Explicit K-symplectic methods for nonseparable non-canonical Hamiltonian systems

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(Received 8 October 2022; revised manuscript received 27 November 2022; accepted manuscript online 8 December 2022)

We propose efficient numerical methods for nonseparable non-canonical Hamiltonian systems which are explicit, K-symplectic in the extended phase space with long time energy conservation properties. They are based on extending the original phase space to several copies of the phase space and imposing a mechanical restraint on the copies of the phase space. Explicit K-symplectic methods are constructed for two non-canonical Hamiltonian systems. Numerical tests show that the proposed methods exhibit good numerical performance in preserving the phase orbit and the energy of the system over long time, whereas higher order Runge–Kutta methods do not preserve these properties. Numerical tests also show that the K-symplectic methods exhibit better efficiency than that of the same order implicit symplectic, explicit and implicit symplectic methods for the original nonseparable non-canonical systems. On the other hand, the fourth order K-symplectic method is more efficient than the fourth order Yoshida's method, the optimized partitioned Runge–Kutta and Runge–Kutta–Nyström explicit K-symplectic methods for the extended phase space Hamiltonians, but less efficient than the the optimized partitioned Runge–Kutta and Runge–Kutta–Nyström extended phase space symplectic-like methods with the midpoint permutation.

Keywords: non-canonical Hamiltonian systems, nonseparable, explicit K-symplectic methods, splitting method

PACS: 02.60.Jh, 02.60.Cb, 45.20.Jj, 45.20.dh **DOI:** 10.1088/1674-1056/aca9c8

1. Introduction

Many mechanical systems can be expressed as non-canonical Hamiltonian systems, such as the Lotka–Volterra model,[1] the nonlinear Schrödinger equation,[2–5] the charged particle system,[6,7] the guiding center system,[8–10] the Maxwell–Vlasov equations[11,12] and the ideal MHD formualtion.[13] These models appear in many applications of areas. The Lotka–Volterra model[1] is the simplest model of predator–prey interactions and it describes the growth of animal species. It was first established in mathematical biology, then it had been derived independently in the fields of epidemics, combustion theory and economics, and other disciplines. The nonlinear Schrödinger equation[2–5] is a very important completely integrable model in soliton theory. It appears in many physical areas, such as nonlinear optics, plasma physics, and bimolecular dynamics. The motion of charged particles[6,7] in external electromagnetic fields is the most fundamental equation in plasma physics research. It contains the fast gyromotion and the slow gyrocenter motion. If we average out the fast gyromotion from the charged particle motion, the motion of the gyrocenter is obtained. The non-canonical Hamiltonian systems are generalizations of the canonical Hamiltonian systems.[1,14–18] They have non-canonical symplectic structures which are preserved by the K-symplectic methods. K-symplectic methods exhibit advantageous energy preservation properties just like the symplectic methods[3,19–23] for Hamiltonian systems. Therefore, K-symplectic methods are preferred methods for long time simulations of non-canonical Hamiltonian systems. One approach to constructing K-symplectic methods for a non-canonical system is to transform the system to a canonical one by a coordinate transformtion[1,14] and use the symplectic method. The other approach is the generating function method,[15,24] but it is also inevitable to seek for one coordinate transformation. To avoid the difficulty of finding the coordinate transformation, we prefer to use the splitting method for the non-canonical Hamiltonian systems.

Symplectic methods exhibit superior long-term behavior compared with standard integrators such as explicit Runge–Kutta methods. The long-term behaviors include the slower error growth and the approximate preservation of invariants, such as the energy and the angular momentum, without secular drift. Symplectic methods can be classified as the explicit ones and the implicit ones. If the Hamiltonian can be separated into several integrable parts, then explicit symplectic methods can be constructed by composing the analytical solutions of the sub-Hamiltonians. The typical examples of explicit symplectic methods are the second-order leapfrog method,[25] the fourth-order Forest–Ruth method,[26] and the Yoshida's fourth-order method.[23] For nonseparable Hamiltonian sys-

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tems, implicit symplectic methods are always available. Implicit symplectic methods have completely implicit symplectic methods including the implicit midpoint rule,[27,28] the implicit Gauss–Legendre Runge–Kutta symplectic method,[29,30] and the explicit and implicit mixed symplectic methods.[31–34] The implicit methods are numerically more expensive than the explicit methods because one of the iteration methods is required to solve the equations. On the other hand, the implicit methods perform better in solving stiff equations than that of the explicit ones.[35]

Recently, a fourth order non-canonical explicit and implicit symplectic integrator for post-Newtonian (PN) Hamiltonian of spinning compact binaries was constructed by splitting the Hamiltonian to orbital and spin contributions and the integrator exhibited excellent long-term performance.[31] Using the canonical spin variables suggested in Ref. [36], some canonical symplectic methods for PN Hamiltonian of spinning compact binaries were obtained.[32–34] By splitting the Hamiltonian into separable and nonseparable parts, Zhong *et al.* developed the fourth-order explicit and implicit mixed symplectic integrators.[32] The explicit leapfrog method was used to calculate the separable Hamiltonians while the implicit midpoint rule was used to solve the nonseparable Hamiltonians.[32] Mei *et al.* discussed the numerical performances of the Forest–Ruth symplectic method and the Yoshida symplectic method by several examples including the PN Hamiltonian formulation of non-spin compact binaries.[33] For the 10-dimensional PN canonical conservative Hamiltonian system, Mei *et al.* explored the influences of the spin effects of black hole pairs on the dynamics and showed that the chaos occurs when the spin–spin effects of the two spinning bodies were included by combining the numerical tests.[34] In fact, when the dissipative force $\boldsymbol{F}$ is set to zero, the non-canonical post-Newtonian Hamiltonian of spinning compact binaries takes the form

$$\dot{\boldsymbol{X}} = \frac{\partial H}{\partial \boldsymbol{P}}, \tag{1}$$

$$\dot{\boldsymbol{P}} = -\frac{\partial H}{\partial \boldsymbol{X}}, \tag{2}$$

$$\dot{\boldsymbol{S}}_a = \frac{\partial H}{\partial \boldsymbol{S}_a} \times \boldsymbol{S}_a, \tag{3}$$

where $\boldsymbol{X}$ are positions, $\boldsymbol{P}$ are momenta, $\boldsymbol{S}_a$ $(a=1,2)$ are spins and $\times$ denotes the usual vector cross product. As we know that $\frac{\partial H}{\partial \boldsymbol{S}_a} \times \boldsymbol{S}_a = \tilde{\boldsymbol{S}}_a \frac{\partial H}{\partial \boldsymbol{S}_a}$ where $\tilde{\boldsymbol{S}}_a$ is an anti-symmetric matrix, then the system (1)–(3) becomes a non-canonical Hamiltonian system or a Poisson system with the expression

$$\dot{Z} = \boldsymbol{P}(\boldsymbol{Z})\nabla H(\boldsymbol{Z}), \quad \boldsymbol{Z} = (\boldsymbol{X}, \boldsymbol{P}, \boldsymbol{S}_1, \boldsymbol{S}_2), \tag{4}$$

where $\boldsymbol{P}(\boldsymbol{Z})$ is an anti-symmetric matrix and satisfies the Jacobi identity which is defined below in Eq. (10). Poisson systems are generalized non-canonical Hamiltonian systems. The matrix $\boldsymbol{P}(\boldsymbol{Z})$ in Poisson systems can be singular. When the matrix $\boldsymbol{P}(\boldsymbol{Z})$ is nonsingular, the Poisson system becomes the non-canonical Hamiltonian system.

A class of explicit symplectic integrators based on operator splitting and composing have been developed recently for nonseparable systems, such as the charged particles around Schwarzschild black holes,[25,37–39] Reissner–Nordström black holes,[40–42] and Kerr black holes.[43–45] By splitting the Hamiltonian of Schwarzschild spacetime geometry into four integrable parts whose analytical solutions can be expressed as explicit functions, second order and fourth order explicit symplectic integrators were constructed.[25] The same technique was also used to construct explicit symplectic integrators for charged particles moving around a Reissner–Nordström black hole with an external magnetic field[40] and Reissner–Nordström–(anti)-de Sitter black hole with an external magnetic field.[41] Second order and fourth order explicit symplectic integrators were proposed for the Kerr spacetime geometry by using a time transformation function to obtain a transformed Hamiltonian where the operator splitting and composing can be directly used.[45] Following the work of Wu *et al.*,[45] explicit symplectic integrators were applied to study chaos of charged particles around the magnetized Kerr black hole.[43] How the small changes of parameters effect the dynamics of charged particles around the Kerr black holes immersed in an external magnetic field were also investigated.[44] Furthermore, by using the technique of the time-transformed explicit symplectic integrators for the Kerr-type spacetimes introduced in Ref. [45], Zhang *et al.* proposed explicit symplectic integrators for the deformed Schwarzschild black hole immersed in an external magnetic field and the obtained integrators exhibited good long-term performance for both regular orbits and chaotic orbits.[38] All the explicit symplectic integrators constructed above are applied to the canonical Hamiltonian system

$$\dot{\boldsymbol{Z}} = \boldsymbol{J}^{-1}\nabla H(\boldsymbol{Z}), \tag{5}$$

where the symplectic matrix $\boldsymbol{J}$ is defined in Eq. (11). If the Hamiltonian H can be separated into two parts $H(\boldsymbol{Z}) = H_1(\boldsymbol{Z}) + H_2(\boldsymbol{Z})$ with $\boldsymbol{Z} = (\boldsymbol{P}, \boldsymbol{Q}) \in \mathbb{R}^{2n}$, we can define two differential operators

$$\mathscr{A} = \sum_{i=1}^{n} \left(\frac{\partial H_1}{\partial P_i}\frac{\partial}{\partial Q_i} - \frac{\partial H_1}{\partial Q_i}\frac{\partial}{\partial P_i} \right), \tag{6}$$

$$\mathscr{B} = \sum_{i=1}^{n} \left(\frac{\partial H_2}{\partial P_i}\frac{\partial}{\partial Q_i} - \frac{\partial H_2}{\partial Q_i}\frac{\partial}{\partial P_i} \right). \tag{7}$$

If the two sub-Hamiltonians have analytical solutions which can be expressed as explicit functions, then the composing integrator $\exp h\mathscr{B} \exp h\mathscr{A}(\boldsymbol{Z}_0)$ is a first order explicit symplectic integrator. Higher order explicit symplectic integrators can be constructed by composing $\exp h\mathscr{B}$ and $\exp h\mathscr{A}$. This operator splitting and composing technique can also be applied

to the non-canonical Hamiltonian system (4) with nonsingular $\boldsymbol{P}(\boldsymbol{Z})$, but the differential operators are defined in a different way. Assuming that we split the Hamiltonian H into $H(\boldsymbol{Z}) = H_1(\boldsymbol{Z}) + H_2(\boldsymbol{Z})$, the two differential operators $\mathscr{D}_1$ and $\mathscr{D}_2$ acting on a function F are defined as follows:

$$\mathscr{D}_i F = \nabla F^{\top} \boldsymbol{P}(\boldsymbol{Z}) \nabla H_i, \quad i = 1, 2. \tag{8}$$

With the above two operators, if the two sub-Hamiltonians have explicit analytical solutions, then we know that the integrator $\exp h\mathscr{D}_2 \exp h\mathscr{D}_1(\boldsymbol{Z}_0)$ is a first order explicit K-symplectic integrator. Higher order explicit K-symplectic integrators can also be constructed by using composing technique.

The splitting method is widely used to construct explicit symplectic methods for separable Hamiltonian systems[1,46,47] and explicit K-symplectic methods for non-canonical Hamiltonian systems.[6,48,49] Blanes and Moan used the splitting method to construct an efficient fourth order symplectic method for non-autonomous Hamiltonian systems.[46] He *et al.* used the splitting method[6] to construct the explicit K-sympletic methods for the non-canonical charged particle system. Zhu *et al.* constructed the explicit K-symplectic methods for both the bright solitons motion and the dark solitons motion of the nonlinear Schrödinger equation.[48,49] The explicit symplectic methods and K-symplectic methods had been constructed for separable systems while the work is much less for the nonseparable systems. For several subclasses of nonseparable Hamiltonian systems, Pihajoki constructed the explicit extended phase space symplectic-like methods based on the idea of extending the phase space by making two copies of it and using the splitting method.[50] These methods have good long-term performance in preserving the energy but are not symplectic both in the original phase space and the extended phase space because they are combined with coordinate mixing transformations. Inspired by the Pihajoki's work, several researchers developed the phase space mixing maps.[51,52] Liu *et al.* compared several mixing maps and showed that the leapfrog method with the sequent permutations of coordinates and momenta can provide the most accurate results and the best long-term stable error behaviour.[51] A fourth order extended phase space explicit symplectic-like method with the sequent permutations of coordinates and momenta were proposed to solve four-dimensional metric of relativistic core-shell models with nonseparable Hamiltonian and the dynamics of chaos of the system was investigated.[53] Then, the midpoint permutation map was proposed and proved to have better performance. Luo *et al.* developed the midpoint permutation map for the fourth-order Yoshida's method and showed that the midpoint permutation is more powerful in restraining the original phase space and the copying ones than that of the sequent permutations of coordinates and momenta.[52] Li *et al*. developed three fourth order explicit symplectic-like integrators by combining the extended phase space with the midpoint permutation and the sequent permutations of coordinates and momenta and got the same conclusion as Luo *et al*. that the midpoint permutation has the best performance.[54] The Yoshida's fourth order extended phase space symplectic-like method with the midpoint permutation was applied to the problem of neutral particles around a Schwarzschild black hole and the dynamics of generic orbits by using this numerical method was surveyed.[55] Pan *et al*. also applied the Yoshida's fourth order extended phase space symplectic-like method with the midpoint permutation to solve the coherent post-Newtonian Euler–Lagrange equations and showed that the method behaves well in energy and/or angular momentum conservation over long time.[56] To overcome the short-term simulation problem of the Pihajoki's work, Tao imposed a mechanical restraint with a control parameter Ω on the two copies of the phase space and successfully realized the long-term simulation.[57] The recent literature pointed out that there is no universal method that can find the best choice of the control parameter in the Tao's methods.[26] On the other hand, it was shown that the fourth order symplectic Yoshida's method and Suziki-like method which are constructed based on the Tao's idea were inferior to the fourth order nonsymplectic symmetric Forest–Ruth-like method with the midpoint permutation.[26] The Tao's methods were also shown not superior to the extended phase space symplectic-like methods with the midpoint permutation proposed by Luo *et al*.[52] at the same order in accuracy.[39] Recently, semi-explicit symplectic integrators for nonseparable Hamiltonian systems, which are symplectic in both the original phase space and the extended phase space, were proposed.[58,59] These methods have good long-term performance in preserving the invariants and exhibit the same and even better efficiency than that of the Tao's method. All the articles mentioned above construct symplectic methods or symplectic-like methods for nonseparable Hamiltonian systems. Different from them, we concentrate on the nonseparable non-canonical Hamiltonian systems. Our work is based on the pioneer work of Pihajoki and Tao, we construct the explicit K-symplectic methods for nonseparable non-canonical Hamiltonian systems by using the splitting method. As the non-canonical systems are more complicate than the canonical systems, in some cases the two copies of the phase space are not enough to construct explicit K-symplectic methods, thus we need to make more copies.

Nonseparable systems are important gradients of non-canonical Hamiltonian systems. The guiding center system,[8–10] the reduced magnetohydrodynamics equations,[60] and the Ablowitz–Ladik model of the nonlinear Schrödinger equation under periodic condition[1] are all nonseparable non-canonical Hamiltonian systems. Thus, it is critical to construct K-symplectic methods with long-term

conservation property for nonseparable non-canonical systems. The idea is to extend the phase space and make several copies of the phase space and to impose an artificial restraint for the several copies of the phase space. The extended phase space Hamiltonian consists of several copies of the original Hamiltonian and another Hamiltonian H_c with control parameter Ω that are used to control the copies of the variables. The constructed method is explicit and K-symplectic in the extended phase space. We extend the non-canonical systems in two ways according to their structures and analyze in which situation that the explicit K-symplectic methods can be constructed. Then we propose a second-order and a fourth-order explicit methods which are K-symplectic in the extend phase space but not K-symplectic in the original phase space. In order to characterize the distance between the new Hamiltonian $\hat{H}$ which is exactly preserved by a p-th order K-symplectic method and the extended phase space Hamiltonian $\bar{H}$, we provide an error analysis on the Hamiltonian. The error analysis shows that the $\hat{H}$ provides an approximation to $\bar{H}$. To show the superiority of the K-symplectic methods in structure preservation and efficiency, we compare them with higher order explicit Runge–Kutta methods,[61,62] the implicit symplectic methods, the explicit and implicit symplectic methods for the original nonseparable noncanonical Hamiltonians, several other fourth order explicit K-symplectic methods for the extended phase space Hamiltonians, and several fourth order extended phase space K-symplectic-like methods with the midpoint permutation.

The paper is organized as follows. Section 2 is focus on constructing K-symplectic methods for the nonseparable systems with special structure and analyzing the situation in which the explicit K-symplectic methods can be constructed. In Section 3, the nonseparable systems are general systems and we make several copies of the phase space in order to construct explicit K-symplectic methods. Section 4 provides an error analysis from the view of Hamiltonian. In Section 5, all the numerical methods are listed and the numerical results in two nonseparable systems are provided. Finally, we give a short conclusion in Section 6.

2. Explicit K-symplectic methods for nonseparable systems with special structure

Consider the non-canonical Hamiltonian system

$$\dot{\boldsymbol{Z}} = \boldsymbol{K}^{-1}(\boldsymbol{Z})\nabla H(\boldsymbol{Z}), \quad \boldsymbol{z} = (\boldsymbol{P},\boldsymbol{Q})^{\top} \in \mathbb{R}^{2n}, \tag{9}$$

where the dot $\cdot$ represents the derivative with respect to time t and the function H is the Hamiltonian. The matrix $\boldsymbol{K} = (l_{ij})_{2n\times 2n}$ is anti-symmetric, i.e., $l_{ij} = -l_{ji}$. It is nonsingular, i.e., $\det \boldsymbol{K}(\boldsymbol{Z}) \neq 0$. Meanwhile, it satisfies the Jacobi identity

$$\frac{\partial l_{ab}}{\partial z_c} + \frac{\partial l_{bc}}{\partial z_a} + \frac{\partial l_{ca}}{\partial z_b} = 0, \quad 1 \le a,b,c \le 2n\,. \tag{10}$$

If we replace the matrix $\boldsymbol{K}^{-1}(\boldsymbol{Z})$ with the constant matrix $\boldsymbol{J}^{-1}$ where

$$\boldsymbol{J} = \begin{pmatrix} \boldsymbol{O}_n & \boldsymbol{I}_n \\ -\boldsymbol{I}_n & \boldsymbol{O}_n \end{pmatrix}, \tag{11}$$

then the non-canonical Hamiltonian system (9) becomes a canonical Hamiltonian system $\dot{Z} = \boldsymbol{J}^{-1}\nabla H(\boldsymbol{Z})$. According to the Darboux's theorem,[1,14] there exists a coordinate transformation $\boldsymbol{y} = \zeta(\boldsymbol{Z})$ that transforms the non-canonical Hamiltonian system (9) to a canonical Hamiltonian system. We assume that $\boldsymbol{y} = \zeta(\boldsymbol{Z})$ exists, then the system (9) can be rewritten as

$$\dot{\boldsymbol{y}} = \Big[\frac{\partial \zeta(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big]\boldsymbol{K}^{-1}(\boldsymbol{Z})\Big[\frac{\partial \zeta(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big]^{\top}\nabla \tilde{H}(\boldsymbol{y}), \tag{12}$$

where $H(\boldsymbol{Z}) = H \circ \zeta^{-1}(\boldsymbol{y}) = \tilde{H}(\boldsymbol{y})$. If the transformation satisfies

$$\Big[\frac{\partial \zeta(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big]\boldsymbol{K}^{-1}(\boldsymbol{Z})\Big[\frac{\partial \zeta(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big]^{\top} = \boldsymbol{J}^{-1}, \tag{13}$$

or

$$\Big[\frac{\partial \zeta(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big]^{\top}\boldsymbol{J}\Big[\frac{\partial \zeta(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big] = \boldsymbol{K}(\boldsymbol{Z}), \tag{14}$$

then the system (9) becomes a canonical Hamiltonian system $\dot{\boldsymbol{y}} = \boldsymbol{J}^{-1}\nabla \tilde{H}(\boldsymbol{y})$.

The non-canonical Hamiltonian system (9) has the general symplectic structure which is defined by the following 2-form

$$W = \sum_{1\le i,j\le 2n} l_{ij}(\boldsymbol{Z})\,\mathrm{d}z_i \wedge \mathrm{d}z_j. \tag{15}$$

The above 2-form[14] is closed, i.e., $\mathrm{d}W = 0$. The general symplectic structure is also called K-symplectic structure which is related to the matrix $\boldsymbol{K}(\boldsymbol{Z})$. The exact phase flow (exact solution) $\varphi_t(\boldsymbol{Z})$ of the non-canonical Hamiltonian system is usually difficult to solve. However, we can use numerical methods that exactly preserve the K-symplectic structure of the non-canonical system. This kind of numerical methods is called K-symplectic methods. It is well known that the exact flow $\varphi_t(\boldsymbol{Z})$ is one of the K-symplectic methods. On the other hand, the Hamiltonian is exactly preserved by the exact phase flow $\varphi_t(\boldsymbol{Z})$, i.e.,

$$\begin{aligned} \frac{\mathrm{d}H(\varphi_t(\boldsymbol{Z}))}{\mathrm{d}t} &= \frac{\partial H(\varphi_t(\boldsymbol{Z}))}{\partial \varphi_t(\boldsymbol{Z})}\frac{\mathrm{d}\varphi_t(\boldsymbol{Z})}{\mathrm{d}t} \\ &= \big(\nabla H(\varphi_t(\boldsymbol{Z}))\big)^{\top}\boldsymbol{K}^{-1}(\varphi_t(\boldsymbol{Z}))\nabla H(\varphi_t(\boldsymbol{Z})) \\ &= 0, \end{aligned} \tag{16}$$

the last equality holds because $\boldsymbol{K}^{-1}$ is an anti-symmetric matrix. Thus $H(\varphi_t(\boldsymbol{Z})) = H(\varphi_0(\boldsymbol{Z})) = H(\boldsymbol{Z}_0)$. Now we give the definition of the K-symplectic methods.

Definition 1 Given a numerical method $G_\tau : \boldsymbol{Z} \to \hat{\boldsymbol{Z}}$, if its Jacobian satisfies

$$\Big[\frac{\partial G_\tau(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big]^\top \boldsymbol{K}(G_\tau(\boldsymbol{Z}))\Big[\frac{\partial G_\tau(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\Big] = \boldsymbol{K}(\boldsymbol{Z}), \tag{17}$$

we call it as a K-symplectic method.[1]

It is a difficult task to construct the K-symplectic methods for the general non-canonical Hamiltonian systems.[1] However, we can construct the K-symplectic methods for the separable non-canonical Hamiltonian systems by using the splitting method in some cases. The problem is whether we can use the splitting method to construct the K-symplectic methods for the nonseparable non-canonical Hamiltonian systems.

Here the form of the matrix $\boldsymbol{K}^{-1}$ is assumed as

$$\boldsymbol{K}^{-1}(\boldsymbol{Z}) = \begin{pmatrix} \boldsymbol{O}_n & -\boldsymbol{K}_{12}(\boldsymbol{P},\boldsymbol{Q}) \\ \boldsymbol{K}_{12}^\top(\boldsymbol{P},\boldsymbol{Q}) & \boldsymbol{O}_n \end{pmatrix}, \tag{18}$$

where $\boldsymbol{O}_n$ is the $n\times n$ zero matrix. We approximate the flow of the non-canonical Hamiltonian system with an arbitrary nonseparable $H(\boldsymbol{P},\boldsymbol{Q})$. The Hamiltonian is called separable if $H(\boldsymbol{P},\boldsymbol{Q}) = H_1(\boldsymbol{P}) + H_2(\boldsymbol{Q})$.[1] If the Hamiltonian does not satisfy the above form, it is called nonseparable.

We aim at constructing higher order explicit K-symplectic methods of the system (9) with nonseparable H by considering an augmented Hamiltonian[57]

$$\bar{H}(\boldsymbol{p},\boldsymbol{q},\boldsymbol{x},\boldsymbol{y}) := H_A + H_B + \Omega H_C, \tag{19}$$

in an extended phase space which is two copies of the original phase space. Here $H_A := H(\boldsymbol{p},\boldsymbol{y})$ and $H_B := H(\boldsymbol{x},\boldsymbol{q})$ correspond to the two copies of the original Hamiltonian with mixed-up momentum and position variables, $H_C := \| \boldsymbol{p}-\boldsymbol{x} \|_2^2 /2 + \| \boldsymbol{q}-\boldsymbol{y} \|_2^2 /2$ is an imposed restraint, and Ω is a constant that controls the binding of the two copies.[57] Then the new system is

$$\begin{pmatrix} \dot{\boldsymbol{p}} \\ \dot{\boldsymbol{q}} \\ \dot{\boldsymbol{x}} \\ \dot{\boldsymbol{y}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{O}_n & -\boldsymbol{K}_{12}(\boldsymbol{p},\boldsymbol{q}) & \boldsymbol{O}_n & \boldsymbol{O}_n \\ \boldsymbol{K}_{12}^\top(\boldsymbol{p},\boldsymbol{q}) & \boldsymbol{O}_n & \boldsymbol{O}_n & \boldsymbol{O}_n \\ \boldsymbol{O}_n & \boldsymbol{O}_n & \boldsymbol{O}_n & -\boldsymbol{K}_{12}(\boldsymbol{x},\boldsymbol{y}) \\ \boldsymbol{O}_n & \boldsymbol{O}_n & \boldsymbol{K}_{12}^\top(\boldsymbol{x},\boldsymbol{y}) & \boldsymbol{O}_n \end{pmatrix} \begin{pmatrix} \partial_{\boldsymbol{p}}\bar{H}(\boldsymbol{p},\boldsymbol{q},\boldsymbol{x},\boldsymbol{y}) \\ \partial_{\boldsymbol{q}}\bar{H}(\boldsymbol{p},\boldsymbol{q},\boldsymbol{x},\boldsymbol{y}) \\ \partial_{\boldsymbol{x}}\bar{H}(\boldsymbol{p},\boldsymbol{q},\boldsymbol{x},\boldsymbol{y}) \\ \partial_{\boldsymbol{y}}\bar{H}(\boldsymbol{p},\boldsymbol{q},\boldsymbol{x},\boldsymbol{y}) \end{pmatrix} = \bar{\boldsymbol{K}}\nabla\bar{H}. \tag{20}$$

The original initial value problem is

$$\begin{cases} \dot{\boldsymbol{P}} = -\boldsymbol{K}_{12}(\boldsymbol{P},\boldsymbol{Q})\partial_{\boldsymbol{Q}}H(\boldsymbol{P},\boldsymbol{Q}), & \boldsymbol{P}(0) = \boldsymbol{P}_0, \\ \dot{\boldsymbol{Q}} = \boldsymbol{K}_{12}^\top(\boldsymbol{P},\boldsymbol{Q})\partial_{\boldsymbol{P}}H(\boldsymbol{P},\boldsymbol{Q}), & \boldsymbol{Q}(0) = \boldsymbol{Q}_0, \end{cases} \tag{21}$$

and the extended system is

$$\begin{cases} \dot{\boldsymbol{p}} = -\boldsymbol{K}_{12}(\boldsymbol{p},\boldsymbol{q})\partial_{\boldsymbol{q}}H(\boldsymbol{x},\boldsymbol{q}) - \boldsymbol{K}_{12}(\boldsymbol{p},\boldsymbol{q})\Omega(\boldsymbol{q}-\boldsymbol{y}), & \boldsymbol{p}(0) = \boldsymbol{P}(0), \\ \dot{\boldsymbol{q}} = \boldsymbol{K}_{12}^\top(\boldsymbol{p},\boldsymbol{q})\partial_{\boldsymbol{p}}H(\boldsymbol{p},\boldsymbol{y}) - \boldsymbol{K}_{12}^\top(\boldsymbol{p},\boldsymbol{q})\Omega(\boldsymbol{p}-\boldsymbol{x}), & \boldsymbol{q}(0) = \boldsymbol{Q}(0), \\ \dot{\boldsymbol{x}} = -\boldsymbol{K}_{12}(\boldsymbol{x},\boldsymbol{y})\partial_{\boldsymbol{y}}H(\boldsymbol{p},\boldsymbol{y}) - \boldsymbol{K}_{12}(\boldsymbol{x},\boldsymbol{y})\Omega(\boldsymbol{y}-\boldsymbol{q}), & \boldsymbol{x}(0) = \boldsymbol{P}(0), \\ \dot{\boldsymbol{y}} = \boldsymbol{K}_{12}^\top(\boldsymbol{x},\boldsymbol{y})\partial_{\boldsymbol{x}}H(\boldsymbol{x},\boldsymbol{q}) + \boldsymbol{K}_{12}^\top(\boldsymbol{x},\boldsymbol{y})\Omega(\boldsymbol{x}-\boldsymbol{p}), & \boldsymbol{y}(0) = \boldsymbol{Q}(0). \end{cases} \tag{22}$$

It should be noted that if $\boldsymbol{p}(t) = \boldsymbol{x}(t)$ in the extended system (22), then the extended system is just the two copies of the original system, thus we have the same exact solution $\boldsymbol{p}(t) = \boldsymbol{x}(t) = \boldsymbol{P}(t)$, $\boldsymbol{q}(t) = \boldsymbol{y}(t) = \boldsymbol{Q}(t)$ if the same initial values are imposed on $\boldsymbol{p}$, $\boldsymbol{x}$, $\boldsymbol{P}$ and $\boldsymbol{q}$, $\boldsymbol{y}$, $\boldsymbol{Q}$.

Denote the time-τ flow of H_A and H_B by $\phi_{H_A}^\tau$ and $\phi_{H_B}^\tau$. H_C can be separated into two parts $H_C^1 = \| \boldsymbol{p}-\boldsymbol{x} \|_2^2 /2$ and $H_C^2 = \| \boldsymbol{q}-\boldsymbol{y} \|_2^2 /2$. We denote the exact solution of the subsystem with Hamiltonian H_C^1 by $\phi_{\Omega H_C^1}^\tau$ and that with H_C^2 by $\phi_{\Omega H_C^2}^\tau$. Then we have the following four subsystems:

subsystem I

$$\begin{cases} \dot{\boldsymbol{p}} = 0, \\ \dot{\boldsymbol{q}} = \boldsymbol{K}_{12}^\top(\boldsymbol{p},\boldsymbol{q})\partial_{\boldsymbol{p}}H(\boldsymbol{p},\boldsymbol{y}), \\ \dot{\boldsymbol{x}} = -\boldsymbol{K}_{12}(\boldsymbol{x},\boldsymbol{y})\partial_{\boldsymbol{y}}H(\boldsymbol{p},\boldsymbol{y}), \\ \dot{\boldsymbol{y}} = 0, \end{cases} \tag{23}$$

subsystem II

$$\begin{cases} \dot{\boldsymbol{p}} = -\boldsymbol{K}_{12}(\boldsymbol{p},\boldsymbol{q})\partial_{\boldsymbol{q}}H(\boldsymbol{x},\boldsymbol{q}), \\ \dot{\boldsymbol{q}} = 0, \\ \dot{\boldsymbol{x}} = 0, \\ \dot{\boldsymbol{y}} = \boldsymbol{K}_{12}^\top(\boldsymbol{x},\boldsymbol{y})\partial_{\boldsymbol{x}}H(\boldsymbol{x},\boldsymbol{q}), \end{cases} \tag{24}$$

subsystem III

$$\begin{cases} \dot{\boldsymbol{p}} = 0, \\ \dot{\boldsymbol{q}} = \boldsymbol{K}_{12}^\top(\boldsymbol{p},\boldsymbol{q})\Omega(\boldsymbol{p}-\boldsymbol{x}), \\ \dot{\boldsymbol{x}} = 0, \\ \dot{\boldsymbol{y}} = \boldsymbol{K}_{12}^\top(\boldsymbol{x},\boldsymbol{y})\Omega(\boldsymbol{x}-\boldsymbol{p}), \end{cases} \tag{25}$$

and subsystem IV

$$\begin{cases} \dot{\boldsymbol{p}} = -\boldsymbol{K}_{12}(\boldsymbol{p},\boldsymbol{q})\Omega(\boldsymbol{q}-\boldsymbol{y}), \\ \dot{\boldsymbol{q}} = 0, \\ \dot{\boldsymbol{x}} = -\boldsymbol{K}_{12}(\boldsymbol{x},\boldsymbol{y})\Omega(\boldsymbol{y}-\boldsymbol{q}), \\ \dot{\boldsymbol{y}} = 0. \end{cases} \tag{26}$$

The problem is that under which situation, the four subsystems can be solved explicitly and the explicit K-symplectic methods can be constructed. For the above problem, we have the following theorem.

Theorem 1 In the following situation, the above four subsystems (23), (24), (25), and (26) can be solved explicitly.

If the elements

$$\boldsymbol{K}_{12} = \mathrm{diag}(g_1(p_1,q_1), g_2(p_2,q_2), \ldots, g_n(p_n,q_n)),$$

there exist continuous functions $F_i(p_i,q_i)$ and $G_i(p_i,q_i)$ such that $\frac{\mathrm{d}F_i(p_i,q_i)}{\mathrm{d}p_i} = \frac{1}{g_i(p_i,q_i)}$ and $\frac{\mathrm{d}G_i(p_i,q_i)}{\mathrm{d}q_i} = \frac{1}{g_i(p_i,q_i)}$, and p_i and q_i can be solved in closed forms from the two functions $F_i(p_i,q_i)$ and $G_i(p_i,q_i)$ for each $i = 1,2,\ldots,n$.[49]

Proof For the proof we refer to the details in Ref. [49].

If all the four subsystems (23)–(26) can be solved explicitly, K-symplectic methods can be constructed by composing the analytical solutions of all the subsystems. To prove this, we simplify the case with just two subsystems. Assume that the Hamiltonian H of the non-canonical Hamiltonian system (9) can be split into two parts, i.e., $H = H_A + H_B$, then the system (9) can be separated into two subsystems

$$\dot{\boldsymbol{Z}} = \boldsymbol{K}^{-1}(\boldsymbol{Z})\nabla_{\boldsymbol{Z}} H_A, \tag{27}$$

and

$$\dot{\boldsymbol{Z}} = \boldsymbol{K}^{-1}(\boldsymbol{Z})\nabla_{\boldsymbol{Z}} H_B. \tag{28}$$

Theorem 2 If we denote the exact solutions (exact flows) of the two subsystems by $\phi^{\tau}_{H_A}$ and $\phi^{\tau}_{H_B}$, then the method $\phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}$ is a first order K-symplectic method.

Proof To prove the method $\phi^{\tau}_{H_A} \circ \phi^{\tau}_{H_B}$ is a K-symplectic method, we need to prove that it satisfies the Eq. (17) in Definition 1. Thus we need to prove

$$\begin{aligned}&\left[\frac{\partial \phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\right]^{\top} \boldsymbol{K}(\phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}(\boldsymbol{Z}))\\ &\times \left[\frac{\partial \phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}(\boldsymbol{Z})}{\partial \boldsymbol{Z}}\right] = \boldsymbol{K}(\boldsymbol{Z}).\end{aligned} \tag{29}$$

Denote $\tilde{\boldsymbol{Z}} = \phi^{\tau}_{H_A}(\boldsymbol{Z})$, then the above Eq. (29) is equivalent to

$$\begin{aligned}&\left[\frac{\partial \phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}})}{\partial \tilde{\boldsymbol{Z}}}\frac{\partial \tilde{\boldsymbol{Z}}}{\partial \boldsymbol{Z}}\right]^{\top} \boldsymbol{K}(\phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}}))\\ &\times \left[\frac{\partial \phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}})}{\partial \tilde{\boldsymbol{Z}}}\frac{\partial \tilde{\boldsymbol{Z}}}{\partial \boldsymbol{Z}}\right] = \boldsymbol{K}(\boldsymbol{Z}).\end{aligned} \tag{30}$$

The above Eq. (30) is equivalent to

$$\begin{aligned}&\left[\frac{\partial \tilde{\boldsymbol{Z}}}{\partial \boldsymbol{Z}}\right]^{\top}\left[\frac{\partial \phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}})}{\partial \tilde{\boldsymbol{Z}}}\right]^{\top} \boldsymbol{K}(\phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}}))\\ &\times \left[\frac{\partial \phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}})}{\partial \tilde{\boldsymbol{Z}}}\right]\left[\frac{\partial \tilde{\boldsymbol{Z}}}{\partial \boldsymbol{Z}}\right] = \boldsymbol{K}(\boldsymbol{Z}).\end{aligned} \tag{31}$$

As $\phi^{\tau}_{H_B}$ is the exact solution of the subsystem (28), thus it is a K-symplectic method, therefore, it satisfies the Eq. (17) in Definition 1, i.e.,

$$\left[\frac{\partial \phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}})}{\partial \tilde{\boldsymbol{Z}}}\right]^{\top} \boldsymbol{K}(\phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}}))\left[\frac{\partial \phi^{\tau}_{H_B}(\tilde{\boldsymbol{Z}})}{\partial \tilde{\boldsymbol{Z}}}\right] = \boldsymbol{K}(\tilde{\boldsymbol{Z}}). \tag{32}$$

As a result, the Eq. (31) is equivalent to

$$\left[\frac{\partial \tilde{\boldsymbol{Z}}}{\partial \boldsymbol{Z}}\right]^{\top} \boldsymbol{K}(\tilde{\boldsymbol{Z}})\left[\frac{\partial \tilde{\boldsymbol{Z}}}{\partial \boldsymbol{Z}}\right] = \boldsymbol{K}(\boldsymbol{Z}). \tag{33}$$

As $\tilde{\boldsymbol{Z}} = \phi^{\tau}_{H_A}(\boldsymbol{Z})$, it represents the exact solution of the subsystem (27), thus it is also a K-symplectic method, furthermore, we know that the Eq. (33) always holds. As a result, we prove that $\phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}$ is a first order K-symplectic method. The proof is completed.

Remark 1 According to the proof of Theorem 2, if $\phi^{\tau}_{H_A}$ and $\phi^{\tau}_{H_B}$ are two K-symplectic methods, then the composition method $\phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}$ is also a K-symplectic method.

If $\phi^{\tau}_{H_A}, \phi^{\tau}_{H_B}, \phi^{\tau}_{\Omega H^1_C}$, and $\phi^{\tau}_{\Omega H^2_C}$ can be written in close forms where τ represents the time stepsize, then similar to the proof in Theorem 2, we can prove the method $\phi^{\tau}_{\Omega H^2_C} \circ \phi^{\tau}_{\Omega H^1_C} \circ \phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}$ is a first order explicit K-symplectic method. Denote this method by Φ_τ, then

$$\Phi_\tau = \phi^{\tau}_{\Omega H^2_C} \circ \phi^{\tau}_{\Omega H^1_C} \circ \phi^{\tau}_{H_B} \circ \phi^{\tau}_{H_A}. \tag{34}$$

The method Φ^*_τ represents the adjoint method of Φ_τ which is

$$\Phi^*_\tau = \phi^{\tau}_{H_A} \circ \phi^{\tau}_{H_B} \circ \phi^{\tau}_{\Omega H^1_C} \circ \phi^{\tau}_{\Omega H^2_C}. \tag{35}$$

The method Φ^*_τ is also a first order K-symplectic method. According to Remark 1, the composition method

$$\begin{aligned}\Psi^2_\tau &\equiv \Phi^*_{\tau/2} \circ \Phi_{\tau/2}\\ &= \phi^{\tau/2}_{H_A} \circ \phi^{\tau/2}_{H_B} \circ \phi^{\tau/2}_{\Omega H^1_C} \circ \phi^{\tau}_{\Omega H^2_C} \circ \phi^{\tau/2}_{\Omega H^1_C} \circ \phi^{\tau/2}_{H_B} \circ \phi^{\tau/2}_{H_A},\end{aligned} \tag{36}$$

which is a second order explicit K-symplectic method.[63] Higher order explicit K-symplectic methods can be constructed by composing the first order K-symplectic method.

Remark 2 For arbitrary two dimensional nonseparable non-canonical Hamiltonian system, the four subsystems can be solved exactly. Thus the K-symplectic methods can be constructed in the extended phase space by composing the exact solution of the four subsystems.

For high dimensional non-separable systems, if the matrix $\boldsymbol{K}^{-1}$ has the special structure as Eq. (18) and satisfies the requirements in the above Theorem 1, then we only need to make two copies of the phase space to construct explicit K-symplectic methods. If the matrix does not have the special structure, we will show another way to construct explicit K-symplectic methods in the next section.

3. Explicit K-symplectic methods for general nonseparable systems

Let $d = 2n$, we consider the d dimensional non-canonical Hamiltonian system (9) with nonseparable Hamiltonian $H(\boldsymbol{P}) = H(p_1, p_2, \ldots, p_d)$. The skew-symmetric matrix $\boldsymbol{K}^{-1}(\boldsymbol{Z})$ has no special structure. Denote by $\boldsymbol{K}^{-1} = (k_{ij})_{d\times d}$. We extend the d dimensional phase space to d^2 dimensional phase space. Denote by $\boldsymbol{P}_1 = (p_{11}, p_{12}, \ldots, p_{1d})$, $\boldsymbol{P}_2 = (p_{21}, p_{22}, \ldots, p_{2d}), \ldots, \boldsymbol{P}_d = (p_{d1}, p_{d2}, \ldots, p_{dd})$.

We first consider the augmented Hamiltonian with mix-up variables as follows:

$$\bar{H}(\boldsymbol{P}_1, \ldots, \boldsymbol{P}_d) = \sum_{i=1}^{d} H(p_{d+1-i,1}, p_{d+2-i,2}, \ldots, p_{d,i}, p_{1,i+1}, \ldots, p_{d-i,d}) + \Omega H_{\mathrm{c}}. \quad (37)$$

Denote by

$$H_1 = H(p_{d1}, p_{12}, p_{23}, \ldots, p_{d-1,d}), \quad (38)$$

$$H_2 = H(p_{d-1,1}, p_{d2}, p_{13}, \ldots, p_{d-2,d}), \quad (39)$$

$$\vdots$$

$$H_{d-1} = H(p_{21}, p_{32}, \ldots, p_{d,d-1}, p_{1d}), \quad (40)$$

$$H_d = H(p_{11}, p_{22}, \ldots, p_{d-1,d-1}, p_{dd}), \quad (41)$$

then $\bar{H} = H_1 + H_2 + \cdots + H_d + \Omega H_{\mathrm{c}}$ for any $1 \le i \le d$, H_i takes one variable from P_j, $1 \le j \le d$. The function H_{c} is a constraint with

$$H_{\mathrm{c}} = \sum_{j=2}^{d} \frac{\| \boldsymbol{P}_1 - \boldsymbol{P}_j \|_2^2}{2} + \sum_{j=3}^{d} \frac{\| \boldsymbol{P}_2 - \boldsymbol{P}_j \|_2^2}{2} + \cdots + \sum_{j=d-1}^{d} \frac{\| \boldsymbol{P}_{d-2} - \boldsymbol{P}_j \|_2^2}{2} + \frac{\| \boldsymbol{P}_{d-1} - \boldsymbol{P}_d \|_2^2}{2}. \quad (42)$$

Then the new system is

$$\begin{pmatrix} \dot{\boldsymbol{P}}_1 \\ \dot{\boldsymbol{P}}_2 \\ \vdots \\ \dot{\boldsymbol{P}}_d \end{pmatrix} = \begin{pmatrix} \boldsymbol{K}^{-1}(\boldsymbol{P}_1) & & & \\ & \boldsymbol{K}^{-1}(\boldsymbol{P}_2) & & \\ & & \ddots & \\ & & & \boldsymbol{K}^{-1}(\boldsymbol{P}_d) \end{pmatrix} \begin{pmatrix} \partial_{\boldsymbol{P}_1} \bar{H}(\boldsymbol{P}_1, \boldsymbol{P}_2, \ldots, \boldsymbol{P}_d) \\ \partial_{\boldsymbol{P}_2} \bar{H}(\boldsymbol{P}_1, \boldsymbol{P}_2, \ldots, \boldsymbol{P}_d) \\ \vdots \\ \partial_{\boldsymbol{P}_d} \bar{H}(\boldsymbol{P}_1, \boldsymbol{P}_2, \ldots, \boldsymbol{P}_d) \end{pmatrix} = \bar{\boldsymbol{K}} \nabla \bar{H}. \quad (43)$$

It can be verified that if the conditions $\boldsymbol{P}_1(t) = \boldsymbol{P}_2(t) = \cdots = \boldsymbol{P}_d(t)$ hold, the above system (43) is the d copies of the original system (9), thus we have $\boldsymbol{P}_1(t) = \boldsymbol{P}_2(t) = \cdots = \boldsymbol{P}_d(t) = P(t)$ if the same initial condition is imposed on $\boldsymbol{P}$ and each $\boldsymbol{P}_i$, $1 \le i \le d$.

The next step is to explicitly solve each subsystem with the Hamiltonian H_i for $1 \le i \le d$. Here we present the subsystem with $H_1 = H(p_{d1}, p_{12}, p_{23}, \ldots, p_{d-1,d})$

$$\begin{cases} \dot{p}_{1i} = k_{i,2}(\boldsymbol{P}_1) \frac{\partial H_1}{\partial p_{12}}, & i = 1,3,4,\ldots,d, \\ \dot{p}_{12} = 0, \\ \dot{p}_{2i} = k_{i,3}(\boldsymbol{P}_2) \frac{\partial H_1}{\partial p_{23}}, & i = 1,2,4,\ldots,d, \\ \dot{p}_{23} = 0, \\ \cdots\cdots\cdots \\ \dot{p}_{d1} = 0, \\ \dot{p}_{d,i} = k_{i,1}(\boldsymbol{P}_d) \frac{\partial H_1}{\partial p_{d1}}, & i = 2,3,\ldots,d. \end{cases} \quad (44)$$

It can be seen that $p_{12}, p_{23}, \ldots, p_{d1}$ are all constants as their derivatives are zero. As the Hamiltonian H_1 is just a function of constants $p_{12}, p_{23}, \ldots, p_{d1}$, therefore its partial derivatives are all constants. Thus, whether the d subsystems can be solved explicitly depends on k_{ij}, $i, j = 1, \ldots, d$.

For the constraint function ΩH_{c}, we separate it into $\Omega H_{\mathrm{c}} = \sum_{i=d+1}^{d^2} \Omega H_i$ with $H_{d+i} = \sum_{j=2}^{d} \frac{(p_{1i}-p_{ji})^2}{2}$, $H_{2d+i} = \sum_{j=3}^{d} \frac{(p_{2i}-p_{ji})^2}{2}$, …, $H_{(d-1)d+i} = \frac{(p_{d-1,i}-p_{di})^2}{2}$, $i = 1,2,\ldots,d$. Here we only present the subsystem with Hamiltonian ΩH_{d+1}

$$\begin{cases} \dot{p}_{11} = 0, \\ \dot{p}_{1i} = k_{i1}(\boldsymbol{P}_1)\Omega(p_{11} - p_{21} + p_{11} - p_{31} + \cdots + p_{11} - p_{d1}), \\ \quad i = 2,3,\ldots,d, \\ \dot{p}_{21} = 0, \\ \dot{p}_{2i} = k_{i1}(\boldsymbol{P}_2)\Omega(p_{21} - p_{11}), \quad i = 2,3,\ldots,d, \\ \cdots \\ \dot{p}_{d1} = 0, \\ \dot{p}_{d,i} = k_{i1}(\boldsymbol{P}_d)\Omega(p_{d1} - p_{11}), \quad i = 2,3,\ldots,d. \end{cases} \quad (45)$$

We can find that p_{11}, p_{21}, …, p_{d1} are all constants.

Theorem 3 In the following situation, the above d^2 subsystems can be solved explicitly.

If the form of the matrix $\boldsymbol{K}^{-1}$ is under the variable $\boldsymbol{P} = (p_1, p_2, \ldots, p_d)$ is

$$\boldsymbol{K}^{-1}(\boldsymbol{P}) = \begin{pmatrix} 0 & k_{12}(p_1,p_2) & k_{13}(p_1,p_3) & \ldots & k_{1d}(p_1,p_d) \\ -k_{12}(p_1,p_2) & 0 & k_{23}(p_2,p_3) & \ldots & k_{2d}(p_2,p_d) \\ -k_{13}(p_1,p_3) & -k_{23}(p_2,p_3) & 0 & \ldots & k_{3d}(p_3,p_d) \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ -k_{1d}(p_1,p_d) & -k_{2d}(p_2,p_d) & -k_{3d}(p_3,p_d) & \ldots & 0 \end{pmatrix}, \quad (46)$$

where $\boldsymbol{K}^{-1}(\boldsymbol{P}) = (k_{ij}(p_i,p_j))_{d\times d}$ and there exist continuous functions $F_{ij}(p_i,p_j)$ and $G_{ij}(p_i,p_j)$ such that $\frac{\mathrm{d}F_{ij}(p_i,p_j)}{\mathrm{d}p_i} = \frac{1}{k_{ij}(p_i,p_j)}$ and $\frac{\mathrm{d}G_{ij}(p_i,p_j)}{\mathrm{d}p_j} = \frac{1}{k_{ij}(p_i,p_j)}$ and p_i and p_j can be solved in closed forms from the functions $F_{ij}(p_i,p_j)$ and $G_{ij}(p_i,p_j)$ for any $1 \le i,j \le d, i \ne j$.

Proof For the proof we refer to the details in Ref. [64].

Remark 3 By extending the d dimensional phase space to the d^2 dimensional phase space, whether the subsystems can be solved exactly depends totally on the elements of the skew-symmetric matrix $\boldsymbol{K}^{-1}$.

If all the d^2 subsystems can be solved explicitly, then the first order explicit K-symplectic method can be constructed by composing all the exact solutions. The higher order explicit K-symplectic methods can be constructed by composing the first order K-symplectic method. More specifically, denote the exact solution of each subsystem by $\phi^{\tau}_{H_i}$, $i = 1,2,\ldots,d^2$ and denote τ by the time stepsize, then the first order K-symplectic method Φ_τ is

$$\Phi_\tau = \phi^{\tau}_{H_{d^2}} \circ \phi^{\tau}_{H_{d^2-1}} \circ \ldots \circ \phi^{\tau}_{H_2} \circ \phi^{\tau}_{H_1}. \tag{47}$$

Its adjoint method Φ^*_τ is

$$\Phi^*_\tau = \phi^{\tau}_{H_1} \circ \phi^{\tau}_{H_2} \circ \ldots \circ \phi^{\tau}_{H_{d^2-1}} \circ \phi^{\tau}_{H_{d^2}}. \tag{48}$$

Meanwhile, we can compose Φ_τ to obtain a higher order K-symplectic method

$$\Psi_\tau \equiv \Phi_{\alpha_s\tau} \circ \Phi^*_{\beta_s\tau} \circ \ldots \circ \Phi^*_{\beta_2\tau} \circ \Phi_{\alpha_1\tau} \circ \Phi^*_{\beta_1\tau}, \tag{49}$$

with the coefficients $\alpha_i = \beta_{s+1-i}, 1 \le i \le s$. Here Φ^*_τ is the adjoint method of Φ_τ.

In many real problems, the high dimensional problem can be decoupled into several lower dimensional problems, thus one can solve the lower dimensional problems. For example, the equation for the distribution function f of the Vlasov–Maxwell equations can be rewritten as a $6n$ dimensional Hamiltonian system by expressing f as a sum of Dirac masses[65] and the $6n$ dimensional system can be decoupled into n charged particle systems of 6 dimension.

4. Error analysis

The K-symplectic methods can preserve the K-symplectic structure of the non-canonical Hamiltonian system. Another property of the K-symplectic methods is that they can nearly preserve the Hamiltonian without secular drift over long time. The Hamiltonian of the non-canonical Hamiltonian system is also called the energy of the system. Different from the energy-conserving methods which can exactly preserve the energy,[66–70] the K-symplectic methods only possess near energy conservation property. The near energy conservation property of the K-symplectic methods can be seen from the following theorem. The theory of backward error analysis is the main approach to investigating the long-term behavior of the K-symplectic methods. The main idea of backward error analysis is to view the numerical solution obtained by one numerical method as the exact solution of a new system with a new vector field that is an approximation of the original vector field. More specifically, we assume that a numerical method $G_\tau(\boldsymbol{Z})$ proceeds a series of numerical solution $\boldsymbol{Z}_i$, $i = 1,2,\ldots,m$, where $\boldsymbol{Z}_i$ is the value at the i-th time step. Given a differential equation $\dot{\boldsymbol{Z}} = f(\boldsymbol{Z})$ and the numerical method $G_\tau(\boldsymbol{Z})$, the idea of backward error analysis is to search for a modified equation

$$\dot{\hat{\boldsymbol{Z}}} = f(\hat{\boldsymbol{Z}}) + \tau f_2(\hat{\boldsymbol{Z}}) + \tau^2 f_3(\hat{\boldsymbol{Z}}) + \cdots, \quad \hat{\boldsymbol{Z}} \in \mathbb{R}^{2n}, \tag{50}$$

such that $\boldsymbol{Z}_n = \hat{\boldsymbol{Z}}(n\tau)$ where $\hat{\boldsymbol{Z}}(n\tau)$ is the exact solution of the modified Eq. (50) at time $n\tau$.

Theorem 4 Assume that the numerical method $G_\tau(\boldsymbol{Z})$ applied to the differential equation $\dot{\boldsymbol{Z}} = f(\boldsymbol{Z})$ is of order p, i.e.,

$$G_\tau(\boldsymbol{Z}) = \varphi_\tau(\boldsymbol{Z}) + \tau^{p+1}\delta_{p+1}(\boldsymbol{Z}) + \mathcal{O}(\tau^{p+2}), \tag{51}$$

where $\varphi_\tau(\boldsymbol{Z})$ represents the exact solution of the system $\dot{\boldsymbol{Z}} = f(\boldsymbol{Z})$, and the term $\tau^{p+1}\delta_{p+1}(\boldsymbol{Z})$ is the leading term of the local truncation error, then the modified equation of the method $G_\tau(\boldsymbol{Z})$ satisfies

$$\begin{aligned} &\dot{\hat{\boldsymbol{Z}}} = f(\hat{\boldsymbol{Z}}) + \tau^p f_{p+1}(\hat{\boldsymbol{Z}}) + \tau^{p+1} f_{p+2}(\hat{\boldsymbol{Z}}) + \cdots, \\ &\hat{\boldsymbol{Z}}(0) = \boldsymbol{Z}_0, \end{aligned} \tag{52}$$

with $f_{p+1}(\boldsymbol{Z}) = \delta_{p+1}(\boldsymbol{Z})$.[1]

Proof For the proof, please see the proof of Theorem 1.2 of Chapter IX in Ref. [1].

If the differential equation is a non-canonical Hamiltonian system and the method is a K-symplectic method, then we have the following theorem.

Theorem 5 If the numerical method $G_\tau(\boldsymbol{Z})$ of order p applied to the non-canonical Hamiltonian system (9) is K-symplectic, then its modified equation is also a non-canonical Hamiltonian system with the new Hamiltonian $\hat{H}$. To be specific, for every initial value $\boldsymbol{Z}_0 \in \mathbb{R}^{2n}$, there exists a neighborhood U and smooth functions $H_j : U \to \mathbb{R}$, $j = p+1, p+2, \ldots$ such that the modified equation of the method $G_\tau(\boldsymbol{Z})$ satisfies[1]

$$\begin{aligned} \dot{\hat{\boldsymbol{Z}}} = {} & K^{-1}(\hat{\boldsymbol{Z}})(\nabla H(\hat{\boldsymbol{Z}}) + \tau^p \nabla H_{p+1}(\hat{\boldsymbol{Z}}) \\ & + \tau^{p+1} H_{p+2}(\hat{\boldsymbol{Z}}) + \cdots), \quad \hat{\boldsymbol{Z}} \in U, \end{aligned} \tag{53}$$

the new Hamiltonian $\hat{H} = H + \tau^p H_{p+1} + \tau^{p+1} H_{p+2} + \cdots$ is also called the formal energy of $G_\tau(\boldsymbol{Z})$.

Proof For the proof, please see the proof of Theorem 3.5 of Chapter IX in Ref. [1].

According to Theorem 5, we know that the difference of the Hamiltonian H at two adjoint two steps is

$$H(\boldsymbol{Z}_{n+1}) - H(\boldsymbol{Z}_n) = \hat{H}(\boldsymbol{Z}_{n+1}) - \hat{H}(\boldsymbol{Z}_n) + \mathcal{O}(h^p). \tag{54}$$

As the values $\boldsymbol{Z}_n$ and $\boldsymbol{Z}_{n+1}$ calculated by the K-symplectic method $G_\tau(\boldsymbol{Z})$ are the exact solutions of the modified Eq. (53), together with the fact that the Hamiltonian is exactly preserved by the exact solution, then we know that $\hat{H}(\boldsymbol{Z}_{n+1}) = \hat{H}(\boldsymbol{Z}_n)$. Therefore, we obtain that $H(\boldsymbol{Z}_{n+1}) - H(\boldsymbol{Z}_n) = \mathcal{O}(h^p)$.

The near energy conservation property of the K-symplectic methods is explained above. But for the K-symplectic method of the non-canonical Hamiltonian system (20) or (43) with a control parameter Ω whose value might be big, we should further explore the relationship between the difference of the two Hamiltonians $\hat{H} - \bar{H}$ and the parameter Ω. So, we want to quantify the magnitude of the leading term H_{p+1} in the formal energy $\hat{H}$ for the p-th order K-symplectic method of the extended phase space Hamiltonian. Take the first order K-symplectic method $\Phi_\tau = \phi^\tau_{\Omega H_C^2} \circ \phi^\tau_{\Omega H_C^1} \circ \phi^\tau_{H_B} \circ \phi^\tau_{H_A}$ in Section 2 as an example, then according to Theorem 5, the formal energy of Φ_τ is $\hat{H} = H + hH_2 + h^2 H_3 + \cdots$. Denote the Lie derivatives of the subsystems with $\bar{\boldsymbol{K}}\nabla H_A$, $\bar{\boldsymbol{K}}\nabla H_B$, $\bar{\boldsymbol{K}}\Omega\nabla H_C^1$, and $\bar{\boldsymbol{K}}\Omega\nabla H_C^2$ by D_{H_A}, D_{H_B}, $D_{H_C^1}$, and $D_{H_C^2}$, respectively, then we have[1]

$$\Phi_\tau = \exp(\tau D_{H_A})\exp(\tau D_{H_B})\exp(\tau D_{H_C^1})\exp(\tau D_{H_C^2})I_d. \quad (55)$$

By using the BCH formula, we can get

$$\Phi_h = \exp(\tau \tilde{D})I_d, \quad (56)$$

where

$$\begin{aligned}\tilde{D} \;=\; & D_{H_A} + D_{H_B} + D_{H_C^1} + D_{H_C^2} \\ & + \tau\Big(\frac{1}{2}[D_{H_A}, D_{H_B}] + \frac{1}{2}[D_{H_A}, D_{H_C^1}] \\ & + \frac{1}{2}[D_{H_B}, D_{H_C^1}] + \frac{1}{2}[D_{H_A}, D_{H_C^2}] + \frac{1}{2}[D_{H_B}, D_{H_C^2}] \\ & + \frac{1}{2}[D_{H_C^1}, D_{H_C^2}]\Big) + \tau^2\tilde{H}_2 + \tau^3\tilde{H}_3 + \cdots. \end{aligned} \quad (57)$$

The Lie bracket is defined by

$$[D_1, D_2] = D_1 D_2 - D_2 D_1. \quad (58)$$

According to the Lemma 3.1 in the Ref. [1], if D_{H_A} and D_{H_B} are Lie derivatives of $\bar{\boldsymbol{K}}\nabla H_A$ and $\bar{\boldsymbol{K}}\nabla H_B$, respectively, then $[D_{H_A}, D_{H_B}]$ is the Lie bracket of $\bar{\boldsymbol{K}}\nabla\{H_B, H_A\}$ where $\{H_B, H_A\}$ is a Poisson bracket defined by $\nabla H_B^\top \bar{\boldsymbol{K}}\nabla H_A$. Thus, we can know that the second term H_2 in the modified equation is

$$\begin{aligned} H_2 \;=\; & \frac{1}{2}\{H_B, H_A\} + \frac{1}{2}\Omega\{H_C^1, H_A\} \\ & + \frac{1}{2}\Omega\{H_C^1, H_B\} + \frac{1}{2}\Omega\{H_C^2, H_A\} \\ & + \frac{1}{2}\Omega\{H_C^2, H_B\} + \frac{1}{2}\Omega^2\{H_C^2, H_C^1\}. \end{aligned} \quad (59)$$

Therefore, we know that H_2 is the sum of some Poisson brackets containing two Hamiltonians. Then we can obtain that if the K-symplectic method is of order p, the second term H_{p+1} in the modified Eq. (53) is the sum of some terms of p nested Poisson brackets containing $p+1$ Hamiltonians.

For the first order method Φ_τ, we assume that $\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{x}, \boldsymbol{y}$ and H_2 are bounded, and the Hamiltonian $\hat{H}$ of the modified equation is conserved by the K-symplectic methods, thus ΩH_c is bounded. As a result, we know that $\| \boldsymbol{p} - \boldsymbol{x} \| = \mathcal{O}(1/\sqrt{\Omega})$ and $\| \boldsymbol{q} - \boldsymbol{y} \| = \mathcal{O}(1/\sqrt{\Omega})$. Thus, we obtain that

$$\nabla H_C^1 = \mathcal{O}(1/\sqrt{\Omega}), \quad \nabla H_C^2 = \mathcal{O}(1/\sqrt{\Omega}). \quad (60)$$

Therefore, we know that H_2 of the first order K-symplectic method Φ_h is of magnitude Ω, i.e., the difference between $\bar{H}$ and the formal energy $\hat{H}$ of the first order K-symplectic method Φ_τ is

$$\hat{H} - \bar{H} = \mathcal{O}(\tau\Omega). \quad (61)$$

In a similar way, we can prove that the difference between $\bar{H}$ and the formal energy $\hat{H}$ of the p-th order K-symplectic method is

$$\hat{H} - \bar{H} = \mathcal{O}(\tau^p \Omega^{(p+1)/2}), \quad (62)$$

because the p nested Poisson brackets contains the $p+1$ Hamiltonians, and the total number of ΩH_C^1 or ΩH_C^2 that appeared in the Poisson brackets is at most $p+1$. According to the above analysis, we know that the formal energy $\hat{H}$ of the p-th order K-symplectic method provides an approximation to the extended phase space Hamiltonian $\bar{H}$. Thus the time stepsize constraint is $\tau \ll \Omega^{-\frac{p+1}{2p}}$. The energy error analysis of the K-symplectic method for the general nonseparable system in Section 3 is similar.

The above error analysis is a rough error estimate, the true error bound may be even smaller. But the error bound provides a constraint on the time stepsize.

5. Numerical experiments

5.1. Numerical methods

To demonstrate the superiority in the structure preservation and efficiency of the K-symplectic methods, we compare them with higher order Runge–Kutta methods, the implicit symplectic methods, the explicit and implicit symplectic methods for the original nonseparable noncanonical Hamiltonians, several other fourth order explicit K-symplectic methods for the extended phase space Hamiltonians, and several fourth order extended phase space K-symplectic-like methods with the midpoint permutation. Denote Φ_τ by the first order K-symplectic method composed by the exact solution of all subsystems which is defined in Eqs. (34) and (47).

2ndKSYM: the second order K-symplectic method for the extended non-canonical Hamiltonian system, which is the composition of Φ_τ and its adjoint method is Φ_τ^*[63]

$$\Psi_\tau^2 \equiv \Phi^*_{\tau/2} \circ \Phi_{\tau/2}. \quad (63)$$

4thKSYM: the fourth order K-symplectic method for the extended non-canonical Hamiltonian system, which is composed by[71]

$$\Psi_\tau^4 \equiv \Phi_{\alpha_5\tau} \circ \Phi^*_{\beta_5\tau} \circ \ldots \circ \Phi^*_{\beta_2\tau} \circ \Phi_{\alpha_1\tau} \circ \Phi^*_{\beta_1\tau}. \tag{64}$$

The values of the parameters $\alpha_1, \beta_1, \ldots, \alpha_5, \beta_5$ are given as follows:

$$\beta_1 = \alpha_5 = \frac{14-\sqrt{19}}{108}, \quad \alpha_1 = \beta_5 = \frac{146+5\sqrt{19}}{540}, \tag{65}$$

$$\beta_2 = \alpha_4 = \frac{-23-20\sqrt{19}}{270},$$

$$\alpha_2 = \beta_4 = \frac{-2+10\sqrt{19}}{135}, \quad \beta_3 = \alpha_3 = \frac{1}{5}. \tag{66}$$

According to Remark 1, we can prove that both the 2ndKSYM method and the 4thKSYM method are K-symplectic methods. It should be noticed that both the 2ndKSYM method and the 4thKSYM method are not applied to the original non-canonical Hamiltonian system, thus they are not K-symplectic in the original system.

3rdRK: the third-order explicit Runge–Kutta method (Heun method).[72] It can be applied to both the extended non-canonical Hamiltonian system and the original non-canonical Hamiltonian system.

5thRK: the explicit Runge–Kutta method with effective order 5 (Butcher method).[62,72] It can be applied to both the extended non-canonical Hamiltonian system and the original non-canonical Hamiltonian system.

2ndMIDP: the second-order implicit midpoint rule[27,28] for the original non-canonical Hamiltonian system (9). This method is symmetric and symplectic for the Hamiltonian systems.

2ndSV: the second-order Stömer–Verlet method[1] for the original non-canonical Hamiltonian system (9). This method is semi-implicit and symmetric. It is also symplectic for the Hamiltonian systems. We denote it by SV_τ^2.

4thBPRK: the optimized fourth-order partitioned Runge–Kutta method for the extended non-canonical Hamiltonian system proposed in Refs. [39,73]. The method is composed by

$$\Gamma_\tau^4 \equiv \Phi_{\alpha_6\tau} \circ \Phi^*_{\beta_6\tau} \circ \ldots \circ \Phi^*_{\beta_2\tau} \circ \Phi_{\alpha_1\tau} \circ \Phi^*_{\beta_1\tau}. \tag{67}$$

The values of the parameters $\alpha_1, \beta_1, \ldots, \alpha_6, \beta_6$ are given as follows:

$$\begin{aligned} \beta_1 &= \alpha_6 = 0.079203696431196, \\ \alpha_1 &= \beta_6 = 0.130311410182166, \\ \beta_2 &= \alpha_5 = 0.222861495867608, \end{aligned} \tag{68}$$

$$\begin{aligned} \alpha_2 &= \beta_5 = -0.366713268047426, \\ \beta_3 &= \alpha_4 = 0.324648188689706, \end{aligned} \tag{69}$$

$$\alpha_3 = \beta_4 = 0.109688477876750. \tag{70}$$

4thBRKN: the optimized fourth-order Runge–Kutta–Nyström method for the extended non-canonical Hamiltonian system proposed in Refs. [39,73]. The method is composed by

$$\Theta_\tau^4 \equiv \Phi_{\alpha_6\tau} \circ \Phi^*_{\beta_6\tau} \circ \ldots \circ \Phi^*_{\beta_2\tau} \circ \Phi_{\alpha_1\tau} \circ \Phi^*_{\beta_1\tau}. \tag{71}$$

The values of the parameters $\alpha_1, \beta_1, \ldots, \alpha_6, \beta_6$ are given as follows:

$$\begin{aligned} \beta_1 &= \alpha_6 = 0.082984406417405, \\ \alpha_1 &= \beta_6 = 0.16231455076687, \end{aligned} \tag{72}$$

$$\begin{aligned} \beta_2 &= \alpha_5 = 0.23399525073150, \\ \alpha_2 &= \beta_5 = 0.37087741497958, \end{aligned} \tag{73}$$

$$\begin{aligned} \beta_3 &= \alpha_4 = -0.40993371990193, \\ \alpha_3 &= \beta_4 = 0.059762097006575. \end{aligned} \tag{74}$$

4thYOS: the fourth-order Yoshida's K-symplectic methods for the extended non-canonical Hamiltonian system.[23] The method is composed by

$$\Upsilon_\tau^4 \equiv \Psi^2_{\lambda_3\tau} \circ \Psi^2_{\lambda_2\tau} \circ \Psi^2_{\lambda_1\tau}, \tag{75}$$

where $\lambda_1 = \lambda_3 = \frac{1}{2-2^{1/3}}, \lambda_2 = 1-2\lambda_1$.

4thBPRK–MP: the optimized fourth-order partitioned Runge–Kutta K-symplectic-like method with the midpoint permutation.[52] The midpoint permutation is

$$M: \frac{\boldsymbol{p}+\boldsymbol{x}}{2} \to \boldsymbol{p} = \boldsymbol{x}, \quad \frac{\boldsymbol{q}+\boldsymbol{y}}{2} \to \boldsymbol{q} = \boldsymbol{y}, \tag{76}$$

for the extended system (20) with two copies. Meanwhile, for the extended system (43) with d copies, the midpoint permutation is

$$M: \quad \frac{p_{11}+p_{21}+\cdots+p_{d1}}{d} \to p_{11} = p_{21} = \cdots = p_{d1}, \tag{77}$$

$$\frac{p_{12}+p_{22}+\cdots+p_{d2}}{d} \to p_{12} = p_{22} = \cdots = p_{d2}, \tag{78}$$

$$\vdots$$

$$\frac{p_{1d}+p_{2d}+\cdots+p_{dd}}{d} \to p_{1d} = p_{2d} = \cdots = p_{dd}. \tag{79}$$

The 4thBPRK–MP method is the fourth-order partitioned Runge–Kutta method Γ_τ^4 combined with the midpoint permutation

$$M\Gamma_\tau^4 = M \otimes \Gamma_\tau^4. \tag{80}$$

It should be noticed that for the method 4thBPRK–MP, the midpoint permutation is chosen to control the copies of the variables, thus Ω is no longer needed, therefore $\Omega = 0$ in the method Γ_τ^4.

4thBRKN–MP: the optimized fourth-order Runge–Kutta–Nyström K-symplectic-like method with the midpoint permutation.[52] The 4thBRKN–MP method is the fourth-order Runge–Kutta–Nyström method Θ_τ^4 combined with the midpoint permutation

$$M\Theta_\tau^4 = M \otimes \Theta_\tau^4. \tag{81}$$

It should be noticed that for the method 4thBRKN–MP, the midpoint permutation is chosen to control the copies of the variables, thus $\Omega = 0$ in the method Θ^4_τ.

4thYOS–MP: the fourth-order Yoshida's symplectic-like method with the midpoint permutation.[52] The method is the fourth-order Yoshida's method Υ^4_τ combined with the midpoint permutation

$$M\Upsilon^4_\tau = M \otimes \Upsilon^4_\tau. \tag{82}$$

It should be noticed that for the method 4thYOS–MP, $\Omega = 0$ in the method Υ^4_τ.

4thGAUSS: the fourth order implicit Gauss–Legendre Runge–Kutta symplectic method[1,29,30] for the original non-canonical Hamiltonian system (9). It is symmetric and symplectic for the Hamiltonian systems.

4thSVCOMP: the fourth order method composed by the second-order Stömer–Verlet method for the original non-canonical Hamiltonian system (9). The method is composed by

$$SV^4_\tau \equiv SV^2_{\lambda_3\tau} \circ SV^2_{\lambda_2\tau} \circ SV^2_{\lambda_1\tau}, \tag{83}$$

where $\lambda_1 = \lambda_3 = \frac{1}{2-2^{1/3}}, \lambda_2 = 1 - 2\lambda_1$. It is symmetric and symplectic for the Hamiltonian systems.

We note here the 2ndMIDP, the 2ndSV, the 4thGAUSS, and the 4thSVCOMP are applied to the original non-canonical Hamiltonian system. As they are implicit or semi-implicit methods, the Newton iteration method is used to solve them. The tolerance error for both second order methods is 1×10^{-12} while the tolerance error for both fourth order methods is 1×10^{-15}.

5.2. The first numerical demonstration for Ablowitz–Ladik model

The Ablowitz–Ladik model is one of the space discretization of the nonlinear Schrödinger equation[1,74–76] with the form of

$$\begin{aligned} &\mathrm{i}\dot{W}_k + \frac{1}{h^2}(W_{k+1} - 2W_k + W_{k-1}) \\ &+ |W_k|^2(W_{k+1} + W_{k-1}) = 0, \end{aligned} \tag{84}$$

where the dot represents the derivative with respect to the time t and h is the space stepsize. Under the periodic condition $W_{k+N} = W_k (h = \frac{1}{N})$, it is an integral system. It is well known that the integral system possesses an infinite number of conserved quantities. Nonlinear Schrödinger equation also possesses an infinite number of invariants, such as the charge, the momentum, the energy and so on. We list two of them as follows:

$$D_1 = \int_{-\infty}^{+\infty} |W|^2 \mathrm{d}x, \tag{85}$$

$$D_2 = \int_{-\infty}^{+\infty} \left\{ W \frac{\mathrm{d}\overline{W}}{\mathrm{d}x} - \overline{W} \frac{\mathrm{d}W}{\mathrm{d}x} \right\} \mathrm{d}x, \tag{86}$$

where $\overline{W}$ represents the conjugate of W. After using the central difference formula, the above invariants can be approximated as

$$F_1 = h \sum_{i=1}^{N} W_{l+1} \overline{W}_l, \tag{87}$$

$$F_2 = \sum_{i=1}^{N} (W_l \overline{W}_{l+1} - W_{l+1} \overline{W}_l). \tag{88}$$

We denote FI1 and FR1 as the imaginary and the real part of F_1, respectively. The notations for the invariant F_2 are similar.

By separating the variable W_k into real and imaginary parts, $W_k = u_k + \mathrm{i}v_k$, then we obtain a non-canonical Hamiltonian system with[1]

$$\begin{aligned} \begin{pmatrix} \dot{\boldsymbol{u}} \\ \dot{\boldsymbol{v}} \end{pmatrix} &= \begin{pmatrix} O & -\boldsymbol{D} \\ \boldsymbol{D} & O \end{pmatrix} \begin{pmatrix} \partial_{\boldsymbol{u}} H(\boldsymbol{u}, \boldsymbol{v}) \\ \partial_{\boldsymbol{v}} H(\boldsymbol{u}, \boldsymbol{v}) \end{pmatrix} \\ &= \boldsymbol{K}^{-1}(\boldsymbol{u}, \boldsymbol{v}) \nabla H(\boldsymbol{u}, \boldsymbol{v}), \end{aligned} \tag{89}$$

where $\boldsymbol{u} = (u_1, \ldots, u_N)$, $\boldsymbol{v} = (v_1, \ldots, v_n)$, $\boldsymbol{D} = \mathrm{diag}(d_1, d_2, \ldots, d_N)$ is a diagonal matrix with the elements

$$d_k(\boldsymbol{u}, \boldsymbol{v}) = 1 + h^2(u_k^2 + v_k^2), \quad k = 1, 2 \ldots, N, \tag{90}$$

and the Hamiltonian is

$$\begin{aligned} H(\boldsymbol{u}, \boldsymbol{v}) \ = \ & \frac{1}{h^2} \sum_{i=1}^{N} (u_i u_{i-1} + v_i v_{i-1}) \\ & - \frac{1}{h^4} \sum_{i=1}^{N} \ln(1 + h^2(u_i^2 + v_i^2)). \end{aligned} \tag{91}$$

It should be noticed that the pair of variables (u_i, v_i) is not a pair of canonical variables. We can easily prove that the matrix $\boldsymbol{K}^{-1}(\boldsymbol{u}, \boldsymbol{v})$ appeared in the system (89) is anti-symmetric, nonsingular, and satisfies the Jacobi-identity, therefore this matrix is a $\boldsymbol{K}$ matrix. As a result, the system (89) is a non-canonical Hamiltonian system. It can also be seen that the matrix $\boldsymbol{K}^{-1}$ satisfies the requirements in Theorem 1. Thus, we extend the phase space and make the two copies of $(\boldsymbol{u}, \boldsymbol{v})$.

We take $N = 4$ and denote the two copies of $(\boldsymbol{u}, \boldsymbol{v})$ by $\boldsymbol{P} = (p_1, p_2, \ldots, p_8)$ and $\boldsymbol{Q} = (q_1, q_2, \ldots, q_8)$. Thus we consider the augmented Hamiltonian

$$\bar{H} := H_1 + H_2 + \Omega H_{\mathrm{c}}, \tag{92}$$

where

$$H_1 := H(p_1, \ldots, p_4, q_5, \ldots, q_8), \tag{93}$$

$$H_2 := H(q_1, \ldots, q_4, p_5, \ldots, p_8), \tag{94}$$

$$H_{\mathrm{c}} = \frac{\| \boldsymbol{P} - \boldsymbol{Q} \|_2^2}{2} = \sum_{i=1}^{8} \frac{(p_i - q_i)^2}{2}. \tag{95}$$

Then the augmented Hamiltonian is separated into 10 subsystems, with H_1, H_2, and $H_{j+2} = \frac{(p_i - q_i)^2}{2}$, $j = 1, 2, \ldots, 8$. Here we only present the exact solution of the first subsystem with the Hamiltonian H_1

$$\begin{cases} p_i = p_{i0}, & i = 1,2,3,4, \\ p_j = \dfrac{\sqrt{1+h^2p_{j-4,0}^2}}{h}\tan\left(th\dfrac{\partial H_1}{\partial p_{j-4,0}}\sqrt{1+h^2p_{j-4,0}^2}+\arctan\left(\dfrac{hp_{j0}}{\sqrt{1+h^2p_{j-4,0}^2}}\right)\right), & j = 5,6,7,8, \\ q_j = \dfrac{\sqrt{1+h^2q_{j+4,0}^2}}{h}\tan\left(-th\dfrac{\partial H_1}{\partial q_{j+4,0}}\sqrt{1+h^2q_{j+4,0}^2}+\arctan\left(\dfrac{hq_{j0}}{\sqrt{1+h^2q_{j+4,0}^2}}\right)\right), & i = 1,2,3,4, \\ q_i = q_{i0}, & i = 5,6,7,8, \end{cases} \tag{96}$$

where h is the space stepsize and p_{i0}, q_{i0} are the initial values of p_i, q_i. As the Hamiltonian H_1 is the function of constants $p_{i0}, q_{i+4,0}$, $i = 1,2,3,4$, therefore their partial derivatives with respect to its arguments are all constants. The others subsystems can also be solved explicitly, therefore the explicit K-symplectic methods can be constructed by composing the exact solution of all the subsystems.

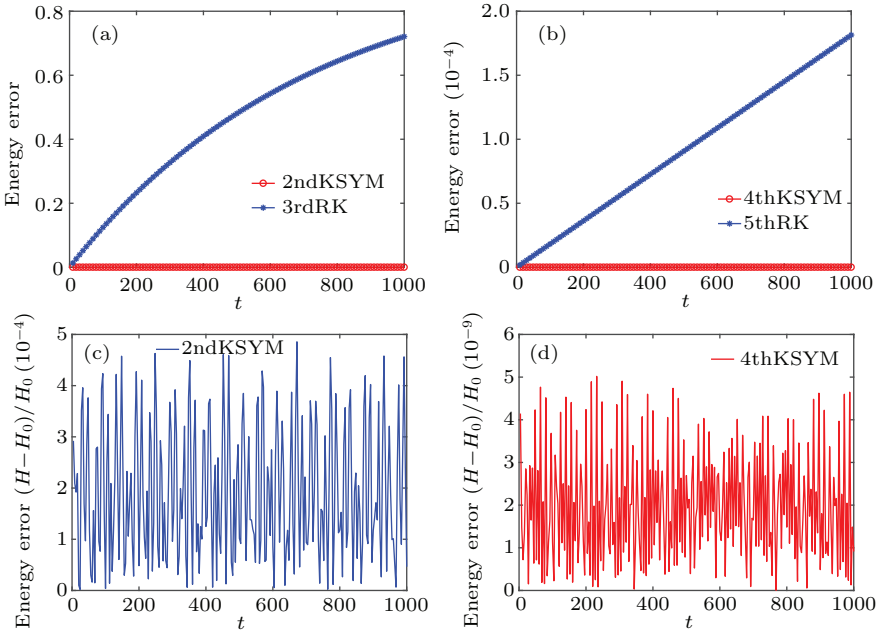


Fig. 1. The energy evolutions of the 2ndKSYM method, the 3rdRK method, the 4thKSYM method, and the 5thRK method. Subfigures (a) and (b) display the relative energy error of the augmented Hamiltonian $\tilde{H}$ for the four methods with $\Omega = 20$ and the time stepsize $\tau = 0.001$. In the first two subfigures the energy error is represented by $|\tilde{H}-\tilde{H}_0|/|\tilde{H}_0|$. Subfigures (c) and (d) display the relative energy error of the original Hamiltonian H with $\Omega = 20$ and $\tau = 0.001$. In the last two subfigures the energy error is represented by $|H-H_0|/|H_0|$.

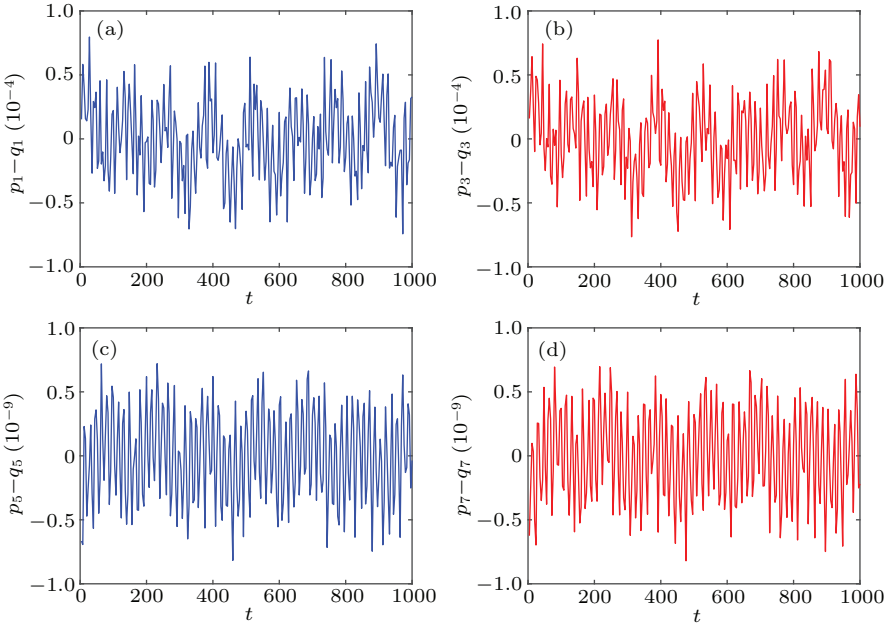


Fig. 2. The difference between the two copies for the four variables u_1, u_3, v_1, and v_3. Subfigures (a) and (b) display the differences between the two copies for the variables u_1 and u_3 obtained by the 2ndKSYM method. Subfigures (c) and (d) display the differences between the two copies for the variables v_1 and v_3 obtained by the 4thKSYM method. Here the time stepsize is $\tau = 0.001$ and $\Omega = 20$, the final time is $T = 1000$.

The initial condition is $u_{10} = 0.2$, $u_{20} = 0.4$, $u_{30} = 0.3$, $u_{40} = 0.5$, $v_{10} = 0.3$, $v_{20} = 0.2$, $v_{30} = 0.3$, $v_{40} = 0.2$. The two copies of the variable $(\boldsymbol{u}, \boldsymbol{v})$ have the same initial condition. The energy evolutions of the augmented Hamiltonian $\bar{H}$ obtained by the 2ndKSYM, 4thKSYM, 3rdRK, and 5thRK methods are displayed in Fig. 1. The energy errors of the K-symplectic methods oscillate with small amplitudes while the energy errors of the Runge–Kutta methods increase without bound as can be seen from Fig. 1. The explicit K-symplectic methods have shown their significant advantages in energy conservation over long-term simulation compared with the higher order Runge–Kutta methods. The energy errors of the original Hamiltonian $H(p_1, \ldots, p_8)$ in the first copy of variables obtained by the two explicit K-symplectic methods are also shown in Fig. 1. As can be seen from Fig. 1 that the energy errors can be bounded at very small intervals. This shows that the explicit K-symplectic methods can also preserve the original Hamiltonian over long time. The two copies of the variable $(\boldsymbol{u}, \boldsymbol{v})$ are also compared. We show the differences between the two copies of u_1, u_3, v_1, v_3 in Fig. 2. The errors in the two copies of u_1, u_3, v_1, v_3 obtained by the two explicit K-symplectic methods are all bounded by small numbers. We display the evolutions of the invariants FI1 and FI2 obtained by the 2ndKSYM method and the 4thKSYM method in Fig. 3. As can be seen from Fig. 3 that the imaginary part of the invariants F_1 and F_2 are both bounded well over long time.

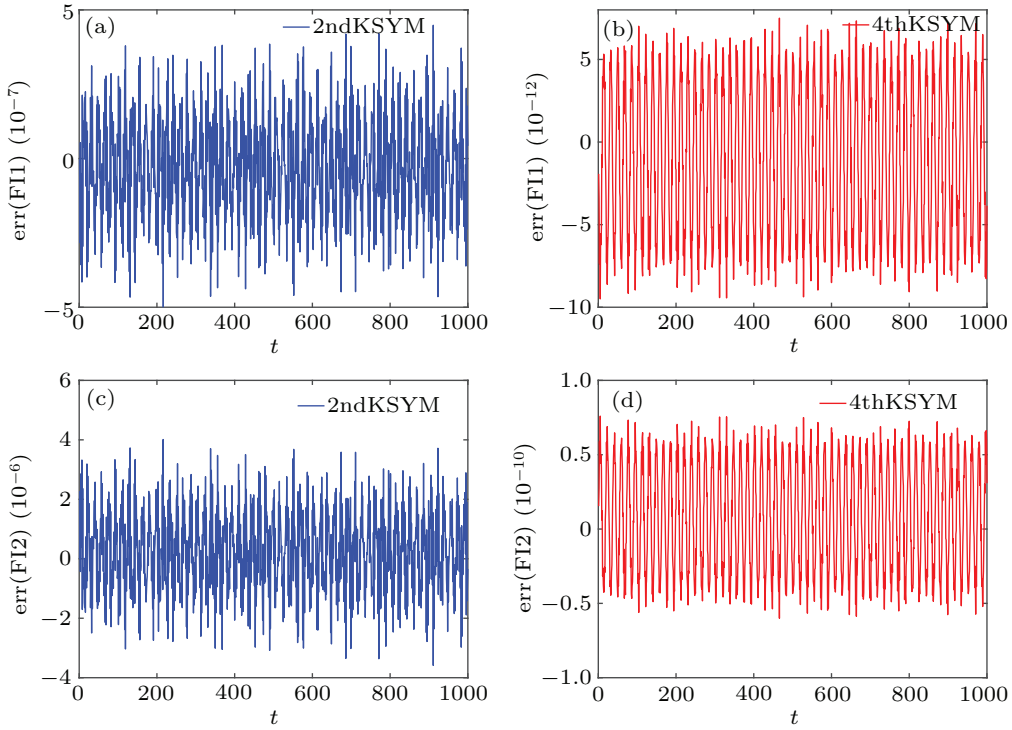


Fig. 3. The errors of the invariant FI1 and FI2 obtain by the 2ndKSYM and 4thKSYM methods. The initial value is the two copies of $(0.2, 0.4, 0.3, 0.5, 0.3, 0.2, 0.3, 0.2)$, the time stepsize $\tau = 0.001$, $\Omega = 20$. The error means the difference between the value at each time step and the value at the initial step.

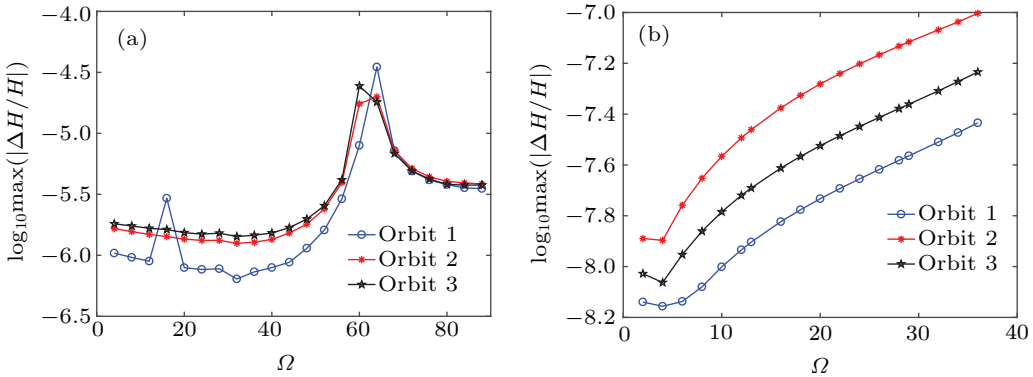


Fig. 4. Dependence of the maximal relative energy error on the parameter Ω for the 2ndKSYM method and the 4thBRKN method solving orbits 1, 2, and 3. In subfigure (a), the initial values for orbit 1, 2, and 3 are two copies of (0.3,0.5,0.1,0.6,0.2,0.3,0.5,0.1), (0.8,0.5,0.6,0.3,0.1,0.4,0.2,0.7), and (0.9,0.5,0.6,0.3,0.2,0.4,0.2,0.7). In subfigure (b), the initial values for orbit 1, 2 and 3 are two copies of (0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8), (0.2,0.2,0.3,0.4,0.6,0.7,0.8,0.9), and (0.6,0.7,0.8,0.9,0.1,0.2,0.3,0.4). Obviously, in subfigure (a) $\Omega = 32$ is an appropriate choice while in subfigure (b) $\Omega = 4$ is an appropriate choice.

As the control parameter Ω is dependent on the algorithms and the initial conditions. We plot the dependence of the maximal relative energy error on the parameter Ω for both the 2ndKSYM method and the 4thBRKN method when solving three orbits in Fig. 4. The three orbits correspond to three different initial conditions. It is shown in Fig. 4(a) that $\Omega = 32$ is an appropriate choice for the 2ndKSYM method. Thus, one of the initial condition in Fig. 4(a) and the chosen Ω are used to compare the computational efficiency of the 2ndKSYM method, the 2ndMIDP method, and the 2ndSV method. The results are shown in Fig. 5(b). It is also shown in Fig. 4(b) that $\Omega = 4$ is an appropriate choice for the 4thBRKN method. One of the initial condition in Fig. 4(b) and the chosen Ω are used to compare the computational efficiency of all the fourth-order methods and the results are shown in Figs. 5(c) and 5(d).

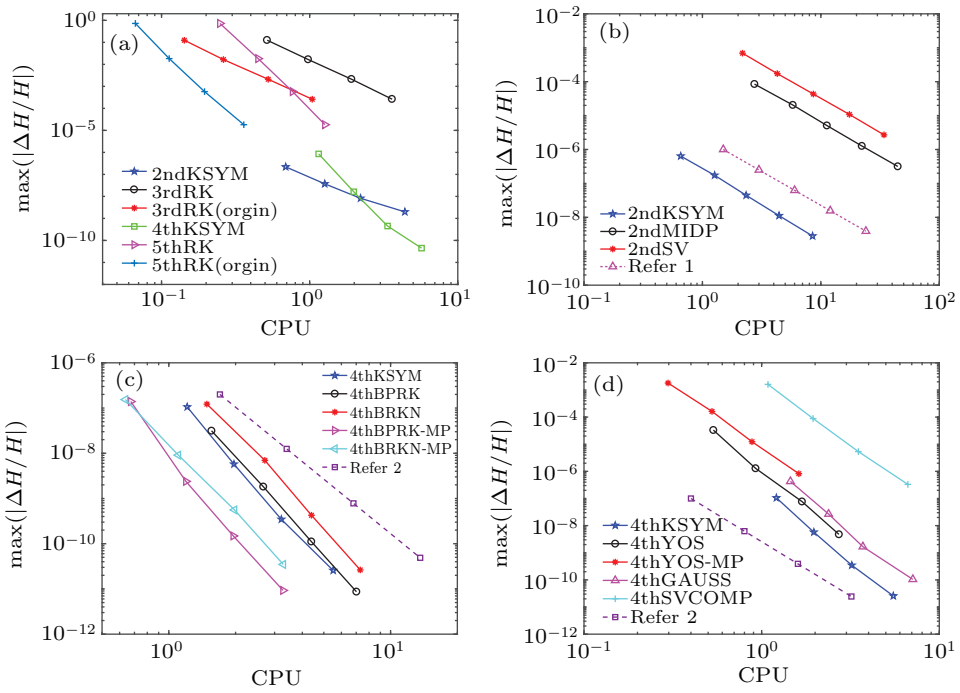


Fig. 5. The log–log plot for the computational efficiency for each method over the interval $[0, T]$. In subfigure (a), the time stepsize τ for the 2ndKSYM and 3rdRK method is $\tau = 0.001/2^i$, $i = 0, 1, 2, 3$, the τ for the 4thKSYM and 5thRK method is $\tau = 0.008/2^i$, $i = 0, 1, 2, 3$, the initial value is $(0.2, 0.4, 0.3, 0.5, 0.3, 0.2, 0.3, 0.2)$, $\Omega = 20$ and $T = 100$. In subfigure (b), the time stepsize τ for the three methods is $\tau = 0.001/2^i$, $i = 0, 1, \ldots, 4$, the initial value is (0.3,0.5,0.1,0.6,0.2,0.3,0.5,0.1), $\Omega = 32$ and $T = 100$. In subfigures (c) and (d), the time stepsize τ for these methods is $\tau = 0.008/2^i$, $i = 0, 1, 2, 3$, the initial value is (0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8), $\Omega = 4$ and $T = 100$.

Figure 5 shows the computational efficiency of all the methods listed in the Subsection 5.1. Figure 5(a) displays the computational efficiency of the 2ndKSYM, the 4thKSYM, the 3rdRK, and the 5thRK method. It is shown that under the time stepsize $\tau = 0.001$, the energy error of the 2ndKSYM method is about six orders of magnitude smaller than that of the 3rdRK method. Under all the stepsizes, the energy errors of the 2ndKSYM method are much smaller than those of the 3rdRK method. The CPU time of the 2ndKSYM method is a bit bigger than that of the 3rdRK method applied to the extended non-canonical Hamiltonian system. The energy errors of the 3rdRK method applied to the original system and the extended system are nearly the same, while the CPU time of the 3rdRK method applied to the original system is less. It can also be seen that the energy errors of the 4thKSYM method are also much smaller than those of the 5thRK method under all the stepsizes. The reason why the energy error of the 2ndKSYM method at the top point is less than that of the 4thKSYM method at the top point is that the time stepsize for the 2ndKSYM method is much less. And the reason why we choose larger stepsizes for the 4thKSYM method is to clearly show the order of the method. Figure 5(a) shows that the K-symplectic methods exhibit much better energy behavior than the higher order Runge–Kutta methods. Figure 5(b) shows the computational efficiency for the three second order methods. One method is said to be more efficient than the other method if it takes less CPU time to obtain the same order magnitude of error. As is shown in Fig. 5(b) that to obtain the same energy error, like 10^{-6}, the CPU time of the 2ndKSYM method is much less than those of the 2ndMIDP and the 2ndSV methods. This shows that the 2ndKSYM method is more efficient than the 2ndMIDP method and the 2ndSV method. The computational efficiency of all the fourth-order methods are displayed in Figs. 5(c) and 5(d). As can be seen from Fig. 5(c) that although the energy error of the 4thKSYM method is larger than that of the 4thBPRK method at the same

stepsize, but to obtain the same order magnitude of energy error, the CPU time of the 4thKSYM method is less than that of the 4thBPRK method. This shows that the 4thKSYM method is more efficient than the 4thBPRK method. The energy error of the 4thKSYM method is nearly the same as that of the 4thBRKN method, but its CPU time is less than that of the 4thBRKN method. This also exhibits that the 4thKSYM method is more efficient than the 4thBPRK method. When we compare the 4thKSYM method with the 4thBPRK–MP method and the 4thBRKN–MP method, the CPU time of the 4thKSYM method is larger than those of the two methods, but the energy error of the 4thKSYM method is slightly small. The reason why the 4thKSYM method takes more CPU time is that the number of subsystems is two times of the 4thBPRK–MP and the 4thBRKN–MP methods. Displayed in Fig. 5(d) is the comparison between the 4thKSYM method and the others fourth order methods. As can be seen from Fig. 5(d) that the 4thKSYM method can not only obtain less energy error, but also take less CPU time than the 4thGAUSS, the 4thYOS, the 4thYOS–MP, and 4thSVCOMP methods. This shows that the 4thKSYM method exhibits much better efficiency than the others four methods.

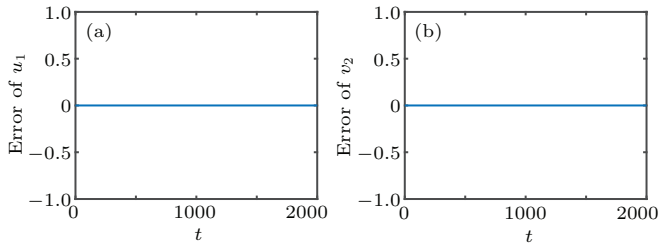


Fig. 6. The error of variables u_1 and v_2 between solution in the original phase space and that in the extended phase space. The initial value is (0.2,0.4,0.3,0.5,0.3,0.2,0.3,0.2) and $\Omega = 20$. Subfigure (a) displays the error between the original u_1 and the first copy of u_1, subfigure (b) displays the error between the original v_2 and the second copy of v_2.

We also plot the errors between the solution in the original phase space and that in the extended phase space in Fig. 6. The initial value of the extended system is the two copies of the original ones. The both solutions are calculated by using the ode45 function in Matlab. The relative tolerance and the absolute tolerance are set to be 10^{-12} and 10^{-12}, respectively. As can be seen from Fig. 6 that there is no difference between the solution in the original phase space and that in the extended phase space for the Ablowitz–Ladik model.

5.3. The second numerical demonstration for gyrocenter system

Gyrocenter system[8–10] plays a fundamental role in plasma physics research. Many neoclassical phenomena in tokamak experiments, such as the bootstrap current, are underlied by gyrocenter dynamics. As is mentioned above, the gyrocenter motion is obtained by averaging out the fast gyromotion from the charged particle dynamics. It is a non-canonical Hamiltonian system

$$\dot{\boldsymbol{Z}} = \boldsymbol{K}^{-1}(\boldsymbol{Z})\nabla H(\boldsymbol{Z}), \quad \boldsymbol{Z} = (x,y,z,u)^{\top}, \tag{97}$$

with the Hamiltonian $H = \frac{1}{2}u^2 + \mu|B(\boldsymbol{X})| + \varphi(\boldsymbol{X})$ and

$$\boldsymbol{K}^{-1}(\boldsymbol{Z}) = \frac{1}{a_{12}b_3 - a_{13}b_2 + a_{23}b_1} \times \begin{pmatrix} 0 & -b_3 & b_2 & a_{23} \\ b_3 & 0 & -b_1 & -a_{13} \\ -b_2 & b_1 & 0 & a_{12} \\ -a_{23} & a_{13} & -a_{12} & 0 \end{pmatrix}. \tag{98}$$

Given a vector potential $\boldsymbol{A}(\boldsymbol{X}) = (f,g,h)^{\top}$, the magnetic field is $\boldsymbol{B}(\boldsymbol{X}) = \nabla \times \boldsymbol{A}(\boldsymbol{X})$, $\boldsymbol{b}(\boldsymbol{X}) = (b_1,b_2,b_3)^{\top} = \frac{\boldsymbol{B}(\boldsymbol{X})}{|\boldsymbol{B}(\boldsymbol{X})|}$ and the elements in $\boldsymbol{K}^{-1}(\boldsymbol{Z})$ are

$$a_{12} = g_x - f_y + u\left(\frac{\partial b_2}{\partial x} - \frac{\partial b_1}{\partial y}\right), \tag{99}$$

$$a_{13} = h_x - f_z + u\left(\frac{\partial b_3}{\partial x} - \frac{\partial b_1}{\partial z}\right), \tag{100}$$

$$a_{23} = h_y - g_z + u\left(\frac{\partial b_3}{\partial y} - \frac{\partial b_2}{\partial z}\right). \tag{101}$$

We set the magnetic field to $\boldsymbol{B}(\boldsymbol{X}) = (0,0,\sec^2(xy))$. The scalar potential is chosen as $\varphi(\boldsymbol{X}) = 10^{-2}\sqrt{x^2+y^2+z^2}$. As the Hamiltonian is not separable, and the matrix $\boldsymbol{K}^{-1}$ does not have the special structure as (18), thus we make four copies of the phase space (x,y,z,u). Denote the four copies of (x,y,z,u) by $\boldsymbol{P} = (p_1,p_2,p_3,p_4)$, $\boldsymbol{Q} = (q_1,q_2,q_3,q_4)$, $\boldsymbol{R} = (r_1,r_2,r_3,r_4)$, and $\boldsymbol{W} = (w_1,w_2,w_3,w_4)$. The exact solution to the first subsystem with Hamiltonian H_1 can be solved explicitly

$$\begin{cases} p_i = p_{i0}, \quad i = 1,3,4, \\ p_2 = \frac{1}{p_{10}}\arctan\left(\frac{\partial H_1}{\partial p_{10}}p_{10}t + \tan(p_{10}p_{20})\right), \\ q_1 = \frac{1}{q_{20}}\arctan\left(-\frac{\partial H_1}{\partial q_{20}}q_{10}t + \tan(q_{10}q_{20})\right), \\ q_i = q_{i0}, \quad i = 2,3,4, \\ r_i = r_{i0}, \quad i = 1,2,3, \\ r_4 = r_{40} - \frac{\partial H_1}{\partial r_{30}}t, \\ w_i = w_{i0}, \quad i = 1,2,4, \\ w_3 = w_{30} + \frac{\partial H_1}{\partial w_{40}}t, \end{cases} \tag{102}$$

where p_{i0}, q_{i0}, r_{i0}, w_{i0} represent the initial values of p_i, q_i, r_i, w_i for $i = 1,2,3,4$. As the Hamiltonian H_1 is the function of the constants p_1, q_2, r_3, w_4, therefore the partial derivative of H_1 with respect to each argument is also a constant. The others subsystems can also be solved explicitly, thus the explicit K-symplectic methods can be constructed.

The initial condition is $x_0 = 0.003$, $y_0 = 0.002$, $z_0 = 0.004$ and $u_0 = 0.005$. The four copies of the original variables x, y, z, u have the same initial condition. The orbits in $p_1 - p_2$ plane obtained by the 2ndKSYM method and the 3rdRK method are

displayed in Fig. 7. The orbit obtained by the second order K-symplectic method is a closed circle while the orbit obtained by the third order Runge–Kutta method spirals outwards and loses accuracy as can be seen from Fig. 7. The relative energy errors of the augmented Hamiltonian $\bar{H}$ obtained by the four methods are also shown in Fig. 7. The energy errors of the K-symplectic methods can be bounded at small intervals along time while those of the higher order Runge–Kutta methods increase linearly along time. The K-symplectic methods have shown their superiorities in preserving the orbit and the energy over long-term simulation compared with the higher order Runge–Kutta methods. The evolutions of the original H for the two K-symplectic methods are shown in Fig. 8. The energy errors of the two methods oscillate at vey small amplitudes as can be seen from Fig. 8. The explicit K-symplectic methods have the property of preserving the original Hamiltonian over long time. The differences between the four copies in the original variables x, y, z, u are displayed in Fig. 9 and they are all bounded by very small numbers. Displayed in Fig. 10 is the orbits projected on (x,y) plane obtained by the two K-symplectic methods under different magnitudes of electric field $E=-\nabla\varphi$. The phase orbits are all closed ellipses. It can be seen that the orbit obtained by the 4thKSYM method under the $\varphi(\boldsymbol{X})=10^0\sqrt{x^2+y^2+z^2}$ is a bit more accurate than obtained by the 2ndKSYM method. As can be seen from Fig. 10 that the value of y changes rapidly when the electric field turns large. The periods of the orbits are 13.1, 3.4, 1.8, 1.5, and 1.3 when the coefficients in the $\varphi(\boldsymbol{X})$ are 10^{-3}, 10^{-2}, 10^{-1}, $10^{-1/2}$, and 10^0, respectively. This shows that the larger electric field accelerates the motion of the guiding center.

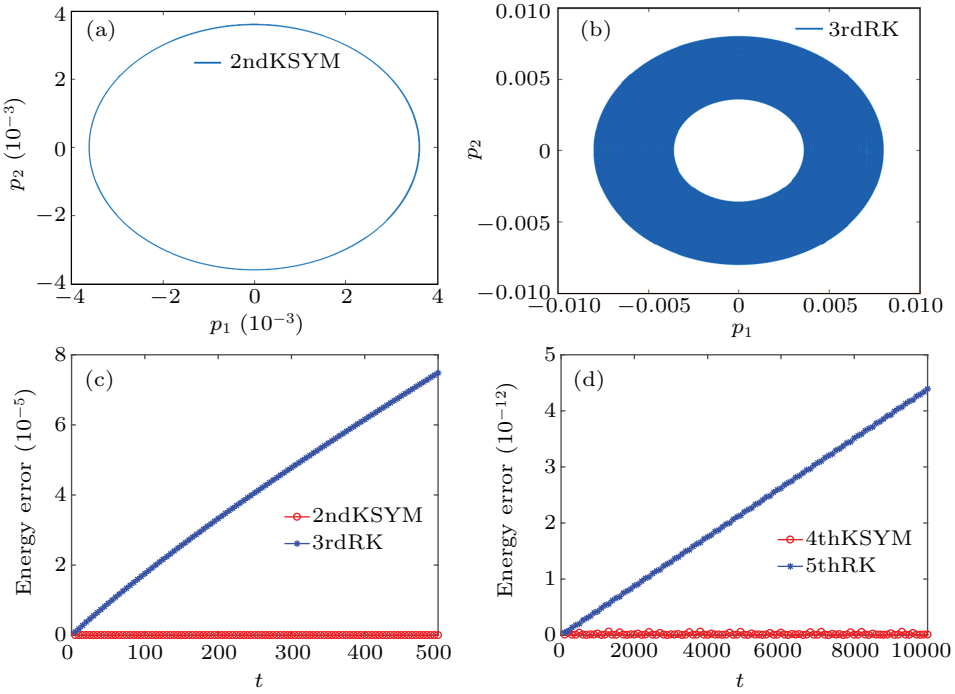


Fig. 7. The phase orbit and the energy error obtained by the 2ndKSYM method, the 3rdRK method, the 4thKSYM method, and the 5thRK method. Subfigures (a) and (b) display the orbit projected to p_1-p_2 plane obtained by the 2ndKSYM method and the 3rdRK method with stepsize $\tau=0.01$, $\Omega=20$ over the time interval $[0,10000]$. Subfigures (c) and (d) display the relative energy error of the augmented Hamiltonian $\bar{H}$ for the four methods with $\Omega=20$. In subfigure (c), the stepsize $\tau=0.01/4$ while in subfigure (d) $\tau=0.01$. The energy error is represented by $|\bar{H}-\bar{H}_0|/|\bar{H}_0|$.

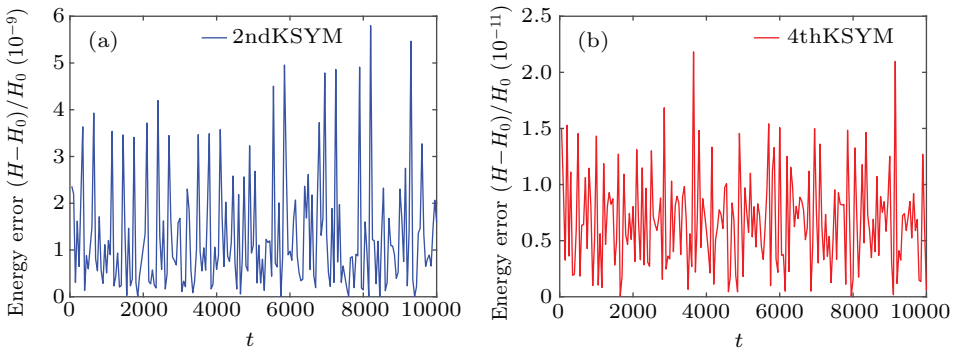


Fig. 8. The relative energy error of the original Hamiltonian $H(p_1,p_2,p_3,p_4)$ obtained by the 2ndKSYM method and the 4thKSYM method. The relative energy error is represented by $(H-H_0)/H_0$. The stepsize is chosen as $\tau=0.01$ and the parameter is $\Omega=20$.

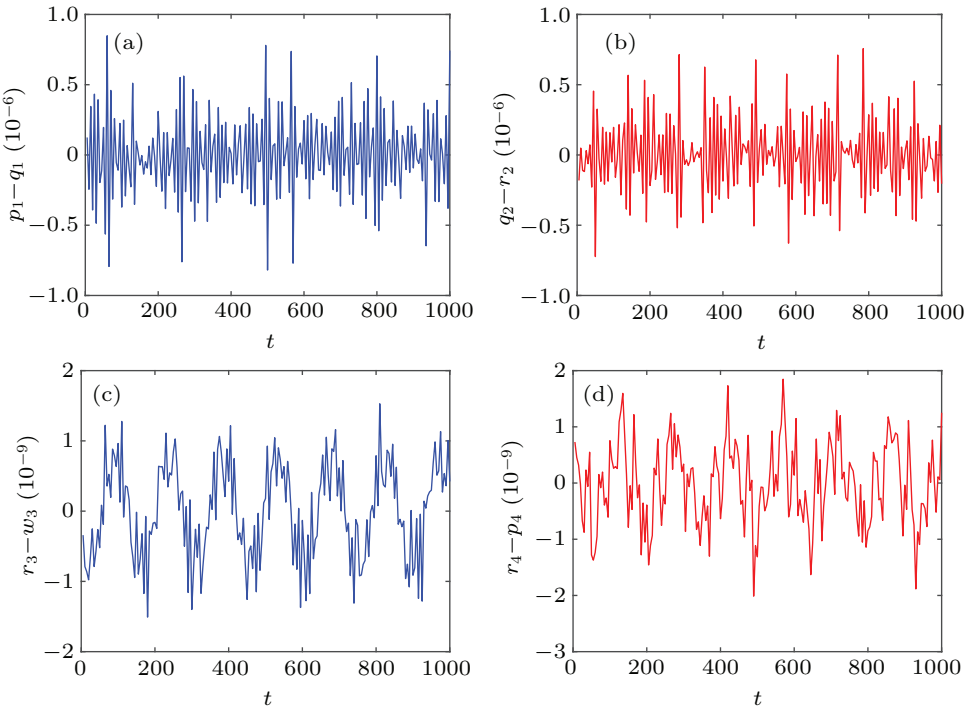


Fig. 9. The difference between the four copies for the four variables. Subfigures (a) and (b) display the differences between the several copies for the variable x and y obtained by the 2ndKSYM method. Subfigures (c) and (d) display the differences between the several copies for z and u obtained by the 4thKSYM method. Here the stepsize is $\tau = 0.01$ and $\Omega = 20$, the final time is $T = 1000$.

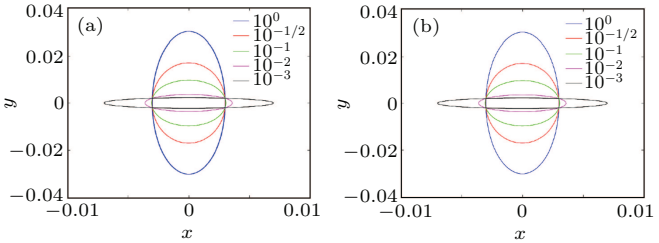


Fig. 10. The phase orbit obtained by the 2ndKSYM and the 4thKSYM methods under different electric field. The initial condition is $(0.003, 0.002, 0.004, 0.005)$, $\Omega = 20$ and $T = 100$. The coefficient in the $\varphi(\boldsymbol{X})$ varies from 10^{-3} to 10^{0}. Subfigure (a) is the result obtained by the 2ndKSYM method while subfigure (b) is the result obtained by the 4thKSYM method.

Figure 11 shows the dependence of the maximal relative energy error on the parameter Ω for the 2ndKSYM method and the 4thBPRK method when solving three orbits. The three orbits correspond to three different initial conditions. It is shown in Fig. 11(a) that the energy error is nearly the same no matter how big the Ω is, thus we choose $\Omega = 18$. One of the initial condition in Fig. 11(a) and the chosen Ω are used to compare the computational efficiency of the 2ndKSYM method, the 2ndMIDP method, and the 2ndSV method and the results are shown in Fig. 12(b). As can be seen from Fig. 11(b) that $\Omega = 6$ is an appropriate choice for the 4thBPRK method. One of the initial condition in Fig. 11(b) and the chosen Ω are used to compare the computational efficiency of all the fourth-order methods and the results are shown in Figs. 12(c) and 12(d).

Figure 12 shows the computational efficiency of all the numerical methods. Figure 12(a) displays the computational efficiency of the 2ndKSYM, the 4thKSYM, the 3rdRK, and the 5thRK method. It is shown that to obtain the same order magnitude of energy error, the CPU time of the 2ndKSYM method is less than that of the 3rdRK method applied to the extended phase space Hamiltonian. Thus the 2ndKSYM method is more efficient than the 3rdRK method applied to the extended phase space Hamiltonian. It can also be seen from Fig. 12(a) that the 4thKSYM method is more efficient than the 5thRK method applied to the extended phase space Hamiltonian. The K-symplectic methods are less efficient than the higher-order Runge–Kutta methods applied to the original non-canonical Hamiltonian system. Figure 12(b) shows the computational efficiency for the three second order methods. As shown in Fig. 12(b) that the energy error of the 2ndMIDP method is less than that of the 2ndKSYM method at each time stepsize. But to obtain the same order magnitude of error, like 10^{-10}, the CPU time of the 2ndKSYM method is less than that of 2ndMIDP method. This exhibits that the 2ndKSYM method is more efficient than the 2ndMIDP method. As shown in Fig. 12(b) that the 2ndKSYM method is more efficient than the 2ndSV method. The computational efficiency of all the fourth order methods are displayed in Figs. 12(c) and 12(d). It can be seen from Fig. 12(c) that the 4thKSYM method is more efficient than the 4thBPRK method and the 4thBRKN method. It is also shown in Fig. 12(c) that both the energy error and the CPU time of the 4thBPRK–MP and the 4thBRKN–MP methods are less than those of 4thKSYM methods. The reason why the 4thKSYM method takes more CPU time is that more subsystems are required to be calcu-

lated. Thus, the 4thBPRK–MP method and the 4thBRKN–MP method are more efficient than the 4thKSYM method. Displayed in Fig. 12(d) is the comparison between the 4thKSYM method and the others fourth order methods. As can be seen from Fig. 12(d) that the 4thKSYM method is more efficient than the 4thGAUSS method and the 4thYOS method. Furthermore, the energy error of the 4thKSYM method is much less than that of the 4thYOS method under the same stepsize. On the other hand, although at the same stepsize, the energy error of the 4thKSYM method is about two orders of magnitude smaller than that of the 4thYOS–MP method, but the CPU time of the 4thKSYM method is nearly four times of the 4thYOS–MP method. This is because the 4thYOS–MP method calculates less subsystems and only need triple composition of Ψ_τ^2. Figure 12(d) also shows that the 4thKSYM method exhibits much better efficiency than the 4thSVCOMP method.

We also plot the errors between the solution in the original phase space and that in the extended phase space in Fig. 13. The initial value of extended system is the four copies of the original ones. The both solutions are calculated by using the ode45 function in Matlab. The relative tolerance and the absolute tolerance are set to be 10^{-12} and 10^{-12}, respectively. Figure 13 shows that the errors in two variables between the solution in the original phase space and that in the extended phase space are bounded by the machine precision.

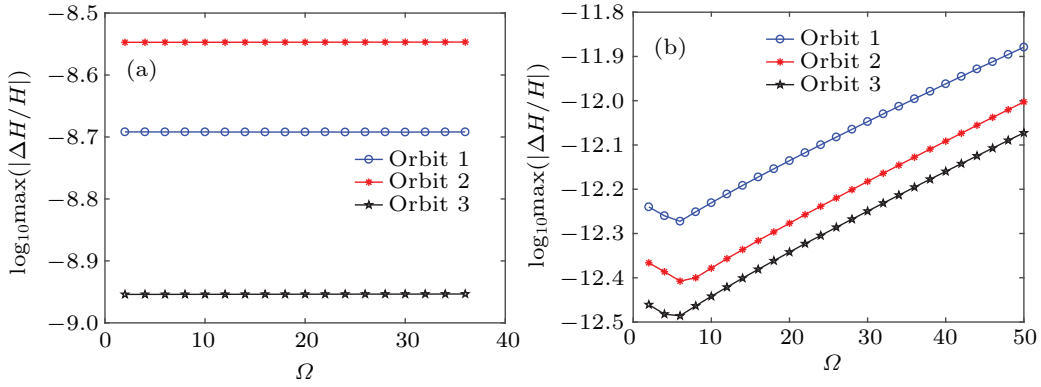


Fig. 11. Dependence of the maximal relative error on the parameter Ω for the 2ndKSYM method and the 4thBPRK method solving orbits 1, 2, and 3. In subfigure (a), the initial values for orbit 1, 2, and 3 are four copies of (0.03,0.05,0.05,0.06), (0.05,0.06,0.05,0.08), and (0.07,0.03,0.02,0.04). In subfigure (b), the initial values for orbit 1, 2, and 3 are four copies of (0.0005,0.0006,0.0005,0.0007), (0.0005,0.0007,0.0005,0.0007), and (0.0006,0.0007,0.0005,0.0008). Obviously, in subfigure (b) $\Omega = 6$ is an appropriate choice.

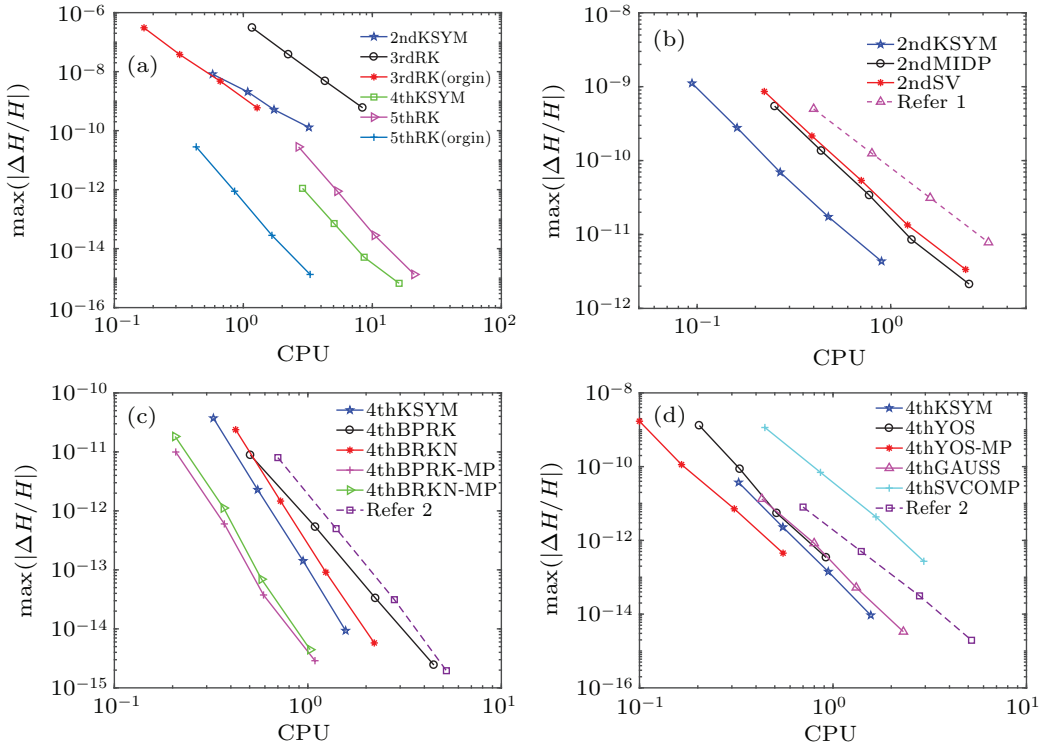


Fig. 12. The log–log plot for the computational efficiency for each method over the interval $[0,T]$. In subfigure (a), the time stepsize τ for the four methods is $\tau = 0.002/2^i$, $i = 0,1,2,3$, the initial value is $(0.003, 0.002, 0.004, 0.005)$, $\Omega = 20$, and $T = 2000$. In subfigure (b), the time stepsize τ for the three methods is $\tau = 0.001/2^i$, $i = 0,1,\ldots,4$, the initial value is (0.07,0.03,0.02,0.04), $\Omega = 18$, and $T = 100$. In subfigures (c) and (d), the time stepsize τ for these methods is $\tau = 0.002/2^i$, $i = 0,1,2,3$, the initial value is (0.0005,0.0006,0.0005,0.0007), $\Omega = 6$, and $T = 100$.

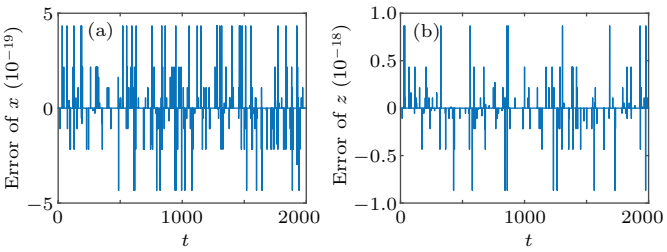


Fig. 13. The error of variables x and z between solution in the original phase space and that in the extended phase space. The initial value is (0.003,0.002,0.004,0.005) and $\Omega = 20$. Subfigure (a) displays the error between the original x and the first copy of x, subfigure (b) displays the error between the original z and the second copy of z.

6. Conclusion

We propose explicit K-symplectic methods for noncanonical Hamiltonian systems with nonseparable Hamiltonian. The idea is to extend the original phase space to several copies of the phase space and to impose a mechanical restraint on the copies of the phase space. Explicit K-symplectic methods have been constructed for two non-separable noncanonical Hamiltonian systems and are compared with higher order explicit Runge–Kutta methods. The numerical results show that the K-symplectic methods have superiority in phase orbit tracking and energy conservation over long-term simulation compared with the higher order Runge–Kutta methods. The differences between the several copies of the variables are also bounded by the K-symplectic methods. The numerical results also show that the 2ndKSYM method is more efficient than the 3rdRK applied to the extended systems, the 2ndMIDP method and the 2ndSV method applied to the original systems. Meanwhile, the 4thKSYM method is more efficient than the 5thRK applied to the extended systems, the 4thBPRK and the 4thBRKN methods for the extended systems and the 4thYOS, the 4thGAUSS, and the 4thSVCOMP methods for the original systems. The energy error of the 4thKSYM method is much less than those of the 4thYOS and the 4thYOS–MP methods under the same time stepsize. The numerical results also show that the 4thKSYM method is less inferior to the 4thBPRK–MP and 4thBRKN–MP in efficiency because less subsystems are required be calculated in the latter two methods, but their energy errors are nearly in the same magnitude. Thus, the 2ndKSYM method and the 4thKSYM method are suitable for long-time simulations of nonseparable noncanonical Hamiltonian systems.

Acknowledgement

Project supported by the National Natural Science Foundation of China (Grant Nos. 11901564 and 12171466).

References

[1] Hairer E, Lubich Ch and Wanner G 2002 *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations* (Berlin Heidelberg: Springer-Verlag)
[2] Brugnano L, Zhang C J and Li D F 2018 *Commun. Nonlinear Sci. Numer. Simulat.* **60** 33
[3] Tang Y F, Pérez-García V and Vázquez L 1997 *Appl. Math. Comput.* **82** 17
[4] Tang Y F, Cao J W, Liu X T and Sun Y C 2007 *J. Phy. A-Math. Theor.* **40** 2425
[5] Vakhnenko O O 2002 *J. Math. Phys.* **43** 2587
[6] He Y, Zhou Z Q, Sun Y J, Liu J and Qin H 2017 *Phys. Lett. A* **381** 568
[7] Zhang R L, Wang Y L, He Y, *et al*. 2018 *Phys. Plasmas* **25** 022117
[8] Littlejohn R 1979 *J. Math. Phys.* **20** 2445
[9] Qin H, Guan X and Tang W 2009 *Phys. Plasmas* **16** 042510
[10] Zhang R L, Liu J, Tang Y F, *et al*. 2014 *Phys. Plasma* **21** 032504
[11] Marsden J and Weinstein A 1982 *Physica D* **4** 394
[12] Morrison P 1980 *Phys. Lett. A* **80** 383
[13] Morrison P and Green J 1980 *Phys. Rev. Lett.* **45** 790
[14] Arnold V 1978 *Mathematical Methods of Classical Mechanics* (Berlin Heidelberg: Springer-Verlag)
[15] Feng K 1995 *Collected Works of Feng Kang (II)* (Beijing: National Defence Industry Press)
[16] Feng K and Qin M Z 2009 *Symplectic Geometric Algorithms for Hamiltonian System* (Berlin Heidelberg: Springer-Verlag)
[17] Sanz-Serna J M and Calvo M P 1994 *Numerical Hamiltonian Problems* (London: Chapman and Hall)
[18] Wang L L and Fu J L 2016 *Chin. Phys. B* **25** 014501
[19] Channell P and Scovel C 1990 *Nonlinearity* **3** 231
[20] Feng K 1985 *Proceedings of 1984 Beijing Symposium on Differential Geometry and Differential Equations* (Beijing: Science Press) pp. 42–58
[21] Forest E and Ruth R 1990 *Physica D* **43** 105
[22] Sanz-Serna J M 1992 *Acta Numer.* **1** 243
[23] Yoshida H 1990 *Phys. Lett. A* **150** 262
[24] Feng K and Wang D L 1991 *J. Comput. Math.* **9** 86
[25] Wang Y, Sun W, Liu F Y and Wu X 2021 *Astrophys. J.* **907** 66
[26] Wu Y L and Wu X 2018 *Int. J. Mod. Phys. C* **29** 1850006
[27] Brown J D 2006 *Phys. Rev. D* **73** 024001
[28] Tsang D, Galley C R, Stein L C and Turner A 2015 *Astrophys. J. Lett.* **809** L9
[29] Kopáček O, Kovář J and Stuchlík Z 2010 *Astrophys. J.* **722** 1240
[30] Seyrich J and Lukes-Gerakopoulos G 2012 *Phys. Rev. D* **86** 124013
[31] Lubich C, Walther B and Brügmann B 2010 *Phys. Rev. D* **81** 104025
[32] Zhong S Y, Wu X, Liu S Q and Deng X F 2010 *Phys. Rev. D* **82** 124040
[33] Mei L J, Wu X and Liu F Y 2013 *Eur. Phys. J. C* **73** 2413
[34] Mei L Y, Ju M J, Wu X and Liu S Q 2013 *Mon. Not. R. Astron. Soc.* **435** 2246
[35] Hairer E and Wanner G 2010 *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems* (Berlin Heidelberg: Springer-Verlag)
[36] Wu X and Xie Y 2010 *Phys. Rev. D* **81** 084045
[37] Yang D Q, Cao W F, Zhou N Y, Zhang H X, Liu W F and Wu X 2022 *Universe* **8** 320
[38] Zhang H X, Zhou N Y, Liu W F and Wu X 2021 *Universe* **7** 488
[39] Zhou N Y, Zhang H X, Liu W F and Wu X 2022 *Astrophys. J.* **927** 160
[40] Wang Y, Sun W, Liu F Y and Wu X 2021 *Astrophys. J.* **909** 22
[41] Wang Y, Sun W, Liu F Y and Wu X 2021 *Astrophys. J. Suppl. S.* **254** 8
[42] Zhang H X, Zhou N Y, Liu W F and Wu X 2022 *Gen. Relat. Gravit.* **54** 110
[43] Sun W, Wang Y, Liu F Y and Wu X 2021 *Eur. Phys. J. C* **81** 785
[44] Sun X, Wu X, Wang Y, Deng C, Liu B R and Liang E W 2021 *Universe* **7** 410
[45] Wu X, Wang Y, Sun W and Liu F Y 2021 *Astrophys. J.* **914** 63
[46] Blanes S and Moan P C 2001 *J. Comput. Phys.* **170** 205
[47] Mclachlan R I and Quispel G 2002 *Acta Numer.* **11** 341
[48] Zhu B B, Zhang R L, Tang Y F, *et al*. 2016 *J. Comput. Phys.* **322** 387
[49] Zhu B B, Zhang R L, Tang Y F and Zhang Y H 2019 *Numer. Algorithms* **81** 1485
[50] Pihajoki P 2015 *Celest. Mech. Dyn. Astr.* **121** 211
[51] Liu L, Wu X, Liu F Y and Huang G Q 2016 *Mon. Not. R. Astron. Soc.* **459** 1968
[52] Luo J J, Wu X, Huang G Q and Liu F Y 2017 *Astrophys. J.* **834** 64
[53] Liu L, Wu X and Huang G Q 2017 *Gen. Relat. Gravit.* **49** 28

[54] Li D and Wu X 2017 *Mon. Not. R. Astron. Soc.* **469** 3031
[55] Li D and Wu X 2019 *Eur. Phys. J. Plus* **134** 96
[56] Pan G F, Wu X and Liang E W 2021 *Phys. Rev. D* **104** 044055
[57] Tao M L 2016 *Phys. Rev. E* **94** 043303
[58] Jayawardana B and Ohsawa T 2023 *Math. Comput.* **92** 251
[59] Ohsawa T 2022 arXiv: 2208.10546
[60] Kaneko Y 2015 *Phys. Plasmas* **22** 092120
[61] Butcher J C 1964 *Math. Comput.* **18** 50
[62] Butcher J C 1969 *Conference on the numerical solution of differential equations, Lecture Notes in Math.*, June 23–27, 1969, Dundee, Scotland, pp. 133–139
[63] Strang G 1968 *Siam J. Numer. Anal.* **5** 506
[64] Zhu B B, Ji L, Zhu A Q and Tang Y F 2022 *Commun. Comput. Phys.* **32** 1129
[65] He Y, Sun Y J, Qin H and Liu J 2016 *Phys. Plasmas* **23** 092108
[66] Bacchini F, Ripperda B, Chen A Y and Sironi L 2018 *Astrophys. J. Suppl. S.* **237** 6
[67] Hu S Y, Wu X, Huang G Q and Liang E W 2019 *Astrophys. J.* **887** 191
[68] Hu S Y, Wu X and Liang E W 2021 *Astrophys. J. Suppl. S.* **253** 55
[69] Hu S Y, Wu X and Liang E W 2021 *Astrophys. J. Suppl. S.* **257** 40
[70] Zhang H, Song S H, Chen X D and Zhou W E 2014 *Chin. Phys. B* **23** 070208
[71] McLachlan R I 1995 *SIAM J. Sci. Comput.* **16** 151
[72] Hairer E, Nørsett S P and Wanner G 1987 *Solving Ordinary Differential Equation I: Nonstiff Problems* (Berlin Heidelberg: Springer-Verlag)
[73] Blanes S and Moan P C 2002 *J. Comput. Appl. Math.* **142** 313
[74] Liu G T 2006 *Chin. Phys.* **15** 2500
[75] Zheng C L, Zhang J F, Sheng Z M and Huang W H 2003 *Chin. Phys.* **12** 11
[76] Fu H, Zhou W E, Qian X, Song S H and Zhang L Y 2016 *Chin. Phys. B* **25** 110201