the standard symplectic matrix, which has the form $J=\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}$. The Hamiltonian function of Hamiltonian canonical equations (5) is

$$H(u,v)=\frac{1}{2}\begin{pmatrix}u^{\mathrm{T}} & v^{\mathrm{T}}\end{pmatrix}G\begin{pmatrix}u\\ v\end{pmatrix}+\frac{q}{4}\sum_{i=1}^{N}(u_i^2+v_i^2)^2, \tag{6}$$

where

$$G=\begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}, \quad S=\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 1 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix}.$$

If the second-order partial derivative is discretized by using the following fourth-order space difference approximation:

$$\text{Method II}: \begin{cases} \dfrac{\partial^2 u_j}{\partial x^2} \approx \dfrac{1}{12h^2}(-u_{j-2}+16u_{j-1}-30u_j+16u_{j+1}-u_{j+2}), \\ \dfrac{\partial^2 v_j}{\partial x^2} \approx \dfrac{1}{12h^2}(-v_{j-2}+16v_{j-1}-30v_j+16v_{j+1}-v_{j+2}), \end{cases} \tag{7}$$

the cubic NSE (1) can be also discretized into the finite dimensional Hamiltonian canonical equations, which has the same formalism of Eq.(5), but the matrix S changes to

$$S=\frac{1}{12h^2}\begin{vmatrix} -30 & 16 & -1 & \cdots & 0 & -1 & 16 \\ 16 & -30 & 16 & -1 & \cdots & 0 & -1 \\ -1 & 16 & -30 & 16 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -1 & 16 & -30 & 16 & -1 \\ -1 & 0 & \cdots & -1 & 16 & -30 & 16 \\ 16 & -1 & 0 & \cdots & -1 & 16 & -30 \end{vmatrix}.$$

Thus the symplectic method can be used to solve the cubic NSE (1) numerically. For example, the second-order symplectic scheme based on the generating function is[20,23]

$$z^{k+1}=z^k+\tau J^{-1}(\nabla H)_{\left(\frac{z^{k+1}+z^k}{2}\right)}, \tag{8}$$

which is the well known Euler centred scheme and the fourth-order symplectic scheme is

$$\begin{aligned} z^{n+1}=&z^n+\tau J^{-1}(\nabla H)_{\left(\frac{z^{n+1}+z^n}{2}\right)} \\ &-\frac{\tau^3}{24}J^{-1}\nabla_z((\nabla H)^{\mathrm{T}}JH_{zz}J\nabla H)_{\left(\frac{z^{n+1}+z^n}{2}\right)}. \end{aligned} \tag{9}$$

Another symplectic scheme of the Runge–Kutta type[25]

$$\begin{aligned} z^{n+1}&=z^n+\frac{\tau}{2}(f(Y_1)+f(Y_2)), \\ Y_1&=z^n+\tau\left(\frac{1}{4}f(Y_1)+\left(\frac{1}{4}-\frac{1}{6}\sqrt{3}\right)f(Y_2)\right), \\ Y_2&=z^n+\tau\left(\left(\frac{1}{4}+\frac{1}{6}\sqrt{3}\right)f(Y_1)+\frac{1}{4}f(Y_2)\right), \end{aligned} \tag{10}$$

is also the fourth-order scheme. Here τ is the time step and $\tau>0$, $t_k=k\tau$, $z^k=(u^k,v^k)^{\mathrm{T}}$, $u^k=u(t_k)$, $v^k=v(t_k)$, $k=0,1,2,\ldots$.

Since the symplectic schemes (8)–(10) are the implicit scheme, we make use of iteration method for each time step to compute the solutions.

For convenience, we call the second-order space difference approximation (4) Method I, while we call the fourth-order space difference approximation (7) Method II.

3. The conserved quantities of the nonlinear Schrödinger equation

We know that the cubic NSE (1) has three conserved quantities, i.e. the quasi-particle number

$$I_1=\int |E|^2\mathrm{d}x, \tag{11}$$

the total momentum

$$I_2=\frac{1}{2}\mathrm{i}\int (EE_x^*-E_xE^*)\mathrm{d}x, \tag{12}$$

and the total energy

$$I_3=\int\left(|E_x|^2-\frac{q}{2}|E|^4\right)\mathrm{d}x. \tag{13}$$

In the numerical simulation, we choose the initial condition as

$$E(x,0) = E_0 + \varepsilon e^{i\theta} \cos(K_{\max} x). \qquad (14)$$

This is a harmonically modulated initial wavefunction, where $K_{\max} = 1$ is the unstable wavenumber corresponding to the maximum instability mode and $E_0 = 1$, ε is a small real constant which is chosen to be $\varepsilon = 0.1$. $\varepsilon e^{i\theta}$ indicates the initial amplitude of the modulation. In this paper, we only consider the case that θ is slightly larger than 45° and choose θ=45.18°. For different cubic nonlinear parameters q, we study the conserved quantities and the dynamic properties of the cubic NSE (1) under the periodic boundary condition (2) with the periodic length being taken to be $L = 2\pi/K_{\max}$ and the large positive integer to be $N = 64$.

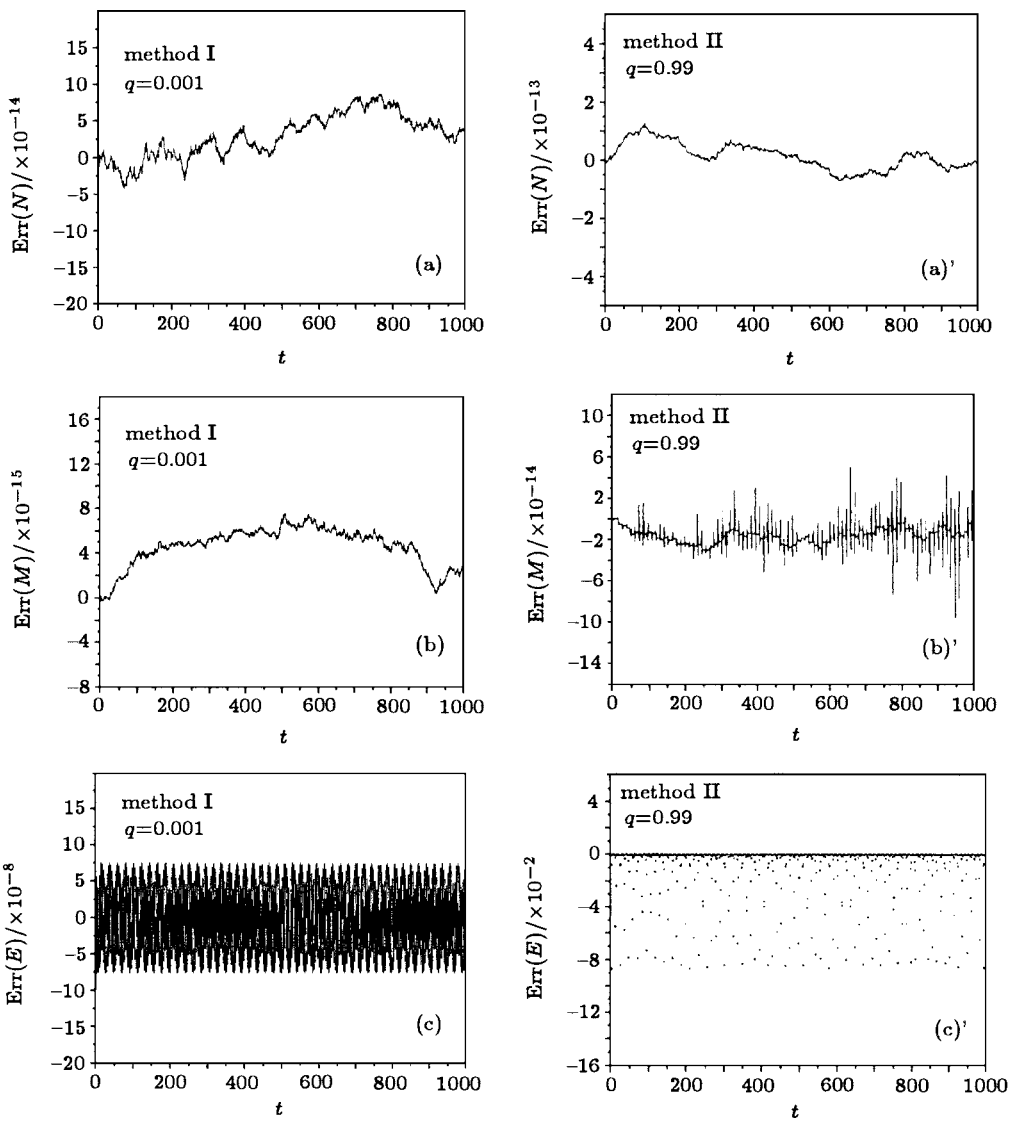


Fig.1. The conserved quantities of the cubic NSE by using the symplectic method with q=0.001 and q=0.99. (a) and (a)' are the evolution of the error of the quasi-particle number [Err(N)]; (b) and (b)' are the evolution of the error of the total momentum [Err(M)]; (c) and (c)' are the evolution of the error of the total energy [Err(E)].

The conserved quantities of the cubic NSE (1) are obtained by using the second-order symplectic scheme (8) with Method I. In the computation, we choose the time step $\tau = 0.001$ and the computational time is from $t = 0$ to $t = 10^6$, and the total computational step number is 10^9. The long-time evolution is almost the same for $t > 10^3$, thus we only discuss the dynamic properties for $0 \le t \le 10^3$. The errors of the conserved

quantities of the cubic NSE (1) obtained by using the symplectic scheme (6) with Method I for q=0.001 and q=0.99 are shown in Fig.1, where Err(N), Err(M) and Err(E) are the errors of the quasi-particle number, the total momentum and the total energy, respectively. Figures 1(a) and (a)' are the evolutions of the error of the quasi-particle number [Err(N)]; it is shown that the quasi-particle number is kept at 10^{-14} and 10^{-13} for q=0.001 and q=0.99, respectively. Figures 1(b) and (b)' are the evolutions of the error of the total momentum [Err(M)]; it is shown that the total momentum is kept at 10^{-15} and 10^{-14} for q=0.001 and q=0.99, respectively. The evolutions of the error of the total energy [Err(E)] for q=0.001 and q=0.99 is shown in Figs.1(c) and (c)', respectively. From Fig.1(c), we can see clearly that the total energy is kept at 10^{-8} and the error of it oscillates periodically about the zero point for q=0.001 for the long-time evolution. When q is increased to 0.99 (Fig.1(c)'), the plot of errors of the total energy indicates that there are some isolated distribution points deviating from the zero point. Figure 2 shows the comparison between the time evolution of the amplitude of fields $A(L/2,t)$ and the evolution of the error of the total energy [Err(E)] for the cubic NSE by using the Method I for q=0.99. It is shown that the isolated distribution points of the total energy is the same as the period of the time evolution of the amplitude of fields $A(L/2,t)$.

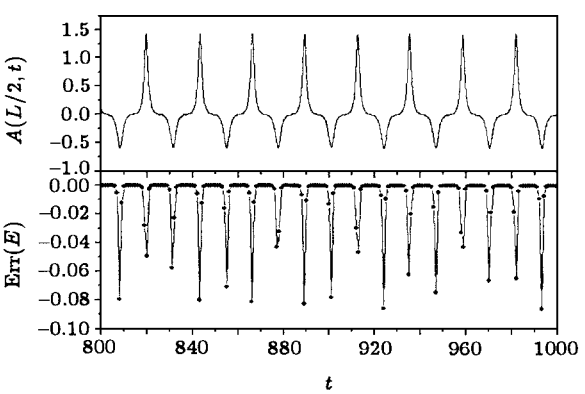


Fig.2. The comparison between the time evolution of the amplitude of fields $A(L/2,t)$ and the evolution of the error of the total energy [Err(E)] for the cubic NSE by using the Method I with q=0.99.

We have also use Method II and symplectic Runge–Kutta scheme (10) to integrate the NSE (1), and the above phenomena about the conserved quantities can also be observed.

4. Numerical experiments

In order to analyse the dynamic properties of the cubic NSE (1) in the long-time evolution, we construct the phase-space diagrams (A, A_t) at $x = L/2$, which are defined as[16]

$$A(L/2,t) = |E(L/2,t)| - 1,$$
$$A_t(L/2,t) = \frac{\mathrm{d}A(L/2,t)}{\mathrm{d}t}. \qquad (15)$$

In Ref.[24], we illustrated that the trajectory in the phase space is the elliptic orbit, and the origin, $(A, A_t) = (0,0)$, could be an elliptic point when we add a weak nonlinearity to it. When the parameter q is increased, the single loop in the phase space will shrink to the origin, $(A, A_t) = (0,0)$, along the $A(L/2,t) = 0$ axis, and become two loops. Meanwhile, the trajectory in the phase space becomes a HMO, and the origin becomes a saddle. This phenomenon occurs in the range of $q > 0.5$. We have also indicated that the system will exhibit irregular motion for large nonlinearity.

The purpose of this paper is to compare the dynamic properties of NSE (1) between Method I and Method II for different nonlinear parameters q. Figures 3 and 4 show the numerical comparison of the cubic NSE (1) obtained by using the second-order symplectic method (8) with Method I and Method II for parameter q=0.6 and 0.9915 respectively, where (a) and (c) are the phase trajectories in the phase space ($A(L/2,t)$, $A_t(L/2,t)$); (b) and (d) are the time evolution of the amplitude of fields $A(L/2,t)$. For weak nonlinear parameters q, the dynamic properties of NSE are exactly the same whether Method I or Method II is used. Figure 3 shows that the long-term behaviour of manifolds in phase space and the time evolution of the amplitude of the field are the same for q=0.6 with different space difference approximations. When q is increased to 0.9915, the trajectories in phase space are regular HMOs, and the time evolution of the amplitude of the fields $|E(x,t)|$ at $x = L/2$ is temporally periodical, as shown in Figs.4(c) and (d) obtained using Method II, while the irregular HMO is observed and the time evolution of the amplitude of the fields is not exactly periodical temporally, as shown in Figs.4(a) and (b) obtained using Method I.

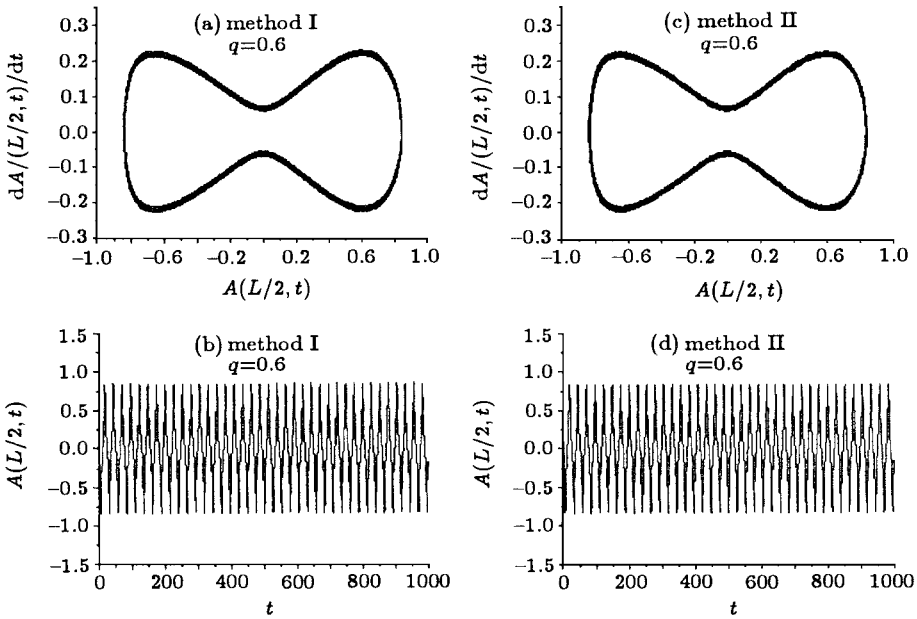


Fig.3. The comparison between Method I and Method II for the cubic NSE with q=0.6: (a) and (c) are the phase trajectories; (b) and (d) are the time evolution of the amplitude of fields $A(L/2,t)$.

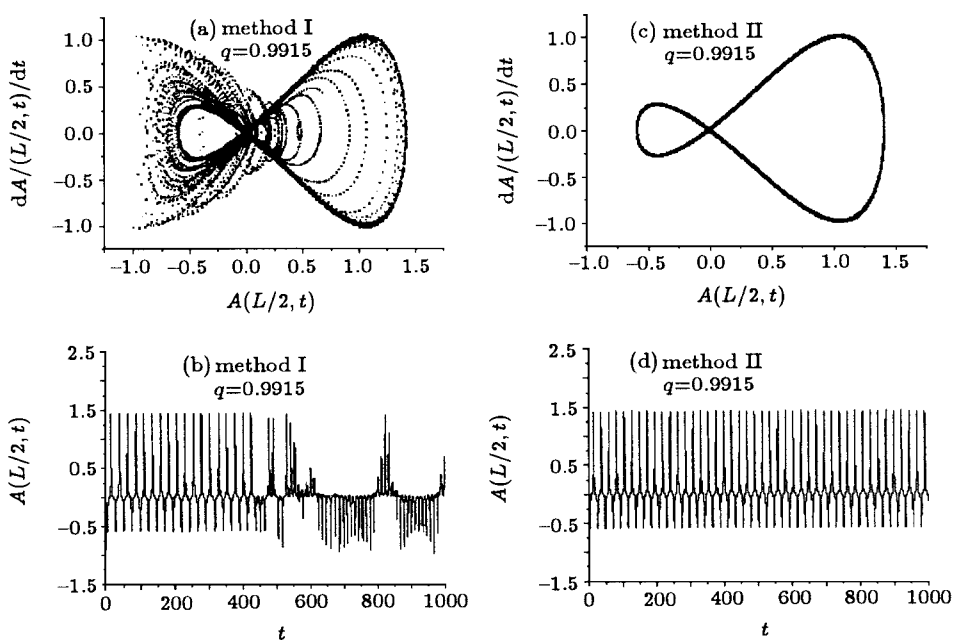


Fig.4. The comparison between Method I and Method II for the cubic NSE with q=0.9915: (a) and (c) are the phase trajectories; (b) and (d) are the time evolution of the amplitude of fields $A(L/2,t)$.

For the cubic nonlinear parameter $q = 1.630$, the phase trajectories in phase space are shown in Fig.5 together with the time evolution of the amplitude of the fields $|E(x,t)|$ at $x = L/2$ in different space difference approximation. The long-term behaviour of the manifolds in phase space becomes a single loop to form a Kolmogorov–Arnold–Moser (KAM) torus which is very thick but is not destroyed using Method II (Fig.5(c)). The time evolution of the amplitude of the fields (Fig.5(d)) indicates that the motion corresponds to the quasi-recurrence. However, the evolution of the trajectories in a long-time scale exhibits irregular motion, as shown in Fig.5(a) using Method I, and the time evolution of the amplitude of the fields (Fig.5(b)) still displays the stochastic motion, where Fig.5(a) is the same as Fig.6(a) of Ref.[24].

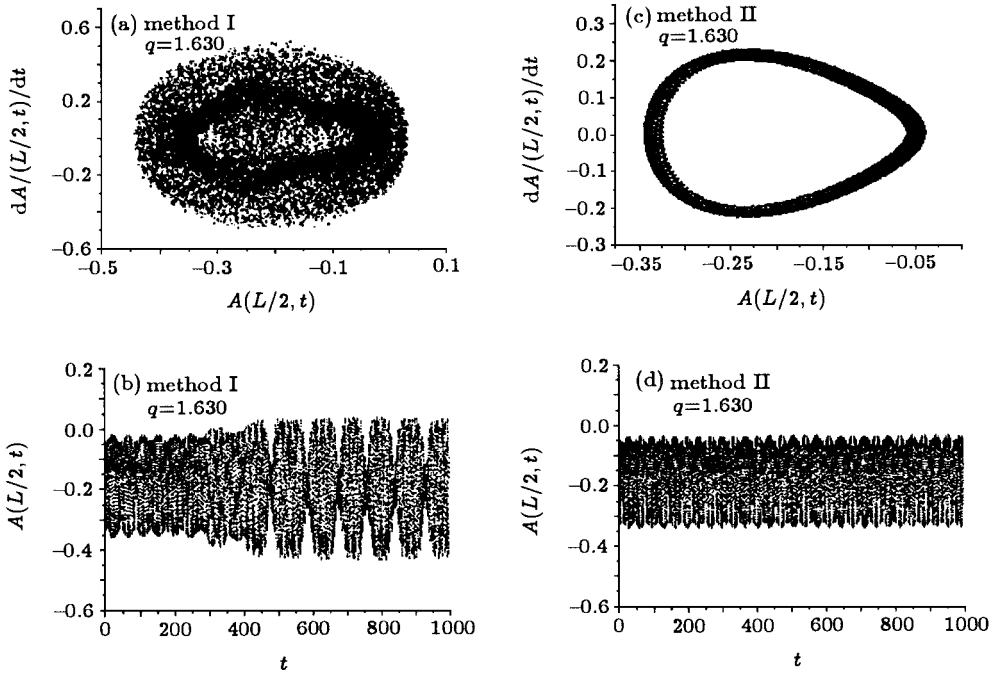


Fig.5. The comparison between Method I and Method II for the cubic NSE with q=1.630: (a) and (c) are the phase trajectories; (b) and (d) are the time evolution of the amplitude of fields $A(L/2,t)$.

We have also used the high-order symplectic Runge–Kutta scheme (10) to integrate the NSE (1) and obtain the same results.

5. Discussions

The basic dynamic behaviour of the cubic NSE (1) is studied using the symplectic scheme in different space difference approximations. The numerical results illustrate that the quasi-particle number, the total momentum and the total energy can be preserved, and the error of the total energy oscillates periodically about zero for long-time computation. For large cubic nonlinear parameters, the error of the total energy appears to be some isolated distribution points deviating from the zero point. We find that the isolated distribution point of the total energy is the same as the period of the time evolution for the amplitude of the fields $A(L/2,t)$. We also indicate that the low-order space difference approximation may induce irregular phase trajectories for large cubic nonlinear parameter, but the high-order space difference approximation may give the correct phase trajectories. The results obtained in this work indicate that the symplectic method is a good one for the calculation of conserved quantities of NSE for long-time computation, and the precision in calculation of space difference approximation is also very important for investigating the dynamic properties of NSE.

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