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Explicit K-Symplectic and Symplectic-like Methods for Charged Particle System in General Magnetic Field

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Abstract: We propose explicit K-symplectic and explicit symplectic-like methods for the charged particle system in a general strong magnetic field. The K-symplectic methods are also symmetric. The charged particle system can be expressed both in a canonical and a non-canonical Hamiltonian system. If the three components of the magnetic field can be integrated in closed forms, we construct explicit K-symplectic methods for the non-canonical charged particle system; otherwise, explicit symplectic-like methods can be constructed for the canonical charged particle system. The symplectic-like methods are constructed by extending the original phase space and obtaining the augmented separable Hamiltonian, and then by using the splitting method and the midpoint permutation. The numerical experiments have shown that compared with the higher order implicit Runge-Kutta method, the explicit K-symplectic and explicit symplectic-like methods have obvious advantages in long-term energy conservation and higher computational efficiency. It is also shown that the influence of the parameter ε in the general strong magnetic field on the Runge-Kutta method is bigger than the two kinds of symplectic methods.

Keywords: K-symplectic method; symplectic-like method; energy conservation; computational efficiency



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1. Introduction

The dynamics of charged particles [1–4] in the electric and the general magnetic field is one of the most fundamental theoretical models in magnetic confinement fusion research. Under the position and velocity variables, the charged particle system can be expressed in the form of a non-canonical Hamiltonian system, which is

$$\dot{\mathbf{Z}} = K^{-1}(\mathbf{Z})\nabla H(\mathbf{Z}) \quad (1)$$

where H is the Hamiltonian function and $K^{-1}(\mathbf{Z})$ is the antisymmetric matrix, depending on variable $\mathbf{Z}$. The non-canonical Hamiltonian system possesses a general symplectic structure. It is also a conservative system that has several conserved quantities, including the energy of the system. Therefore, when constructing numerical methods for the charged particle system, the methods should preserve the intrinsic structure or the conserved quantities [5]. This kind of numerical method is called a structure-preserving algorithm.

A structure-preserving algorithm includes the symplectic methods [6–9], the energy-preserving methods [10,11] and the volume-preserving methods [12,13]. The property that is preserved by the symplectic methods is the intrinsic symplectic structure, which can be expressed as a 2-form of the Hamiltonian system [5,14–17]; thus, they are preferable for simulating the Hamiltonian system. The canonical Hamiltonian system has the expression of

$$\dot{\mathbf{y}} = J^{-1} \nabla H(\mathbf{y}), \quad J = \begin{pmatrix} O_n & I_n \\ -I_n & O_n \end{pmatrix}. \quad (2)$$

and it possesses a symplectic structure that can be exactly preserved by the symplectic methods, while the non-canonical Hamiltonian system possesses a K-symplectic structure that can be exactly preserved by the K-symplectic methods. As the charged particle system can be represented as a non-canonical Hamiltonian system, it can be rewritten as a canonical Hamiltonian system by using a suitable coordinate transformation. The existence of the coordinate transformation is guaranteed by Darboux's theorem [15,18]. Non-canonical Hamiltonian systems are generalized Hamiltonian systems. The well-known Schrödinger equation [19,20] can also be expressed as a non-canonical Hamiltonian system. Developing stable and efficient numerical methods for both the Hamiltonian systems and the non-canonical Hamiltonian systems is of importance. Thus, we prefer developing explicit symplectic and explicit K-symplectic methods that have long-term stability and high efficiency.

Symplectic methods exhibit superior long-term structure-preserving behaviors and long-term stability compared with conventional methods such as Runge-Kutta methods. The slower error growth and the approximate preservation of conserved quantities without secular drift are their long-term behaviors. Symplectic methods consist of the explicit symplectic methods and the implicit ones. If the Hamiltonian function of the Hamiltonian system can be separated into several subsystems, and if the analytical solution of these subsystems can be obtained, then explicit symplectic methods can be proposed by composing the analytical solutions of these subsystems. Explicit K-symplectic methods can also be proposed by using such splitting and composing approaches. The explicit methods exhibit better efficiency than the implicit methods.

Explicit symplectic methods can be constructed for separable canonical Hamiltonian systems by using the splitting methods [15,21]. This splitting technique also applies to separable non-canonical Hamiltonian systems to construct explicit K-symplectic methods [22–24]. Splitting methods are applied for the case when the Hamiltonian is separable. The Hamiltonian H and the Hamiltonian system (2) are called separable if H can be written as $H(q, p) = U(p) + V(q)$ with some functions U and V , and nonseparable otherwise. This separability also applies to the non-canonical Hamiltonian system. If the Hamiltonian is not separable, Pihajoki proposed to extend the phase space to make the Hamiltonian separable for the canonical Hamiltonian systems, i.e., the Hamiltonian $H(\mathbf{q}, \mathbf{p})$ turns to $\tilde{H}(\mathbf{q}, \tilde{\mathbf{q}}, \mathbf{p}, \tilde{\mathbf{p}}) = H_A(\mathbf{q}, \tilde{\mathbf{p}}) + H_B(\tilde{\mathbf{q}}, \mathbf{p})$. Then, symplectic-like methods were constructed with the coordinate-mixing permutation [25]. These methods are not symplectic, but they show the same long-term behavior in energy conservations as symplectic methods. Instead of adding the coordinate-mixing permutation, Tao provided another way to constrain the extended phase space. In addition to the two Pihajoki sub-Hamiltonians H_A and H_B , Tao also added a third sub-Hamiltonian H_C , which is the norm of the difference of the two copies of the phase space with a control parameter ω , i.e., $H_C = \|\mathbf{q} - \tilde{\mathbf{q}}\|_2^2 / 2 + \|\mathbf{p} - \tilde{\mathbf{p}}\|_2^2 / 2$ [26]. These methods are symplectic in the extended phase space, but as is shown, they are inferior to the symplectic-like methods with the midpoint permutation [27]. To construct symplectic methods for general nonseparable canonical Hamiltonian systems, Ohsawa and Jayawardana combined the symmetric projection method with the extended phase space approach proposed by Pihajoki [28,29]. Their methods have better performance than Tao's methods [28].

In this paper, we construct the explicit K-symplectic and explicit symplectic-like methods for the charged particle dynamics in a general strong magnetic field. We have identified that if the three components of the magnetic field can all be integrated explicitly, then we can develop explicit K-symplectic methods. If the above condition does not hold, we can develop explicit symplectic-like methods. The numerical experiments have shown that the explicit K-symplectic and explicit symplectic-like methods have significant

advantage in long-term energy conservation over the higher-order Runge-Kutta methods. The K-symplectic and symplectic-like methods also exhibit better efficiency than the higher-order Runge-Kutta methods. We also point out the influence of the parameter ε appearing in the general strong magnetic field in the numerical methods. The effects of the parameter ε on the Runge-Kutta methods are larger than the symplectic methods, which shows that the two kinds of symplectic methods are more stable than the Runge-Kutta methods.

We organize the rest of the paper as follows. Section 2 gives a brief introduction to the two kinds of expression of the charged particle system. Section 3 indicates how to utilize the splitting method to develop the explicit K-symplectic methods and symplectic-like methods. We identify that if every component of the magnetic field can be integrated explicitly, then we can develop explicit K-symplectic methods; otherwise, we can develop symplectic-like methods by extending the phase space and by using the midpoint permutation. In Section 4, numerical methods that are used to make comparison are presented. In Section 5, the numerical results of the charged particle system are provided. In Section 6, we summarize our work.

2. Charged Particle System

The motion of the charged particle in an electric field $E(\mathbf{X})$ and a general strong magnetic field $\frac{1}{\varepsilon}B(\mathbf{X})$ is governed by the Lorentz force law. The parameter ε is used for adjusting the strength of the magnetic field. It is usually small such that the strength of the magnetic field is strong. Denote the position variable of the charged particle by $\mathbf{X}$ and denote its velocity by $\mathbf{V}$; the charged particle system is of the form

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}, \quad m \frac{d\mathbf{V}}{dt} = q(E(\mathbf{X}) + \frac{1}{\varepsilon} \mathbf{V} \times B(\mathbf{X}))$$

where m is the mass and q is the charge. Denote $\mathbf{Z} = (\mathbf{X}, \mathbf{V})^\top = (x_1, x_2, x_3, v_1, v_2, v_3)^\top$, the charged particle system can be expressed as a non-canonical Hamiltonian system [9,15]

$$\dot{\mathbf{Z}} = K^{-1}(\mathbf{Z}) \nabla H(\mathbf{Z}) \quad (3)$$

where

$$K^{-1}(\mathbf{Z}) = \begin{pmatrix} O & \frac{I}{m} \\ -\frac{I}{m} & -\frac{q\hat{B}(\mathbf{X})}{m^2} \end{pmatrix}$$

with the Hamiltonian being $H(\mathbf{X}, \mathbf{V}) = mv_1^2/2 + mv_2^2/2 + mv_3^2/2 + q\varphi(\mathbf{X})$. Here, I is the 3×3 identity matrix. The scalar potential is $\varphi(\mathbf{X})$ and the electric field is $E(\mathbf{X}) = -\nabla\varphi$. The general magnetic field is $\frac{1}{\varepsilon}B(\mathbf{X}) = \frac{1}{\varepsilon}(B_1(\mathbf{X}), B_2(\mathbf{X}), B_3(\mathbf{X}))$ and the matrix $\hat{B}(\mathbf{X})$ is

$$\hat{B}(\mathbf{X}) = \begin{pmatrix} 0 & -B_3(\mathbf{X}) & B_2(\mathbf{X}) \\ B_3(\mathbf{X}) & 0 & -B_1(\mathbf{X}) \\ -B_2(\mathbf{X}) & B_1(\mathbf{X}) & 0 \end{pmatrix}.$$

The magnetic field satisfies $\nabla \cdot B(\mathbf{X}) = 0$. Then, there exists a vector potential $A(\mathbf{X})$ that satisfies $B(\mathbf{X}) = \nabla \times A(\mathbf{X})$.

According to Darboux's theorem, under a suitable coordinate transformation, the non-canonical Hamiltonian system (3) can be transformed to a canonical Hamiltonian system [7,8,15]

$$\dot{\mathbf{y}} = J^{-1} \nabla H(\mathbf{y}), \quad J = \begin{pmatrix} O_3 & I_3 \\ -I_3 & O_3 \end{pmatrix}. \quad (4)$$

where O_3 is the 3×3 zero matrix and I_3 is the 3×3 identity matrix. The common coordinate transformation is

$$\begin{cases} \mathbf{X} = \mathbf{X}, \\ \mathbf{V} = \mathbf{P} - A(\mathbf{X}), \end{cases} \quad (5)$$

then, under the variable $\mathbf{y} = (\mathbf{P}, \mathbf{X})$, the charged particle system can be rewritten as a canonical Hamiltonian system

$$\begin{cases} \dot{\mathbf{P}} = -\partial_{\mathbf{X}} \tilde{H}(\mathbf{P}, \mathbf{X}), \\ \dot{\mathbf{X}} = \partial_{\mathbf{P}} \tilde{H}(\mathbf{P}, \mathbf{X}) \end{cases} \quad (6)$$

with the Hamiltonian $\tilde{H}(\mathbf{P}, \mathbf{X})$ being

$$\tilde{H} = \frac{1}{2m} (\mathbf{P} - qA(\mathbf{X}))^\top (\mathbf{P} - qA(\mathbf{X})) + q\varphi(\mathbf{X})$$

where X is still the position variable, and $\mathbf{P} = m\dot{\mathbf{X}} + qA(\mathbf{X})$ is the conjugate momentum.

3. K-Symplectic and Symplectic-like Methods Based on Splitting Methods

As the charged particle system can be expressed in both canonical form and non-canonical form, we can develop both the symplectic and K-symplectic methods. Here, we develop the K-symplectic methods for its non-canonical form and the symplectic methods for its canonical form.

3.1. K-Symplectic Methods for the Charged Particle System

For the non-canonical Hamiltonian system (3), it owns a K-symplectic structure, which can be expressed as a 2-form:

$$W = \sum_{i < j} k_{ij}(\mathbf{Z}) dz_i \wedge dz_j$$

where k_{ij} , $1 \leq i, j \leq 6$ are the elements of the matrix K^{-1} , and z_i is the i -th component of the variable $\mathbf{Z}$. This general symplectic structure is exactly preserved by K-symplectic methods.

Definition 1. A numerical method φ_h is a one-step method. Given a variable $\mathbf{v} \in \mathbb{R}^n$ and a time stepsize h , assume that the value of $\mathbf{v}$ at the initial time step is $\mathbf{v}_0$; by using the method φ_h , we can get the value of $\mathbf{v}$ at the next time step, i.e., $\varphi_h(\mathbf{v}_0) \in \mathbb{R}^n$. The method φ_h is called K-symplectic if its Jacobian satisfies

$$\left[\frac{\partial \varphi_h(\mathbf{v}_0)}{\partial \mathbf{v}_0} \right]^T K(\varphi_h(\mathbf{v}_0)) \left[\frac{\partial \varphi_h(\mathbf{v}_0)}{\partial \mathbf{v}_0} \right] = K(\mathbf{v}_0).$$

The Jacobian means the matrix composed by the partial derivatives of every component $(\varphi_h(\mathbf{v}_0))_i$, $1 \leq i \leq n$ of $\varphi_h(\mathbf{v}_0)$ with respect to every component $(\mathbf{v}_0)_j$, $1 \leq j \leq n$ of $\mathbf{v}_0$.

There is no common approach to construct K-symplectic methods for all non-canonical Hamiltonian systems (3). However, in some special cases where the Hamiltonian H is separable or it can be separated into several parts, the K-symplectic methods can be constructed by using the splitting and composing technique.

For the charged particle system, its Hamiltonian can be separated into four parts with the sub-Hamiltonians $H_1 = mv_1^2/2$, $H_2 = mv_2^2/2$, $H_3 = mv_3^2/2$ and $H_4 = q\varphi(\mathbf{X})$. For the first subsystem with $H_1 = mv_1^2/2$, its exact solution is

$$\begin{cases} x_1(t) = x_{10} + tmv_{10}, \\ x_2(t) = x_{20}, \\ x_3(t) = x_{30}, \\ v_1(t) = v_{10}, \\ v_2(t) = -v_{10} \int_0^t B_3(x_{10} + smv_{10}, x_{20}, x_{30}) ds, \\ v_3(t) = v_{10} \int_0^t B_2(x_{10} + smv_{10}, x_{20}, x_{30}) ds. \end{cases} \quad (7)$$

The exact solution to the fourth subsystem with $H_4 = q\varphi(\mathbf{X})$ is

$$\begin{cases} x_1(t) = x_{10}, \\ x_2(t) = x_{20}, \\ x_3(t) = x_{30}, \\ v_1(t) = v_{10} - tq \frac{\partial \varphi(\mathbf{X})}{\partial x_1} \Big|_{\mathbf{x}_0}, \\ v_2(t) = v_{20} - tq \frac{\partial \varphi(\mathbf{X})}{\partial x_2} \Big|_{\mathbf{x}_0}, \\ v_3(t) = v_{30} - tq \frac{\partial \varphi(\mathbf{X})}{\partial x_3} \Big|_{\mathbf{x}_0}. \end{cases} \quad (8)$$

where $\mathbf{X}_0 = (x_{10}, x_{20}, x_{30})$ and $\mathbf{V}_0 = (v_{10}, v_{20}, v_{30})$ are the initial values of $\mathbf{X}$ and $\mathbf{V}$. The exact solutions of the second and the third subsystems can also be written in integral forms.

We assume that the components of the magnetic field $B_i(\mathbf{X})$, $i = 1, 2, 3$ can be explicitly integrated, i.e., there exist primitive functions $F_i(x_1, x_2, x_3, t)$, $i = 1, 2, \dots, 6$ such that

$$\begin{aligned} F_1(x_1, x_2, x_3, t) &= \int_0^t B_1(x_1, x_2 + s, x_3) ds, & F_2(x_1, x_2, x_3, t) &= \int_0^t B_1(x_1, x_2, x_3 + s) ds, \\ F_3(x_1, x_2, x_3, t) &= \int_0^t B_2(x_1 + s, x_2, x_3) ds, & F_4(x_1, x_2, x_3, t) &= \int_0^t B_2(x_1, x_2, x_3 + s) ds, \\ F_5(x_1, x_2, x_3, t) &= \int_0^t B_3(x_1 + s, x_2, x_3) ds, & F_6(x_1, x_2, x_3, t) &= \int_0^t B_3(x_1, x_2 + s, x_3) ds. \end{aligned}$$

If every components of the magnetic field $B_i(\mathbf{X})$, $i = 1, 2, 3$ can be explicitly integrated, then the exact solutions of the four subsystems can be written in explicit forms; thus, we can develop explicit K-symplectic methods. Denote the exact solutions of the four subsystems with sub-Hamiltonians H_i by φ_h^i , $i = 1, 2, 3, 4$, then we know that the composition method

$$\psi_h \equiv \varphi_h^4 \circ \varphi_h^3 \circ \varphi_h^2 \circ \varphi_h^1 \quad (9)$$

is an explicit K-symplectic method of order 1. Another composition method,

$$\psi_h^2 \equiv \psi_{h/2}^* \circ \psi_{h/2} = \varphi_{h/2}^1 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^3 \circ \varphi_h^4 \circ \varphi_{h/2}^3 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^1 \quad (10)$$

is an explicit K-symplectic method of order 2 [30]. The method ψ_h^* represents the adjoint method of ψ_h , and ψ_h^* can be expressed as

$$\psi_h^* \equiv \varphi_h^1 \circ \varphi_h^2 \circ \varphi_h^3 \circ \varphi_h^4. \quad (11)$$

The K-symplectic methods of higher order can be developed by composing the lower-order K-symplectic method. As such, given a $2n$ -th order K-symplectic method χ_h^{2n} , the $2n + 2$ -th order K-symplectic method χ_h^{2n+2} can be obtained in the following way:

$$\chi_h^{2n+2} \equiv \chi_{\alpha_n h}^{2n} \circ \chi_{\beta_n h}^{2n} \circ \chi_{\alpha_n h}^{2n}$$

where $\alpha_n = (2 - 2^{1/(2n+1)})^{-1}$ and $\beta_n = 1 - 2\alpha_n < 0$.

If every component of the magnetic field $B(\mathbf{X})$ can be explicitly integrated, then we use the above splitting and composing technique to develop explicit K-symplectic methods for the charged particle system in the general strong magnetic field.

3.2. Symplectic-like Methods for the Charged Particle System

For the canonical Hamiltonian system (6), it owns a symplectic structure that is defined by the following 2-form:

$$\omega = \sum_{i=1}^3 dy_i \wedge dy_{n+i}$$

where y_i is the i -th component of the variable $\mathbf{y}$. This symplectic structure is exactly preserved by symplectic methods.

Definition 2. A numerical method Φ_h is a one-step method. Given the variable $\mathbf{Z} \in \mathbb{R}^n$ and a time stepsize h , assume that the value of $\mathbf{Z}$ at the initial time step is $\mathbf{Z}_0$; by using the method Φ_h , we can get the value of $\mathbf{Z}$ at the next time step, i.e., $\Phi_h(\mathbf{Z}_0) \in \mathbb{R}^n$. The method Φ_h is called symplectic if its Jacobian satisfies

$$\left[\frac{\partial \Phi_h(\mathbf{Z}_0)}{\partial \mathbf{Z}_0} \right]^\top J \left[\frac{\partial \Phi_h(\mathbf{Z}_0)}{\partial \mathbf{Z}_0} \right] = J. \quad (12)$$

The Jacobian means the matrix composed by the partial derivatives of every component $(\Phi_h(\mathbf{Z}_0))_i, 1 \leq i \leq n$ of $\Phi_h(\mathbf{Z}_0)$ with respect to every component $(\mathbf{Z}_0)_j, 1 \leq j \leq n$ of $\mathbf{Z}_0$.

There are many kinds of symplectic methods, such as symplectic Runge-Kutta methods and symplectic generating function methods. Another approach to constructing symplectic methods is the splitting method. The idea is the same as that in the above subsection.

If one of the component of the magnetic field $B(\mathbf{X})$ can not be explicitly integrated, we can construct symplectic-like methods based on the splitting and composing technique. The charged particle system in the canonical form has the Hamiltonian

$$\tilde{H} = \frac{1}{2m} (\mathbf{P} - qA(\mathbf{X}))^\top (\mathbf{P} - qA(\mathbf{X})) + q\varphi(\mathbf{X})$$

which is not separable. To make the Hamiltonian $\tilde{H}$ separable, we aim at extending the phase space $(\mathbf{P}, \mathbf{X})$ to two copies. Therefore, the extended phase space is $(\mathbf{P}_1, \mathbf{X}_1, \mathbf{P}_2, \mathbf{X}_2)$; thus, we can construct an augmented Hamiltonian

$$\bar{H} := \tilde{H}(\mathbf{P}_1, \mathbf{X}_2) + \tilde{H}(\mathbf{P}_2, \mathbf{X}_1).$$

By extending the original phase space $(\mathbf{P}, \mathbf{X})$ to the extended phase space $(\mathbf{P}_1, \mathbf{X}_1, \mathbf{P}_2, \mathbf{X}_2)$, and considering the augmented Hamiltonian $\bar{H}$, we can find that the augmented Hamiltonian is separable. Thus, we can use the splitting and composing technique to construct explicit symplectic methods for the extended Hamiltonian system (13). In the extended phase space, the symplectic 2-form becomes $d\mathbf{P}_1 \wedge d\mathbf{X}_1 + d\mathbf{P}_2 \wedge d\mathbf{X}_2$. Then, the extended system is

$$\begin{cases} \dot{\mathbf{P}}_1 = -\partial_{\mathbf{X}_1} \tilde{H}, \\ \dot{\mathbf{X}}_1 = \partial_{\mathbf{P}_1} \tilde{H}, \\ \dot{\mathbf{P}}_2 = -\partial_{\mathbf{X}_2} \tilde{H}, \\ \dot{\mathbf{X}}_2 = \partial_{\mathbf{P}_2} \tilde{H}. \end{cases} \quad (13)$$

This augmented system has the same exact solution as the original system (6) if it has the initial condition $\mathbf{P}_{10} = \mathbf{P}_0$, $\mathbf{X}_{10} = \mathbf{X}_0$, $\mathbf{P}_{20} = \mathbf{P}_0$, $\mathbf{X}_{20} = \mathbf{X}_0$, where $\mathbf{P}_0$ and $\mathbf{X}_0$ are the initial conditions of the original system (6) [26,28].

The augmented Hamiltonian $\tilde{H}$ can be separated into two subsystems with subHamiltonians $H_A = \tilde{H}(\mathbf{P}_1, \mathbf{X}_2)$ and $H_B = \tilde{H}(\mathbf{P}_2, \mathbf{X}_1)$. Denote the exact solution of the two subsystems by $\varphi_h^{H_A}$ and $\varphi_h^{H_B}$. The explicit forms of the two exact solutions are

$$\varphi_h^{H_A} : \begin{cases} \mathbf{P}_1(h) = \mathbf{P}_{10}, \\ \mathbf{X}_1(h) = \mathbf{X}_{10} + h\partial_{\mathbf{P}_1} H_A, \\ \mathbf{P}_2(h) = \mathbf{P}_{20} - h\partial_{\mathbf{X}_2} H_A, \\ \mathbf{X}_2(h) = \mathbf{X}_{20}. \end{cases} \quad (14)$$

and

$$\varphi_h^{H_B} : \begin{cases} \mathbf{P}_1(h) = \mathbf{P}_{10} - h\partial_{\mathbf{X}_1} H_B, \\ \mathbf{X}_1(h) = \mathbf{X}_{10}, \\ \mathbf{P}_2(h) = \mathbf{P}_{20}, \\ \mathbf{X}_2(h) = \mathbf{X}_{20} + h\partial_{\mathbf{P}_2} H_B. \end{cases} \quad (15)$$

As the variables in the extended system are mixed, the augmented system is not the two duplicates of the original system. If there is no constraint on the two duplicates of the phase space, the numerical solution of the extended system may not converge to that of the original one; thus, the difference between the two solutions is large. To constrain the two copies of the phase space $(\mathbf{P}_1, \mathbf{X}_1, \mathbf{P}_2, \mathbf{X}_2)$, we set the permutation on them. Here, we prefer to use the midpoint permutation as

$$\kappa : \begin{cases} \frac{\mathbf{P}_1(t) + \mathbf{P}_2(t)}{2} \rightarrow \mathbf{P}_1(t), \\ \frac{\mathbf{P}_1(t) + \mathbf{P}_2(t)}{2} \rightarrow \mathbf{P}_2(t), \\ \frac{\mathbf{X}_1(t) + \mathbf{X}_2(t)}{2} \rightarrow \mathbf{X}_1(t), \\ \frac{\mathbf{X}_1(t) + \mathbf{X}_2(t)}{2} \rightarrow \mathbf{X}_2(t). \end{cases} \quad (16)$$

Thus, we can obtain a first-order explicit symplectic-like method as

$$\chi_h \equiv \kappa \circ \varphi_h^{H_A} \circ \varphi_h^{H_B}$$

and a second-order explicit symplectic-like method as

$$\chi_h^2 \equiv \kappa \circ \varphi_{h/2}^{H_B} \circ \varphi_h^{H_A} \circ \varphi_{h/2}^{H_B}$$

Higher-order symplectic-like methods can be obtained by composing the lower order methods.

4. Numerical Methods

The explicit K-symplectic methods and symplectic-like methods are compared with conventional Runge-Kutta methods to demonstrate their advantage in structure preservation and computational efficiency. Here, we list all the numerical methods we used.

2ndKSYM: the second-order explicit K-symplectic method ψ_h^2 for the non-canonical charged particle system with the expression

$$\psi_h^2 \equiv \varphi_{h/2}^1 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^3 \circ \varphi_h^4 \circ \varphi_{h/2}^3 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^1. \quad (17)$$

We formulate the methods $\varphi_{h/2}^1$, $\varphi_{h/2}^2$, $\varphi_{h/2}^3$ and φ_h^4 with discrete time stepsize h , which can be calculated as follows:

$$\varphi_{h/2}^1 : \begin{cases} x_{11} = x_{10} + \frac{h}{2}mv_{10}, \\ x_{21} = x_{20}, \\ x_{31} = x_{30}, \\ v_{11} = v_{10}, \\ v_{21} = -v_{10} \int_0^{\frac{h}{2}} B_3(x_{10} + smv_{10}, x_{20}, x_{30})ds, \\ v_{31} = v_{10} \int_0^{\frac{h}{2}} B_2(x_{10} + smv_{10}, x_{20}, x_{30})ds. \end{cases} \quad (18)$$

$$\varphi_{h/2}^2 : \begin{cases} x_{12} = x_{11}, \\ x_{22} = x_{21} + \frac{h}{2}mv_{21}, \\ x_{32} = x_{31}, \\ v_{12} = v_{21} \int_0^{\frac{h}{2}} B_3(x_{11}, x_{21} + smv_{21}, x_{31})ds, \\ v_{22} = v_{21}, \\ v_{32} = -v_{21} \int_0^{\frac{h}{2}} B_1(x_{11}, x_{21} + smv_{21}, x_{31})ds. \end{cases} \quad (19)$$

$$\varphi_{h/2}^3 : \begin{cases} x_{13} = x_{12}, \\ x_{23} = x_{22}, \\ x_{33} = x_{32} + \frac{h}{2}mv_{32}, \\ v_{13} = -v_{32} \int_0^{\frac{h}{2}} B_2(x_{12}, x_{22}, x_{32} + smv_{32})ds, \\ v_{23} = v_{32} \int_0^{\frac{h}{2}} B_1(x_{12}, x_{22}, x_{32} + smv_{32})ds, \\ v_{33} = v_{32}. \end{cases} \quad (20)$$

$$\varphi_h^4 : \begin{cases} x_{14} = x_{13}, \\ x_{24} = x_{23}, \\ x_{34} = x_{33}, \\ v_{14} = v_{13} - hq \frac{\partial \varphi}{\partial x_1}(x_{13}, x_{23}, x_{33}), \\ v_{24} = v_{23} - hq \frac{\partial \varphi}{\partial x_2}(x_{13}, x_{23}, x_{33}), \\ v_{34} = v_{33} - hq \frac{\partial \varphi}{\partial x_3}(x_{13}, x_{23}, x_{33}). \end{cases} \quad (21)$$

Therefore, we know that

$$(x_{11}, x_{21}, x_{31}, v_{11}, v_{21}, v_{31}) = \varphi_{h/2}^1(x_{10}, x_{20}, x_{30}, v_{10}, v_{20}, v_{30})$$

where $x_{10}, x_{20}, x_{30}, v_{10}, v_{20}, v_{30}$ are the initial values of $x_1, x_2, x_3, v_1, v_2, v_3$, and $x_{11}, x_{21}, x_{31}, v_{11}, v_{21}, v_{31}$ are the values of the variables at time step $h/2$. The notions are similar for others. Then, we have

$$(x_{12}, x_{22}, x_{32}, v_{12}, v_{22}, v_{32}) = \varphi_{h/2}^2(x_{11}, x_{21}, x_{31}, v_{11}, v_{21}, v_{31}),$$

$$(x_{13}, x_{23}, x_{33}, v_{13}, v_{23}, v_{33}) = \varphi_{h/2}^3(x_{12}, x_{22}, x_{32}, v_{12}, v_{22}, v_{32}),$$

$$(x_{14}, x_{24}, x_{34}, v_{14}, v_{24}, v_{34}) = \varphi_h^4(x_{13}, x_{23}, x_{33}, v_{13}, v_{23}, v_{33}),$$

$$(x_{15}, x_{25}, x_{35}, v_{15}, v_{25}, v_{35}) = \varphi_{h/2}^3(x_{14}, x_{24}, x_{34}, v_{14}, v_{24}, v_{34}),$$

$$(x_{16}, x_{26}, x_{36}, v_{16}, v_{26}, v_{36}) = \varphi_{h/2}^2(x_{15}, x_{25}, x_{35}, v_{15}, v_{25}, v_{35})$$

and

$$(x_{17}, x_{27}, x_{37}, v_{17}, v_{27}, v_{37}) = \varphi_{h/2}^1(x_{16}, x_{26}, x_{36}, v_{16}, v_{26}, v_{36}).$$

Thus, we know that $\psi_h^2(x_{10}, x_{20}, x_{30}, v_{10}, v_{20}, v_{30}) = (x_{17}, x_{27}, x_{37}, v_{17}, v_{27}, v_{37})$.

4thKSYM: the fourth-order explicit K-symplectic method for the non-canonical charged particle system. The fourth-order method is constructed by composing the first-order K-symplectic method ψ_h . We formulate the method ψ_h with discrete time stepsize h . Then, we know that

$$(x_{11}, x_{21}, x_{31}, v_{11}, v_{21}, v_{31}) = \varphi_h^1(x_{10}, x_{20}, x_{30}, v_{10}, v_{20}, v_{30})$$

where $x_{10}, x_{20}, x_{30}, v_{10}, v_{20}, v_{30}$ are the initial values of $x_1, x_2, x_3, v_1, v_2, v_3$. Then

$$(x_{12}, x_{22}, x_{32}, v_{12}, v_{22}, v_{32}) = \varphi_h^2(x_{11}, x_{21}, x_{31}, v_{11}, v_{21}, v_{31}),$$

$$(x_{13}, x_{23}, x_{33}, v_{13}, v_{23}, v_{33}) = \varphi_h^3(x_{12}, x_{22}, x_{32}, v_{12}, v_{22}, v_{32})$$

and

$$(x_{14}, x_{24}, x_{34}, v_{14}, v_{24}, v_{34}) = \varphi_h^4(x_{13}, x_{23}, x_{33}, v_{13}, v_{23}, v_{33}).$$

Therefore, we know that $\psi_h(x_{10}, x_{20}, x_{30}, v_{10}, v_{20}, v_{30}) = (x_{14}, x_{24}, x_{34}, v_{14}, v_{24}, v_{34})$. The composing way is as follows:

$$\psi_h^4 \equiv \psi_{\alpha_6 h} \circ \psi_{\beta_6 h}^* \circ \cdots \circ \psi_{\beta_2 h}^* \circ \psi_{\alpha_1 h} \circ \psi_{\beta_1 h}^*, \quad (22)$$

where ψ_h^* is the adjoint method of the method ψ_h . Values of the parameters $\alpha_1, \beta_1, \dots, \alpha_6, \beta_6$ are given as follows [31].

$$\begin{aligned} \beta_1 &= \alpha_6 = 0.082984406417405, & \alpha_1 &= \beta_6 = 0.16231455076687, \\ \beta_2 &= \alpha_5 = 0.23399525073150, & \alpha_2 &= \beta_5 = 0.37087741497958, \\ \beta_3 &= \alpha_4 = -0.40993371990193, & \alpha_3 &= \beta_4 = 0.059762097006575. \end{aligned}$$

This composing way is a systematic way of obtaining a higher-order method and it is a symmetric composition of the first-order method [15]. The parameters $\alpha_i, \beta_i, i = 1, 2, \dots, 6$ are chosen to satisfy the order conditions of the numerical method [15]. That is to say, the parameters $\alpha_i, \beta_i, i = 1, 2, \dots, 6$ are chosen such that the composing method (22) is of order 4.

2ndSYM: the second-order explicit symplectic-like method χ_h^2 for the canonical charged particle system with the expression

$$\chi_h^2 \equiv \kappa \circ \varphi_{h/2}^{H_B} \circ \varphi_h^{H_A} \circ \varphi_{h/2}^{H_B}. \quad (23)$$

We formulate the methods $\varphi_{h/2}^{H_B}$ and $\varphi_{h/2}^{H_A}$ with discrete time stepsize h , which can be calculated as follows:

$$\varphi_{h/2}^{H_B} : \begin{cases} \mathbf{P}_{11} = \mathbf{P}_{10} - \frac{h}{2} \partial_{\mathbf{X}_1} H_B(\mathbf{P}_{20}, \mathbf{X}_{10}), \\ \mathbf{X}_{11} = \mathbf{X}_{10}, \\ \mathbf{P}_{21} = \mathbf{P}_{20}, \\ \mathbf{X}_{21} = \mathbf{X}_{20} + \frac{h}{2} \partial_{\mathbf{P}_2} H_B(\mathbf{P}_{20}, \mathbf{X}_{10}). \end{cases} \quad (24)$$

$$\varphi_h^{H_A} : \begin{cases} \mathbf{P}_{12} = \mathbf{P}_{11}, \\ \mathbf{X}_{12} = \mathbf{X}_{11} + h \partial_{\mathbf{P}_1} H_A(\mathbf{P}_{11}, \mathbf{X}_{21}), \\ \mathbf{P}_{22} = \mathbf{P}_{21} - h \partial_{\mathbf{X}_2} H_A(\mathbf{P}_{11}, \mathbf{X}_{21}), \\ \mathbf{X}_{22} = \mathbf{X}_{21}. \end{cases} \quad (25)$$

$$\varphi_{h/2}^{H_B} : \begin{cases} \mathbf{P}_{13} = \mathbf{P}_{12} - \frac{h}{2} \partial_{\mathbf{X}_1} H_B(\mathbf{P}_{22}, \mathbf{X}_{12}), \\ \mathbf{X}_{13} = \mathbf{X}_{12}, \\ \mathbf{P}_{23} = \mathbf{P}_{22}, \\ \mathbf{X}_{23} = \mathbf{X}_{22} + \frac{h}{2} \partial_{\mathbf{P}_2} H_B(\mathbf{P}_{22}, \mathbf{X}_{12}). \end{cases} \quad (26)$$

$$\kappa : \begin{cases} \mathbf{P}_{14} = \frac{\mathbf{P}_{13} + \mathbf{P}_{23}}{2}, \\ \mathbf{X}_{14} = \frac{\mathbf{X}_{13} + \mathbf{X}_{23}}{2}, \\ \mathbf{P}_{24} = \frac{\mathbf{P}_{13} + \mathbf{P}_{23}}{2}, \\ \mathbf{X}_{24} = \frac{\mathbf{X}_{13} + \mathbf{X}_{23}}{2}. \end{cases} \quad (27)$$

Therefore, we know that $\chi_h^2(\mathbf{P}_{10}, \mathbf{X}_{10}, \mathbf{P}_{20}, \mathbf{X}_{20}) = (\mathbf{P}_{14}, \mathbf{X}_{14}, \mathbf{P}_{24}, \mathbf{X}_{24})$.

4thSYM: the fourth order explicit symplectic-like method for the non-canonical charged particle system. The fourth-order method is constructed by composing the first-order K-symplectic method χ_h . Here, we formulate χ_h with discrete time stepsize h . Then, we know that

$$(\mathbf{P}_{11}, \mathbf{X}_{11}, \mathbf{P}_{21}, \mathbf{X}_{21}) = \varphi_h^{H_B}(\mathbf{P}_{10}, \mathbf{X}_{10}, \mathbf{P}_{20}, \mathbf{X}_{20}),$$

$$(\mathbf{P}_{12}, \mathbf{X}_{12}, \mathbf{P}_{22}, \mathbf{X}_{22}) = \varphi_h^{H_A}(\mathbf{P}_{11}, \mathbf{X}_{11}, \mathbf{P}_{21}, \mathbf{X}_{21})$$

with $\varphi_h^{H_B}$ and $\varphi_h^{H_A}$ defined in Equations (24) and (25). Then we know that $\chi_h(\mathbf{P}_{10}, \mathbf{X}_{10}, \mathbf{P}_{20}, \mathbf{X}_{20}) = (\mathbf{P}_{12}, \mathbf{X}_{12}, \mathbf{P}_{22}, \mathbf{X}_{22})$. The composing way is as follows:

$$\chi_h^4 \equiv \kappa \circ \chi_{\alpha_6 h} \circ \chi_{\beta_6 h}^* \circ \cdots \circ \chi_{\beta_2 h}^* \circ \chi_{\alpha_1 h} \circ \chi_{\beta_1 h}^* \quad (28)$$

where ψ_h^* is the adjoint method of the method ψ_h . Values of the parameters $\alpha_1, \beta_1, \dots, \alpha_6, \beta_6$ are the same as those in 4thKSYM [31]. The parameters are chosen in the same way as in 4thKSYM.

RK3: the third-order implicit Runge-Kutta method [32,33]. As the RK3 method is implicit, the iteration method is used to solve this method. We set the tolerance error to be 10^{-10} . The RK3 method is displayed as follows:

$$\begin{cases} \mathbf{Z}_{n+1} = \mathbf{Z}_n + \frac{1}{2}hf(\mathbf{W}_1) + \frac{1}{2}hf(\mathbf{W}_2), \\ \mathbf{W}_1 = \mathbf{Z}_n + \frac{1}{2}hf(\mathbf{W}_1) - \frac{\sqrt{3}}{6}hf(\mathbf{W}_2), \\ \mathbf{W}_2 = \mathbf{Z}_n + \frac{\sqrt{3}}{6}hf(\mathbf{W}_1) + \frac{1}{2}hf(\mathbf{W}_2) \end{cases} \quad (29)$$

where $\mathbf{Z} = (x_1, x_2, x_3, v_1, v_2, v_3)$ and $f = K^{-1}\nabla H(\mathbf{Z})$ with the matrix and the Hamiltonian H , which are defined in Section 2.

RK5: the fifth-order implicit Runge-Kutta method [32,33]. As the RK5 method is implicit, the iteration method is used to solve this method. We set the tolerance error to be 10^{-12} . The RK5 method is displayed as follows:

$$\begin{cases} \mathbf{Z}_{n+1} = \mathbf{Z}_n + \frac{1}{9}hf(\mathbf{W}_1) + \frac{16+\sqrt{6}}{36}hf(\mathbf{W}_2) + \frac{16-\sqrt{6}}{36}hf(\mathbf{W}_3), \\ \mathbf{W}_1 = \mathbf{Z}_n + \frac{1}{9}hf(\mathbf{W}_1) + \frac{-1-\sqrt{6}}{18}hf(\mathbf{W}_2) + \frac{-1+\sqrt{6}}{18}hf(\mathbf{W}_3), \\ \mathbf{W}_2 = \mathbf{Z}_n + \frac{1}{9}hf(\mathbf{W}_1) + \frac{88+7\sqrt{6}}{360}hf(\mathbf{W}_2) + \frac{88-43\sqrt{6}}{360}hf(\mathbf{W}_3), \\ \mathbf{W}_3 = \mathbf{Z}_n + \frac{1}{9}hf(\mathbf{W}_1) + \frac{88+43\sqrt{6}}{360}hf(\mathbf{W}_2) + \frac{88-7\sqrt{6}}{360}hf(\mathbf{W}_3) \end{cases} \quad (30)$$

where $\mathbf{Z} = (x_1, x_2, x_3, v_1, v_2, v_3)$ and $f = K^{-1}\nabla H(\mathbf{Z})$ with the matrix and the Hamiltonian H , which are defined in Section 2.

5. Numerical Experiments

Here, we present several examples of a charged particle system under different magnetic fields. In the first two examples, the magnetic fields are integrable, and the integral can be written in closed forms; thus, the explicit K-symplectic methods are constructed. In the last two examples, since the magnetic fields cannot be integrated in closed form, we construct the explicit symplectic-like methods.

5.1. Example 1

The system is normalized according to natural units. We set the particle mass $m = 1$ and electric charge $q = 1$. The electric field is

$$E(\mathbf{X}) = \frac{10^{-2}}{(x_1^2 + x_2^2)^{3/2}}(x_1, x_2, 0) \quad (31)$$

and the scalar potential is $\varphi(X) = \frac{10^{-2}}{\sqrt{x_1^2 + x_2^2}}$. We choose the magnetic field to be

$$B(\mathbf{X}) = (0, 0, \sqrt{2x_1^2 + 3x_2^2}). \quad (32)$$

The integral of the third component of the magnetic field with respect to x_1 can be integrated in closed form

$$\int \sqrt{2x_1^2 + 3x_2^2} dx_1 = \frac{1}{4} \left(2x_1 \sqrt{2x_1^2 + 3x_2^2} + 3\sqrt{2} \ln(2x_1 + \sqrt{4x_1^2 + 6x_2^2}) \right). \quad (33)$$

The integral with respect to x_2 can also be obtained in closed form. Thus, the explicit K-symplectic methods can be constructed for the charged particle system in non-canonical form.

The initial condition is $Z_0 = (0, -1, 0, 0.2, 0.1, 0)$. Displayed in Figure 1a,b are the projections on the $x_1 - x_2$ plane of the phase orbit obtained by the second-order K-symplectic method and the third-order Runge-Kutta method under the parameter $\varepsilon = \frac{1}{5}$. As can be seen from Figure 1a,b, under the same stepsize, the phase orbit of the 2ndKSYM method is preserved well, while the phase orbit of the RK3 method is not accurate. Displayed in Figure 1c,d are the energy errors obtained by the 2ndKSYM method, the RK3 method, the 4thKSYM method and the RK5 method. The energy errors of the 2ndKSYM method and the 4thKSYM method oscillates with small amplitudes over a long time, while those of the RK3 method and the RK5 method increase along time and increase without bound. The K-symplectic methods demonstrate their advantage in orbit preservation and energy preservation over a long time. Figure 2 shows the phase orbit obtained by the two K-symplectic methods and two Runge-Kutta methods under the parameter $\varepsilon = \frac{1}{10}$. Displayed in Figure 2a,b are the phase orbits obtained by the 2ndKSYM and RK3 methods. It can be seen that the phase orbit of the 2ndKSYM method can be preserved under a big stepsize, but the phase orbit of the RK3 method is not accurate even under a very small stepsize. This shows the big influence of the parameter ε on the third-order Runge-Kutta method. When the parameter ε turns big, the stepsize of the third-order Runge-Kutta method should be very small. Displayed in Figure 2c,d are the phase orbits obtained by the 4thKSYM and RK5 methods under the same stepsize. The phase orbit of the 4thKSYM method is accurate over a long period, while the phase orbit of the RK5 method is not accurate. This clearly shows the superior advantage of the two K-symplectic methods in structure-preservation compared with the two higher-order Runge-Kutta methods.

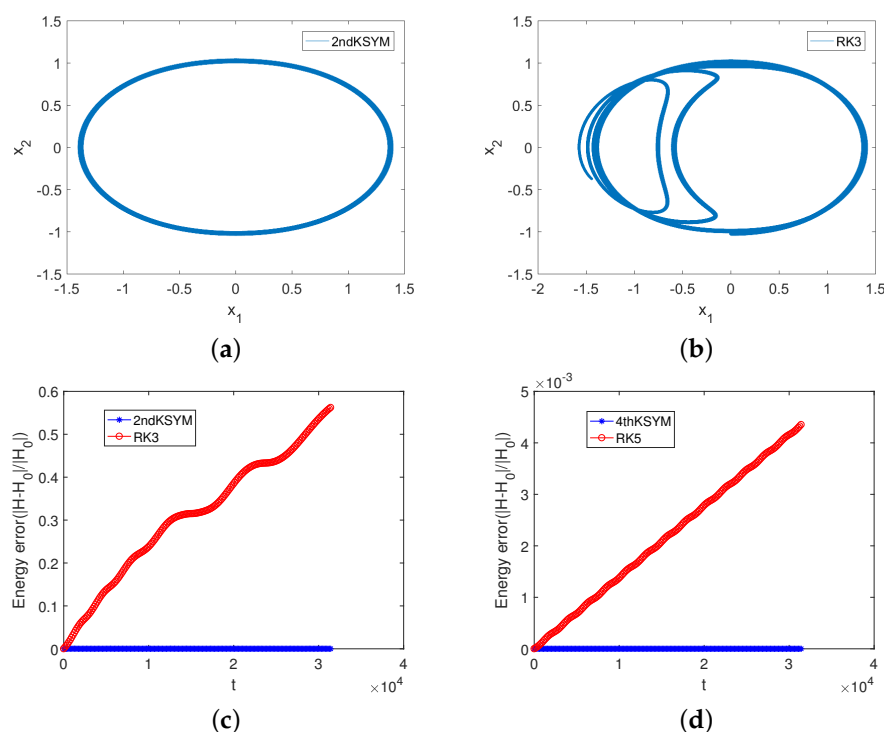


Figure 1. The phase orbit and the energy evolution obtained by the 2ndKSYM, 4thKSYM, RK3 and RK5 methods with the parameter $\varepsilon = 1/5$ in Example 1. The time interval for subfigures (a,b) is $[0, 10^4\pi]$, and the time stepsize is $h = \pi/800$. In subfigure (c), the stepsize is $h = \pi/800$, while in (d), the stepsize is $h = \pi/200$.

Figure 3 shows the computational efficiency of the 2ndKSYM method, the RK3 method, the 4thKSYM method and the RK5 method under two different parameters ϵ . Figure 3a,b are the energy errors versus computational time for the four methods for $\epsilon = \frac{1}{5}$. Figure 3c,d are the energy errors versus computational time for the four methods for $\epsilon = \frac{1}{10}$. Method A is more efficient than method B if A takes less computational (CPU) time to achieve the same magnitude of error than B. We can observe from Figure 3 that under the same stepsize, both the computational times and the energy errors of the two K-symplectic methods are much less than the two Runge-Kutta methods. The computational time of the RK3 method is nearly 8 times of that of the 2ndKSYM method, and the computational time of the RK5 method is nearly 4 times of that of the 4thKSYM method. The energy error of the 2ndKSYM method is nearly $\frac{1}{100}$ times of that of the RK3 method, while the energy error of the 4thKSYM method is nearly $\frac{1}{10000}$ times of that of the RK5 method. To obtain the same order of magnitude of energy error, the two K-symplectic methods need much less computational times compared to the two Runge-Kutta methods. This shows that the two K-symplectic methods are much more efficient than the two higher-order Runge-Kutta methods.

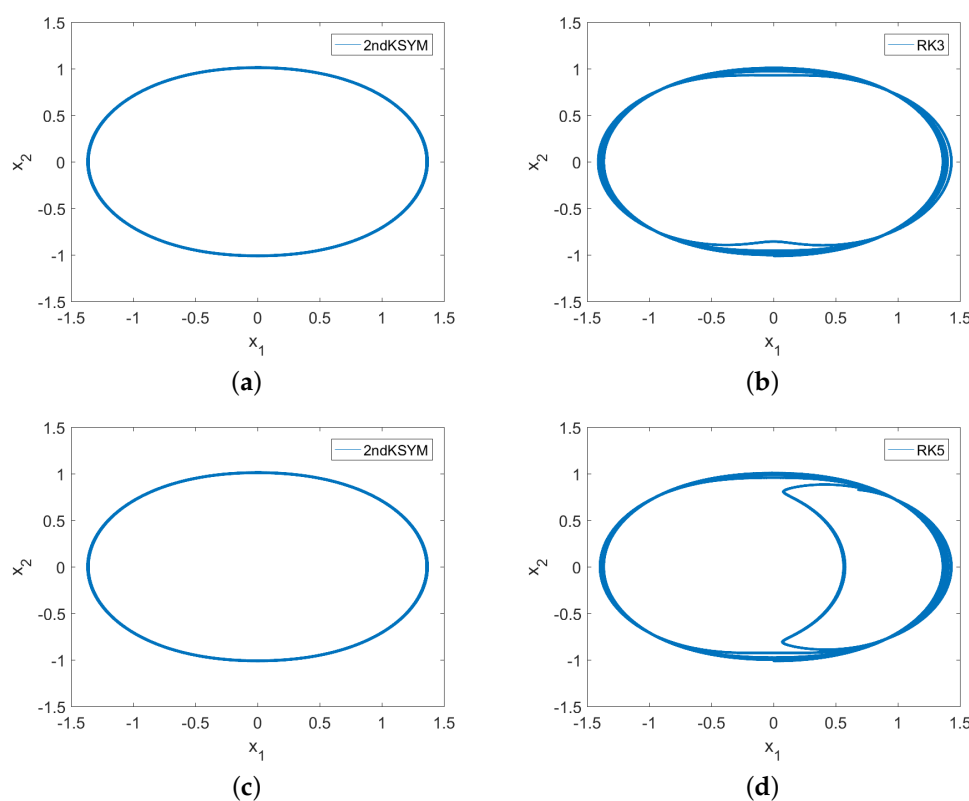


Figure 2. The phase orbit projected on the $x_1 - x_2$ plane of the 2ndKSYM, 4thKSYM, RK3 and RK5 methods with the parameter $\epsilon = 1/10$ in Example 1. The time interval for the four subfigures is $[0, 2 \times 10^4 \pi]$. In subfigure (a), the stepsize is $\pi/400$, and in subfigure (b), the stepsize is $h = \pi/3200$. In subfigure (c), the stepsize is $h = \pi/100$, while in (d), the stepsize is $h = \pi/100$.

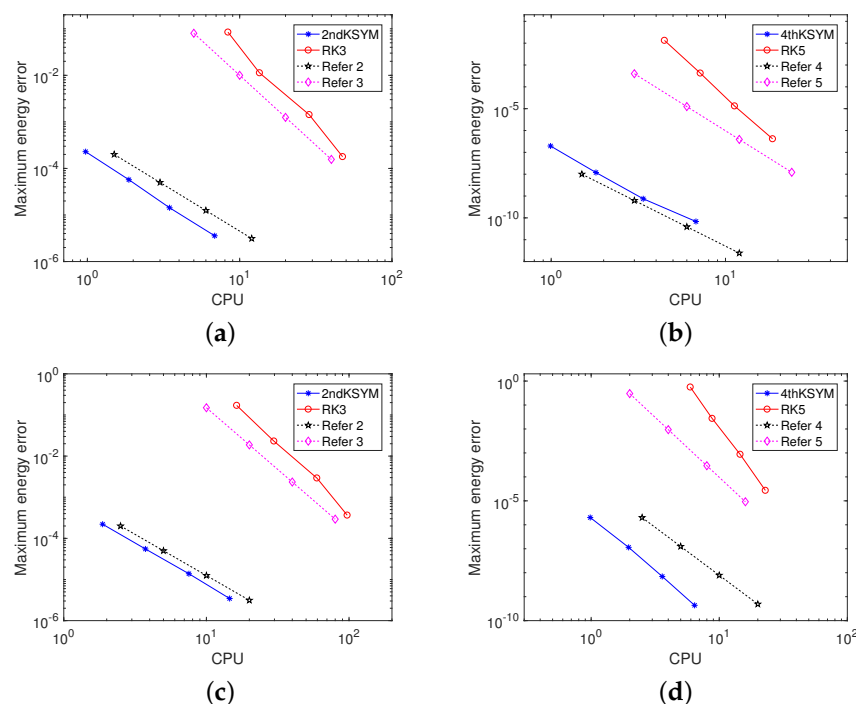


Figure 3. The maximum energy error versus CPU time for the 2ndKSYM, 4thKSYM, RK3 and RK5 methods in Example 1. In subfigures (a,b), $\epsilon = 1/5$ while in subfigures (c,d), $\epsilon = 1/10$. In subfigure (a), the stepsize is $h = \pi/800/2^i, i = 0, 1, 2, 3$, while in (b), the stepsize is $h = \pi/100/2^i, i = 0, 1, 2, 3$. In subfigure (c), the stepsize is $h = \pi/1600/2^i, i = 0, 1, 2, 3$, while in (d), the stepsize is $h = \pi/100/2^i, i = 0, 1, 2, 3$.

5.2. Example 2

The system is normalized according to natural units. We set the particle mass $m = 1$ and electric charge $q = 1$. The electric field is

$$E(\mathbf{X}) = \frac{10^{-2}}{(x_1^2 + x_2^2)^{3/2}}(x_1, x_2, 0) \quad (34)$$

We choose the magnetic field to be

$$B(\mathbf{X}) = \left(-\cos(x_2 + x_3), x_1^2 + x_3^2, \frac{x_1^2}{2} + \frac{x_2^2}{2} \right). \quad (35)$$

As the three components of the magnetic field B can be integrated explicitly, we can construct explicit K-symplectic methods.

The initial condition is $Z_0 = (0.2, -1, 0.2, 0.02, 0.01, 0.01)$. Figure 4 shows the energy error and the computational efficiency of the two K-symplectic methods and the two Runge-Kutta methods under the parameter $\epsilon = \frac{1}{5}$. It can be seen from Figure 4a,b that the defects $|H_n - H_0|/|H_0|$ of the 2ndKSYM method and the 4thKSYM method oscillate within small intervals, but those of the RK3 method and the RK5 method increase without bound. Figure 4c,d shows that to obtain the same magnitude of the defect $|H_n - H_0|/|H_0|$, such as 10^{-4} , the computational time of the 2ndKSYM method is much less than the computational time of the RK3 method. The 2ndKSYM method exhibits better efficiency than the RK3 method. The 4thKSYM method also exhibits better efficiency than the RK5 method. Displayed in Figure 5 are the relative energy errors $|H_n - H_0|/|H_0|$ obtained by the 2ndKSYM method, the RK3 method, the 4thKSYM method and the RK5 method under the parameter $\epsilon = \frac{1}{10}$. As can be seen from Figure 5, the defects $|H_n - H_0|/|H_0|$ of the two

K-symplectic methods can be preserved by small errors, while the defects of the two Runge-Kutta methods do not have boundaries and increase along time. Displayed in Figure 5a,b are the energy errors obtained by the 2ndKSYM and the RK3 methods. Displayed in Figure 5c,d are the energy errors obtained by the 4thKSYM and the RK5 methods. We can observe that the maximum energy errors of the 2ndKSYM method and RK3 under $\varepsilon = \frac{1}{5}$ are of magnitude 10^{-5} and 10^{-3} , while the energy error of the 2ndKSYM method and the RK3 method under $\varepsilon = \frac{1}{10}$ are of magnitude 10^{-4} and 10^{-1} . When the parameter ε turns from $\frac{1}{5}$ to $\frac{1}{10}$, the energy error of the 2ndKSYM method is one order of magnitude larger, while that of the RK3 method is two orders of magnitude larger. This observation also applies to the 4thKSYM method and RK5 method. This shows the big influence of parameter ε on the Runge-Kutta methods, and it also shows that the two kinds of symplectic methods are more stable than the Runge-Kutta methods.

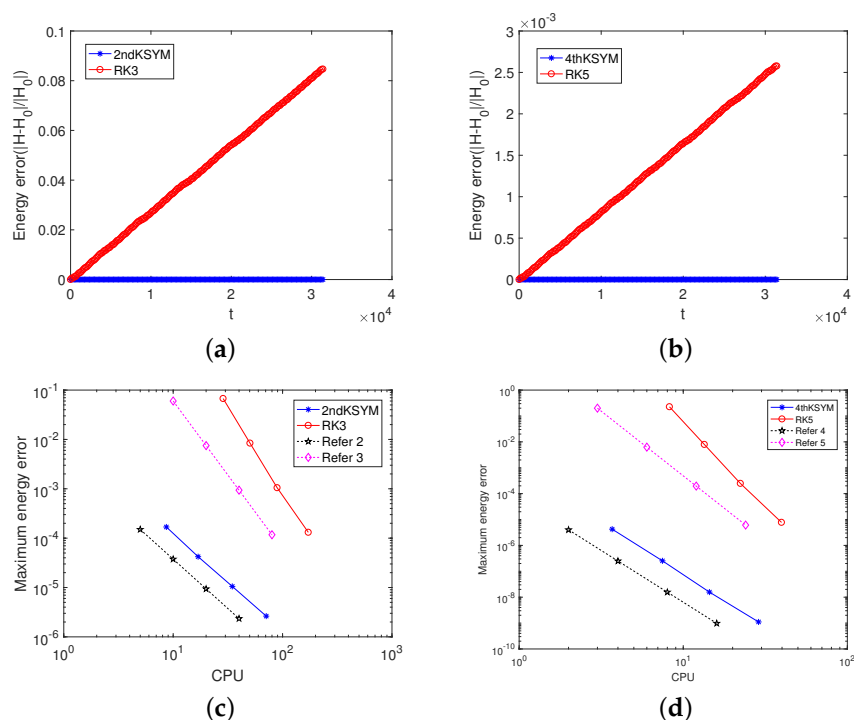


Figure 4. The energy evolution and computational efficiency for the 2ndKSYM, 4thKSYM, RK3 and RK5 methods with the parameter $\varepsilon = 1/2$ in Example 2. In subfigure (a), the stepsize is $h = \pi/6400$, while in subfigure (b), the stepsize is $h = \pi/800$. The time interval is $[0, 10^4\pi]$. In subfigure (c,d), the stepsize for the 2ndKSYM and RK3 methods is $h = \pi/3200/2^i, i = 0, 1, 2, 3$, while that for the 4thKSYM and RK5 methods is $h = \pi/200/2^i, i = 0, 1, 2, 3$.

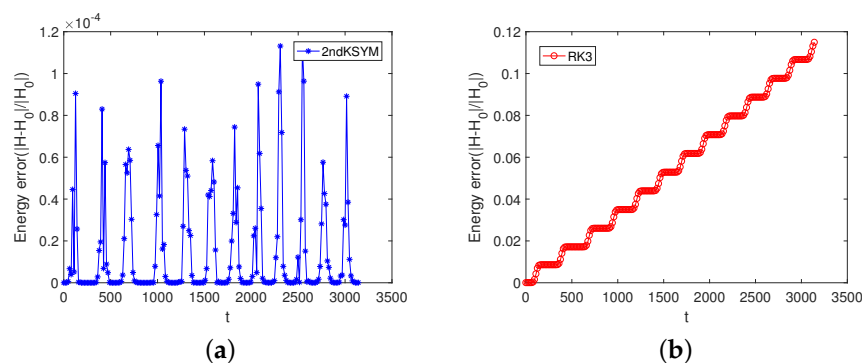


Figure 5. Cont.

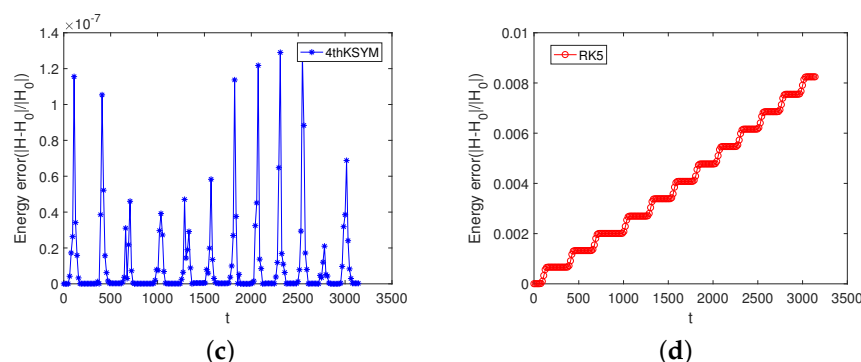


Figure 5. The energy error obtained by the 2ndKSYM, 4thKSYM, RK3 and RK5 methods with the parameter $\epsilon = 1/5$ in Example 2. The stepsize for the 2ndKSYM and RK3 methods is $h = \pi/12,800$, and the stepsize for the 4thKSYM and RK5 methods is $h = \pi/1600$. The time interval is $[0, 1000\pi]$. Subfigures (a,b) are the energy errors obtained by the 2ndKSYM and the RK3 methods. Subfigures (c,d) are the energy errors obtained by the 4thKSYM and the RK5 methods.

5.3. Example 3

The system is normalized according to natural units. We set the particle mass $m = 1$ and electric charge $q = 1$. The electric field is

$$E(\mathbf{X}) = \frac{10^{-2}}{(x_1^2 + x_2^2)^{3/2}}(x_1, x_2, 0) \quad (36)$$

The magnetic field is chosen to be

$$B(\mathbf{X}) = \left(-\frac{3x_1x_3}{r^5}, -\frac{3x_2x_3}{r^5}, -\frac{2x_3^2 - x_1^2 - x_2^2}{r^5} \right) \quad (37)$$

where $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$. When the component of the magnetic field is chosen as the integrand, it can not be integrated explicitly; thus, explicit K-symplectic methods cannot be obtained. Thus, we aim to construct explicit symplectic-like methods for the canonical charged particle system. Accordingly, we can obtain the vector potential as

$$A(\mathbf{X}) = \left(\frac{y}{r^3}, -\frac{x}{r^3}, 0 \right). \quad (38)$$

The initial condition is $Z_0 = (10, 10, 10, 0, 0, 0)$. Displayed in Figure 6 are the orbits projected on the $x_1 - x_2$ plane and the energy evolution of the two symplectic-like methods and two Runge-Kutta methods. It is demonstrated in Figure 6a,b that although the phase orbits of the 2ndSYM method and the RK3 method do not show much difference, the energy error of the 2ndKSYM method is much less than that of the RK3 method. Displayed in Figure 6c,d are the energy errors obtained by the 2ndKSYM, the 4thKSYM, the RK3 and the RK5 methods. The energy error of the 4thSYM method can be bounded within a very small interval, but the energy error of the RK5 method increases without bound. The symplectic-like methods show their long-term energy conservation behavior. Figure 7 shows the computational efficiency of the four methods under two different parameters ϵ . Figure 7a shows the energy error versus the computational time for the four methods for the parameter $\epsilon = \frac{1}{100}$ while Figure 7b shows the energy error versus the computational time for the four methods for $\epsilon = \frac{1}{200}$. Both the energy errors and the CPU times of the two symplectic-like methods are less than those of the two Runge-Kutta methods. The two symplectic-like methods exhibit better efficiency than the two Runge-Kutta methods.

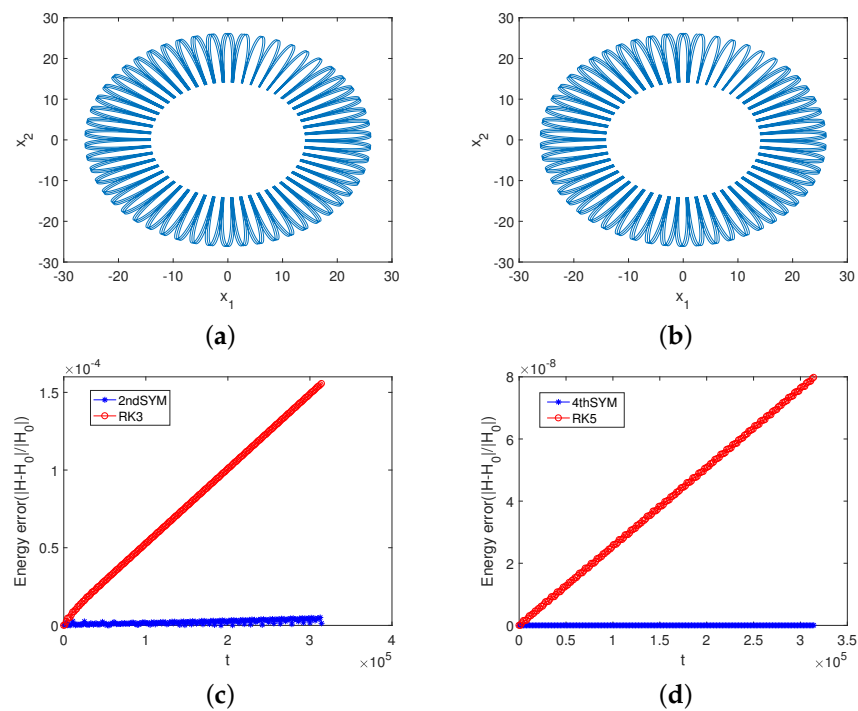


Figure 6. The phase orbit projected on the $x_1 - x_2$ plane and the energy evolution of the 2ndKSYM, 4thKSYM, RK3 and RK5 methods with the parameter $\epsilon = 1/400$ in Example 3. Subfigure (a,b) are the phase orbits obtained by the 2ndKSYM and the RK3 methods with the time interval being $[0, 10^5\pi]$ and the stepsize being $h = \pi/2$. For subfigure (c), the stepsize for the two methods is $h = \pi/2$, while for subfigure (d), the stepsize is $h = \pi$.

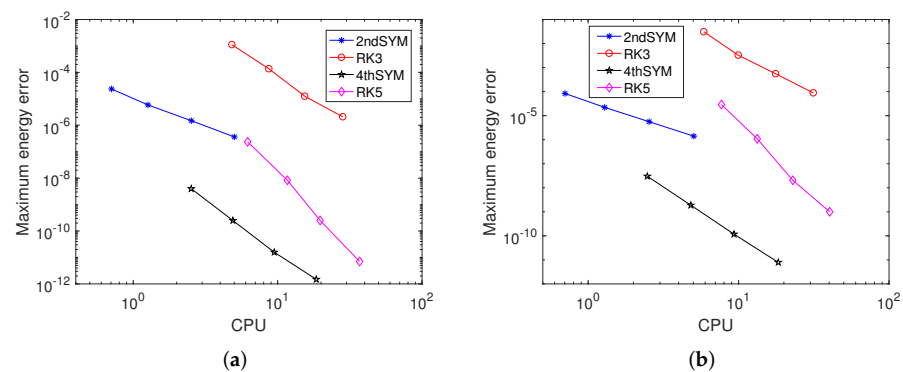


Figure 7. The computational efficiency obtained by the 2ndKSYM, 4thKSYM, RK3 and RK5 methods in Example 3. For subfigure (a), the value is $\epsilon = 1/100$, and the time interval is $[0, 10^5\pi]$. For subfigure (b), the value is $\epsilon = 1/200$, and the time interval is $[0, 10^5\pi]$. In both subfigures, the stepsize for the 2ndKSYM and RK3 methods is $h = \pi/2^i, i = 0, 1, 2, 3$, and the stepsize for the 4thKSYM and RK5 methods is $h = 2\pi/2^i, i = 0, 1, 2, 3$.

5.4. Example 4

The system is normalized according to natural units. We set the particle mass $m = 1$ and electric charge $q = 2$. The electric field is

$$E(\mathbf{X}) = \frac{10^{-2}}{(x_1^2 + x_2^2)^{3/2}}(x_1, x_2, 0). \quad (39)$$

We choose the vector potential as

$$A(\mathbf{X}) = \frac{B_0 r^2}{2Rq} e_\zeta - \ln\left(\frac{R}{R_0}\right) \frac{R_0 B_0}{2} e_{x_3} + \frac{B_0 R_0 x_3}{2R} e_R \quad (40)$$

where $R = \sqrt{x_1^2 + x_2^2}$, $\zeta = \arctan\left(\frac{x_2}{x_1}\right)$. The values are set to be $R_0 = 3$, $B_0 = 1$. Accordingly, we can obtain the magnetic field as

$$B(\mathbf{X}) = \frac{B_0 r}{qR} e_\theta + \frac{B_0 R_0}{R} e_\zeta \quad (41)$$

with the poloidal coordinates being $\theta = \arctan\left(\frac{x_3}{R-R_0}\right)$ and $r = \sqrt{(R-R_0)^2 + x_3^2}$. The initial condition is $Z_0 = (3.15, 0, 0, 0.016, 0.04, 0)$. Displayed in Figure 8 are the energy error and the computational efficiency obtained by the two symplectic-like methods and the two Runge-Kutta methods. The symplectic-like methods have shown their advantage in long-term energy conservation, as shown in Figure 8a,b. The two symplectic-like methods are more efficient than the two Runge-Kutta methods, as shown in Figure 8c,d.

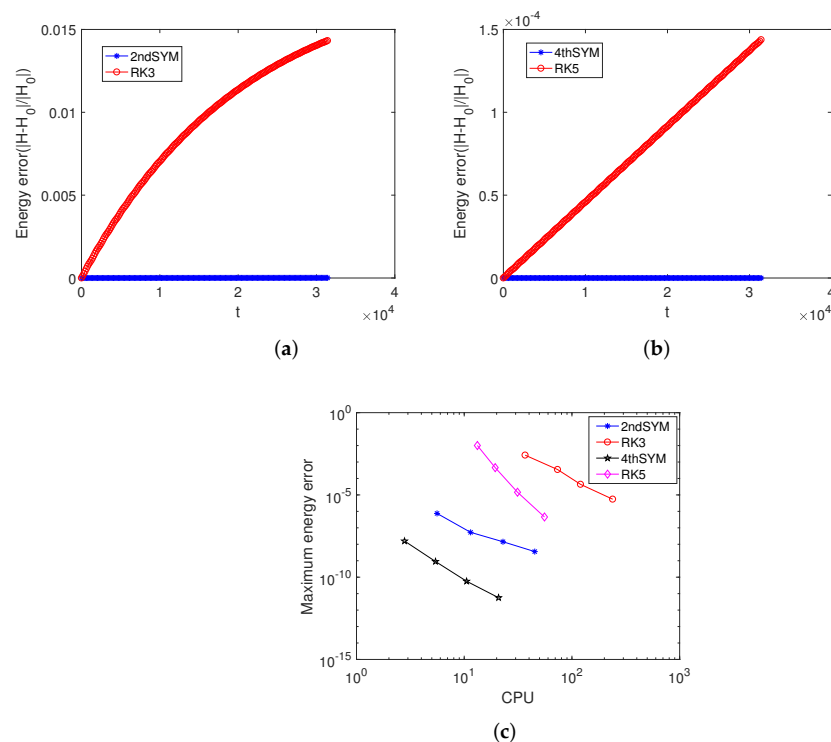


Figure 8. The energy error and the computational efficiency obtained by the 2ndKSYM, 4thKSYM, RK3 and RK5 methods with the parameter $\epsilon = 1/5$ in Example 4. For subfigures (a,b), the time interval is $[0, 10^4 \pi]$. The stepsize for the 2ndKSYM and RK3 methods is $h = \pi/800$, and the stepsize for the 4thKSYM and RK5 methods is $h = \pi/200$. For subfigure (c), the time interval is $[0, 10^3 \pi]$. The stepsize for the 2ndKSYM and RK3 methods is $h = \pi/800/2^i$, $i = 0, 1, 2, 3$, and the stepsize for the 4thKSYM and RK5 methods is $h = \pi/50/2^i$, $i = 0, 1, 2, 3$.

6. Conclusions

We have constructed explicit K-symplectic methods and explicit symplectic-like methods for the charged particle system in the general strong magnetic field. If the three components of the magnetic field can all be integrated explicitly, then we can construct K-symplectic methods; if the above condition does not hold, we can construct symplectic-like methods. Symplectic-like methods can be constructed by extending the original phase

space and obtaining the augmented separable Hamiltonian, and then by using the splitting method and the midpoint permutation. The numerical experiments have shown that the explicit K-symplectic methods and explicit symplectic-like methods have a significant advantage in long-term energy conservation over the higher-order Runge-Kutta methods. Both the K-symplectic methods and the symplectic-like methods exhibit better computational efficiency than the higher-order Runge-Kutta methods. The numerical experiments also show that the effect of the parameter ϵ on the Runge-Kutta methods is larger than the symplectic methods.

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