



Research article

Explicit energy conserving method of two classical dynamical systems

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Abstract: Two classical dynamical systems, the pendulum problem and the Hénon Heiles system, are transformed into the reformulated systems by the nonlinear transformation. These new reformulated systems are transformed into ordinary differential equations on manifolds by the linear transformation. The explicit RKMK method, which is a kind of Lie group method, is applied to solve the differential equations on manifolds. The explicit energy conserving schemes of the two classical dynamical systems are obtained. Numerical simulation investigates the effectiveness of these new schemes in preserving the conservation property of these equations and well simulating dynamical behaviors.

Keywords: Hénon Heiles system; pendulum problem; RKMK method; scalar auxiliary variable approach

Mathematics Subject Classification: 37K05, 65M06

1. Introduction

Dynamical systems have wide applications in vibration problems, fluid dynamics, biological mathematics, etc. Many classical dynamical systems can be written as Hamiltonian systems. The Hamiltonian system has energy conserving property. But the Hamiltonian system has no exact solution in general. Numerical simulation has the important meaning in studying these dynamical systems. Feng et al proposed the symplectic method of the Hamiltonian system [1], which can well simulate the Hamiltonian system for a long time. The symplectic method has been widely applied to different dynamical systems and energy conservation partial differential equations and gained great success. In general, the symplectic method can only approximately preserve the energy conserving property of the Hamiltonian system. Recently, many energy conserving methods for the Hamiltonian dynamical system have also been put forward. McLachlan et al. [2] proposed the discrete gradient method, Quispel et al. [3] proposed the average vector field method, Hairer et al. [4] proposed the

energy conserving collocation method. These energy conserving methods are usually implicit based on the original Hamiltonian dynamical system.

Yang et al proposed the scalar auxiliary variable (SAV) approach for the original Hamiltonian dynamical system by adding new auxiliary variable. The original Hamiltonian dynamical system can be written as the reformulated system by the SAV approach [5, 6]. The reformulated system has the quadratic invariant energy function, which is the same energy as the original Hamiltonian dynamical system [7, 8]. Li et al. [9] transformed the fractional nonlinear Schrödinger (NLS) equations into the reformulated system based on the SAV approach and proposed the implicit energy conserving scheme for the fractional NLS equations. Explicit energy conserving schemes for the reformulated system of the Hamiltonian system have also been proposed by the project method [10, 11].

The reformulated system has quadratic energy conservation. The quadratic energy of the reformulated system is on a manifold. Therefore, the implicit middle scheme can preserve quadratic energy conservation. By the project method, the explicit energy conservation scheme can also be obtained. But the project method needs to change the real value of the numerical solution at every computation step. We find that the reformulated system can be written as the following form by the linear transformation

$$Y(t)' = A(Y(t))Y(t), \quad (1.1)$$

where $Y(t_0) = Y_0$. The solution of Eq (1.1) can be on a manifold. And the corresponding quadratic invariant energy is in fact on the manifold. Many manifold preserving methods were brought up to compute the ordinary differential equation on manifolds, including Crouch-Grossman methods [12], Runge-Kutta-Munthe-Kaas (RKM) method [13, 14], Mangus method [15, 16], the project method [17]. Here, we will apply the famous RKM method to solve the reformulations of the two classical dynamical system: the pendulum problem and the Hénon Heiles equation.

The RKM method, which was a kind of famous Lie group method, is proposed by Munthe-Kaas [13, 14, 18], through which the numerical solution of the Lie group differential equations can be preserved on manifolds exactly. The computation scheme of the RKM method is very simple compared to the other Lie group method [19, 20]. And as a kind of exponential integrator, it also has good stability. The RKM method has been widely used to solve the differential equation on manifolds [21, 22]. In this paper, we present a new explicit energy invariant RKM method for the nonlinear pendulum problem and the Hénon Heiles system based on the nonlinear transformation similar to the SAV approach and RKM method.

The rest of the paper can be organized as follows: In Section 2, the RKM method, which is the Lie group method on a manifold, is introduced. And a fourth-order explicit RKM scheme is presented. In Section 3, the two reformulated systems of the two classical dynamical system, the nonlinear pendulum problem and the Hénon Heiles system, are obtained by the nonlinear transformation similar to the SAV approach. The reformulated systems are changed into the ordinary differential equations on manifolds by the linear transformation. The two reformulated systems are solved by the RKM method. Therefore, the new explicit energy conserving formulas for the two classical dynamical system are proposed. In the last section, numerical simulations investigate the effectiveness of these two new schemes for the two classical dynamical system in preserving property of these equations. Evolution of these dynamical system has also been simulated.

2. The RKMK method on a manifold

The ordinary differential equation on a manifold, which is a n dimensional vector space, can be written as

$$\mathbf{Y}' = \mathbf{A}(\mathbf{Y})\mathbf{Y}, \quad \mathbf{Y}(t_0) = \mathbf{Y}_0 \in R^n, \quad (2.1)$$

$\mathbf{A} : \mathbf{H} \rightarrow h$ is a smooth function, $\mathbf{Y} \in \mathbf{H}$, \mathbf{H} and h are a matrix Lie group and the corresponding Lie algebra. $A(Y)$ is a skew symmetric matrix. It is obvious that the exact solution of Eq (2.1) can be on a manifold

$$\mathbf{M} = \{\mathbf{Y}(t) \mid \mathbf{Y}(t)^T \mathbf{Y}(t) = C\}, \quad (2.2)$$

where C is a constant number.

Calvo, Iserles and Zanna have pointed out that the Lie group is a nonlinear manifold, linear combinations of group elements cannot remain in the group [23]. Therefore, the numerical solution of Eq (2.1) can not stay on the manifold by the classical explicit numerical method, such as the familiar fourth-order Runge-Kutta formula with these coefficients [20].

$$\begin{array}{c|cccc} & 0 & & & \\ & \frac{1}{2} & & & \\ & 0 & \frac{1}{2} & & \\ \hline & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array},$$

cannot guarantee the numerical solution of Eq (2.1) on a manifold exactly.

A classical result was originally given by Felix Hausdorff (1906) that the exact value of Eq (2.1) is expressed as

$$\mathbf{Y}(t) = \exp^{\theta(t)} \mathbf{Y}_0, \quad (2.3)$$

$\exp : g \rightarrow \mathbf{G}$ is the exponential transformation based on Lie algebra g to Lie group \mathbf{G} . $\theta(t) : R \rightarrow g$ means Lie algebra. The solution of Eq (2.1) on a manifold has the Lie group character. Eq (2.1) can also be called Lie group equation. And the matrix function $\theta(t)$ satisfies the Lie algebra differential equation

$$\theta' = \mathbf{dexp}_\theta^{-1} \mathbf{A}(\mathbf{Y}) = \sum_{j=0}^{\infty} g_j \mathbf{ad}^j(\mathbf{A}(\mathbf{Y}), \theta), \quad \theta(t_0) = O, \quad (2.4)$$

where

$$\mathbf{dexp}_\theta^{-1}(\mathbf{A}(\mathbf{Y})) = \mathbf{A}(\mathbf{Y}) - \frac{1}{2}[\theta, \mathbf{A}(\mathbf{Y})] + \frac{1}{12}[\theta, [\theta, \mathbf{A}(\mathbf{Y})]] + \dots = \sum_{j=0}^{\infty} \frac{B_j}{j!} \mathbf{ad}^j(\mathbf{A}(\mathbf{Y}), \theta).$$

The coefficients g_0, g_1, \dots are

$$g_0 = 1, g_1 = B_1 + 1, g_j = \frac{B_j}{j!}, \quad j \geq 2, \quad (2.5)$$

$B_{j=0}^{\infty}$ is the Bernoulli numbers [23–25]. The iterated commutator \mathbf{ad}^j for the matrices W_1 and W_2 is defined as

$$\mathbf{ad}^j(W_1, W_2) = [\mathbf{ad}^{j-1}(W_1, W_2), W_2], \quad j = 1, 2, \dots, \infty. \quad (2.6)$$

And $[., .]$ is the Lie bracket defined by

$$[W_1, W_2] = W_1 W_2 - W_2 W_1, \quad (2.7)$$

$\text{ad}^0(W_1, W_2) = W_1$. When j is taken as the finite number k , the approximation equation of the Lie algebra differential equation

$$\theta' = \sum_{j=0}^k g_j \text{ad}^j(A(Y(t)), \theta), \quad \theta(t_0) = O, \quad (2.8)$$

is obtained. The Lie algebra $\theta(t)$ is a matrix vector space. Munthe-Kaas proposed to solve the approximation matrix Lie algebra differential equation (2.8) by the classical Runge-Kutta method. The computation result approximation Lie algebra equation (2.8) is obtained. Thus, the computation result of Eq (2.1) is also obtained by Eq (2.3). The exponential function is a smooth function, can ensure the correct order of the computation solution. And the computation result of Equation (2.1) can be preserved on a manifold exactly. The method is named for the RKMK method [13, 14]. According to the exponential mapping of the solution of Eq (2.1), a explicit fourth-order RKMK formula can be taken as follows [21]:

We integrate from $Y_n = Y(t_n)$ to $Y_{n+1} = Y(t_{n+1})$

$$\begin{aligned} V_1 &= O, & K_1 &= A(Y_n), \\ V_2 &= \frac{1}{2}hK_1, \\ K_2 &= A(e^{V_2}Y_n) - \frac{1}{2}[V_2, A(e^{V_2}Y_n)] + \frac{1}{12}[V_2, [V_2, A(e^{V_2}Y_n)]], \\ V_3 &= \frac{1}{2}hK_2, \\ K_3 &= A(e^{V_3}Y_n) - \frac{1}{2}[V_3, A(e^{V_3}Y_n)] + \frac{1}{12}[V_3, [V_3, A(e^{V_3}Y_n)]], \\ V_4 &= hK_3, \\ K_4 &= A(e^{V_4}Y_n) - \frac{1}{2}[V_4, A(e^{V_4}Y_n)] + \frac{1}{12}[V_4, [V_4, A(e^{V_4}Y_n)]], \\ \Delta &= h(b_1K_1 + b_2K_2 + b_3K_3 + b_4K_4), \\ Y_{n+1} &= e^\Delta Y_n. \end{aligned} \quad (2.9)$$

3. The reformulations of two classical dynamical systems

3.1. The reformulations of the nonlinear pendulum equation

The nonlinear pendulum always swings regularly around a central value within a certain range. The nonlinear pendulum problem can also be used to illustrate various mechanical phenomena, which is a classical dynamical system. And the motion of this pendulum can be described by the pendulum equation. Here, we consider the following nonlinear pendulum equation [26]

$$\begin{cases} \dot{p} = -\sin q, \\ \dot{q} = p, \end{cases} \quad (3.1)$$

Equation (3.1) can be written as a Hamiltonian system

$$\frac{d\mathbf{z}}{dt} = \mathbf{J} \nabla H(z), \quad (3.2)$$

where $\mathbf{z} = (p, q)^T$,

$$\mathbf{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

with the Hamiltonian function of the nonlinear pendulum equation

$$H(\mathbf{z}) = \frac{1}{2}p^2 + 1 - \cos q. \quad (3.3)$$

By introducing the variable $r = \sqrt{1 - \cos q + c_0}$, where $c_0 > 0$ is a constant number, the SAV reformulation of Eq (3.1) reads

$$\begin{cases} \dot{p} = -2R(q)r, \\ \dot{r} = Rp, \end{cases} \quad (3.4)$$

and

$$\dot{q} = p, \quad (3.5)$$

$$\text{where } R = \frac{\partial r}{\partial q} = \frac{\sin q}{2\sqrt{1-\cos q}}.$$

Equation (3.4) can be written as

$$\frac{d\mathbf{x}}{dt} = \mathbf{D}(q) \nabla_{\mathbf{x}} H, \quad (3.6)$$

where $\mathbf{x} = (p, r)^T$, the corresponding Hamiltonian function is $H(\mathbf{x}) = \frac{1}{2}p^2 + r^2$, and

$$\mathbf{D}(q) = \begin{pmatrix} 0 & -R \\ R & 0 \end{pmatrix}.$$

Equation (3.6) is equivalent to

$$\frac{d\mathbf{x}}{dt} = \mathbf{D}(q) \mathbf{Q} \mathbf{x}, \quad (3.7)$$

where

$$\mathbf{Q} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}.$$

Let $\mathbf{Q} = \mathbf{B}^T \mathbf{B}$, $\mathbf{Y} = \mathbf{B} \mathbf{x}$,

$$\mathbf{B} = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{2} \end{pmatrix},$$

we can obtain the ordinary differential equations

$$\frac{d\mathbf{Y}}{dt} = \mathbf{A}(q) \mathbf{Y} = \mathbf{A}(\mathbf{Y}) \mathbf{Y}, \quad (3.8)$$

where $\mathbf{A}(q) = \mathbf{B} \mathbf{D}(q) \mathbf{B}^T$,

$$\mathbf{A}(q) = \begin{pmatrix} 0 & -\sqrt{2}R \\ \sqrt{2}R & 0 \end{pmatrix}.$$

The solution of Eq (3.8) can be on the manifold

$$M = \{ \mathbf{Y}(t) \mid \mathbf{Y}(t)^T \mathbf{Y}(t) = \frac{1}{2}p^2 + r^2 = C \}, \quad (3.9)$$

where C is a constant. The fourth-order RKMK method (2.9) is applied to solve Eq (3.8). At the same time, Eq (3.6) can be discretized into

$$q^{n+1} = q^n + h(p^{n+1} + p^n)/2. \quad (3.10)$$

Therefore, the new energy conservation scheme of the nonlinear pendulum problem is obtained.

3.2. The reformulations of the Hénon-Heiles system

The Hénon Heiles system describes the motion of particles being confined to a plane, and the potential fields of three body galaxies that limit the motion of particles are symmetrical. The motion of a moving particle in a potential field can be expressed as [27]

$$\begin{cases} \dot{p}_1 = -q_1 - 2q_1q_2, \\ \dot{p}_2 = -q_2 - q_1^2 + q_2^2, \\ \dot{q}_1 = p_1, \\ \dot{q}_2 = p_2. \end{cases} \quad (3.11)$$

Equation (3.11) can be written as the Hamiltonian system

$$\frac{dz}{dt} = \mathbf{J} \nabla H(z), \quad (3.12)$$

where $\mathbf{z} = (p_1, p_2, q_1, q_2)^T$,

$$\mathbf{J} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

with the Hamiltonian function

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2q_2 - \frac{1}{3}q_2^3. \quad (3.13)$$

In the Hénon Heiles system, by introducing a new variable $r = \sqrt{q_1^2q_2 - \frac{1}{3}q_2^3 + c_0}$, ($c_0 > \frac{2}{3}$), where the constant c_0 can ensure the Hamiltonian energy function is positive, we can get an equivalent reformulation

$$\begin{cases} \dot{p}_1 = -q_1 - 2rR_1, \\ \dot{p}_2 = -q_2 - 2rR_2, \\ \dot{q}_1 = p_1, \\ \dot{q}_2 = p_2, \\ \dot{r} = R_1p_1 + R_2p_2, \end{cases} \quad (3.14)$$

where

$$R_1 = \frac{\partial r}{\partial q_1} = \frac{q_1 q_2}{\sqrt{q_1^2 q_2 - \frac{1}{3} q_2^3 + c_0}}, \quad R_2 = \frac{\partial r}{\partial q_2} = \frac{q_1^2 - q_2^2}{2 \sqrt{q_1^2 q_2 - \frac{1}{3} q_2^3 + c_0}}. \quad (3.15)$$

The reformulated Hénon Heiles system (3.14) can be written as

$$\frac{d\mathbf{z}}{dt} = \mathbf{D}(q_1, q_2) \nabla_z H, \quad (3.16)$$

where $\mathbf{z} = (p_1, p_2, q_1, q_2, r)^T$, and

$$\mathbf{D}(q_1, q_2) = \begin{pmatrix} 0 & 0 & -1 & 0 & -R_1 \\ 0 & 0 & 0 & -1 & -R_2 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ R_1 & R_2 & 0 & 0 & 0 \end{pmatrix}.$$

The corresponding Hamiltonian energy function is $H(\mathbf{z}) = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + r^2$. Equation (3.16) is equivalent to

$$\frac{d\mathbf{z}}{dt} = \mathbf{D}(q_1, q_2) \mathbf{Q} \mathbf{z} \quad (3.17)$$

where

$$\mathbf{Q} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}.$$

Let

$$\mathbf{B} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} \end{pmatrix},$$

then $\mathbf{Q} = \mathbf{B}^T \mathbf{B}$, $\mathbf{Y} = \mathbf{B} \mathbf{z}$. We can obtain ordinary differential equations

$$\frac{d\mathbf{Y}}{dt} = \mathbf{A}(q_1, q_2) \mathbf{Y} = \mathbf{A}(\mathbf{Y}) \mathbf{Y}, \quad (3.18)$$

where

$$\mathbf{A}(q_1, q_2) = \mathbf{B} \mathbf{D}(q_1, q_2) \mathbf{B}^T = \begin{pmatrix} 0 & 0 & -1 & 0 & -\sqrt{2}R_1 \\ 0 & 0 & 0 & -1 & -\sqrt{2}R_2 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \sqrt{2}R_1 & \sqrt{2}R_2 & 0 & 0 & 0 \end{pmatrix},$$

is a skew symmetric matrix. The solution of Eq (3.18) can be on the manifold

$$M = \{ \mathbf{Y}(t) \mid \mathbf{Y}(t)^T \mathbf{Y}(t) = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + r^2 = C \}, \quad (3.19)$$

where C is a constant. The fourth-order RKMK method (2.9) is applied to solve Eq (3.18). A new explicit energy-conserving scheme of the Hénon Heiles system is obtained.

4. Simulation of two classical dynamical systems

In the numerical computation part, the explicit fourth-order RKMK formula (2.9) is presented to solve the discrete reformulated system of the nonlinear pendulum problem and the Hénon Heiles system. And $\theta(t)$ is the matrix function. The exponential function $\exp^{\theta(t)}$ is adopted with $\exp(\theta(t))$ in the Matlab software. The discrete energy error is defined as follows:

$$RE(t) = |H(\mathbf{z}^n) - H(\mathbf{z}^0)|. \quad (4.1)$$

In order to compare the energy error, the corresponding fourth order explicit Runge-Kutta (RK) method [20] is utilized to solve the original two Eqs (11) and (21).

4.1. Simulation of the pendulum problem

The initial condition of the pendulum problem (3.1) can be taken as $p = 1, q = 0$, and $c_0 = 1$.

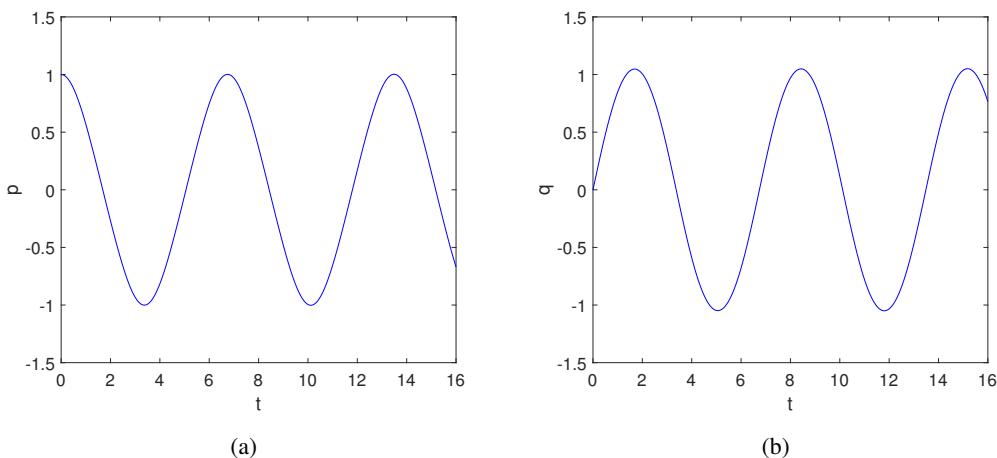


Figure 1. Evolution of solution obtained by RKMK method with $\Delta t = 0.001, t \in [0, 16]$.

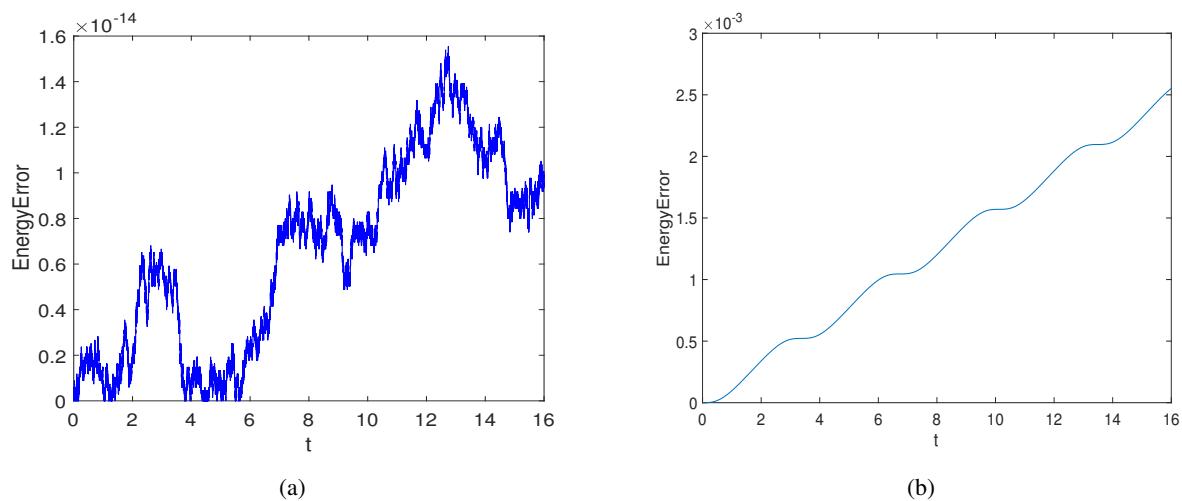


Figure 2. Energy error of Eqs (11) at $t \in [0, 16]$ by (a): RKMK method and (b): RK method.

Figure 1 shows the evolution of the solution $p(t)$ and $q(t)$ at $t \in [0, 16]$. From Figure 1, we can know that the trajectory of the pendulum problem can always swing around the equilibrium position, which reflects the motion of the pendulum. Figure 2(a) shows the discrete energy error of the pendulum problem by the RKMK method. The error is up to 10^{-14} , which can be neglected. Figure 2(b) shows the discrete energy error of the pendulum problem by the RK method. The classical RK method can not preserve the energy invariant of the system exactly. From Figures 1 and 2, we can obtain that the new explicit energy invariant RKMK scheme of the pendulum problem can well simulate the evolution of the solution and preserve the discrete energy conservation of the equation.

4.2. Simulation of the Hénon-Heiles system

As the second example, we choose the initial condition $p_1 = 0, p_2 = 0, q_1 = 0.1, q_2 = -0.5$ at a point local on the boundary of the critical triangular region and $c_0 = 1$.

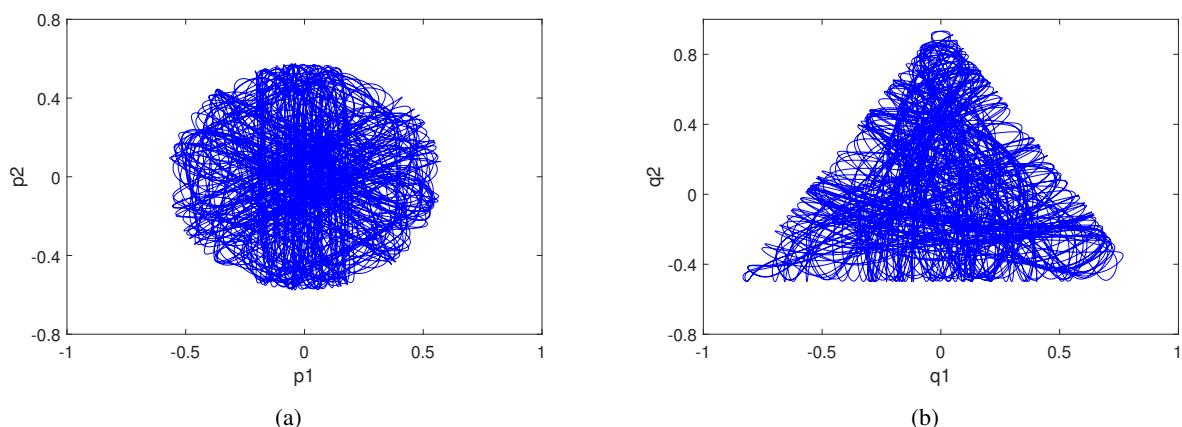


Figure 3. Evolution of solution obtained by RKMK method with $\Delta t = 0.05, t \in [0, 1000]$.

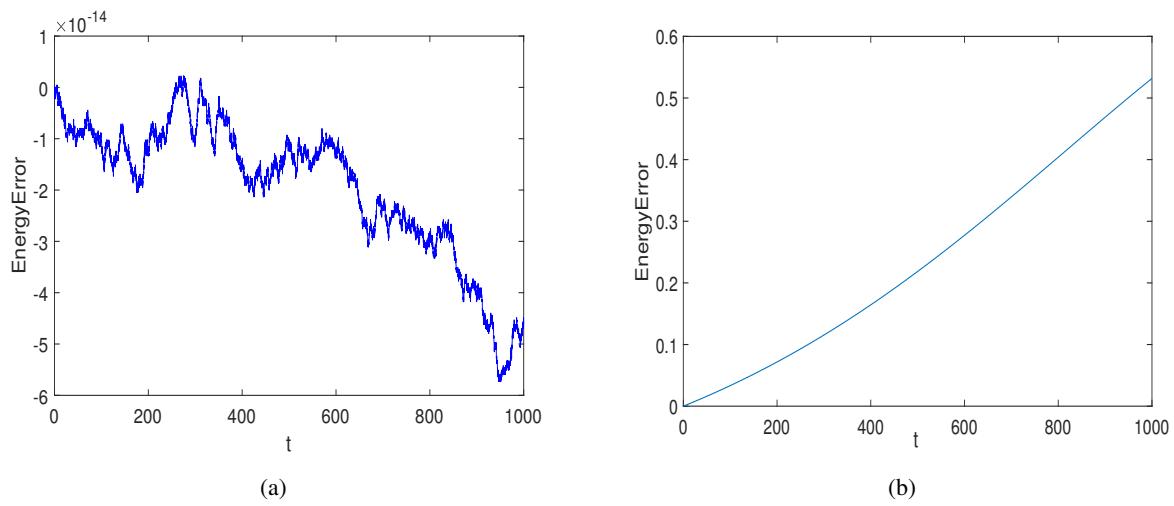


Figure 4. Energy error of Eq (21) at $t \in [0, 1000]$ by (a): RKMK method and (b): RK method.

Figure 3 shows the evolution of the solution of the Hénon Heiles system at $t \in [0, 1000]$ with small temporal step size $\Delta t = 0.05$. The numerical result is consistent with the result in [27]. Figure 4(a) shows the discrete energy error of the Hénon Heiles system at $t \in [0, 1000]$. The error is up to 10^{-14} , which can be neglected. Figure 4(b) shows the discrete energy error of the Hénon Heiles system at $t \in [0, 1000]$ by the RK method. The classical RK method can't preserve the energy invariant of the system. From Figures 3 and 4, we can obtain that the high order explicit energy invariant RKMK scheme of the Hénon-Heiles system can well simulate the evolution of the solution and preserve the discrete energy conservation of the equation.

Then, we choose the initial condition $p_1 = 0, p_2 = 0, q_1 = 0.2, q_2 = -0.3$ at a point local on the boundary of the critical triangular region and $c_0 = 1$.

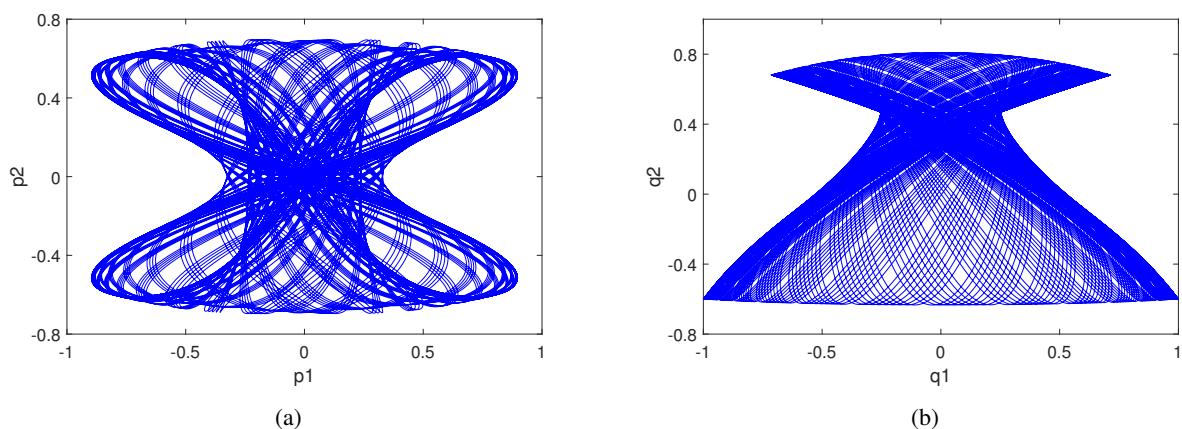


Figure 5. Evolution of solution obtained by RKMK method with $\Delta t = 0.05, t \in [0, 1000]$.

Figure 5 shows the evolution of the solution of the Hénon Heiles system at $t \in [0, 1000]$ with small temporal step size $\Delta t = 0.05$. Figure 6(a) show the discrete energy error of the Hénon Heiles system at

$t \in [0, 1000]$. The error is up to 10^{-14} , which can be neglected. Figure 6(b) shows the discrete energy error of the Hénon Heiles system at $t \in [0, 1000]$ by the RK method. The classical RK method can't preserve the energy invariant of the system. From Figures 5 and 6, we can obtain the high order explicit energy invariant RKMK scheme of the Hénon Heiles system can also well simulate the evolution of the solution and preserve the discrete energy conservation of the equation.

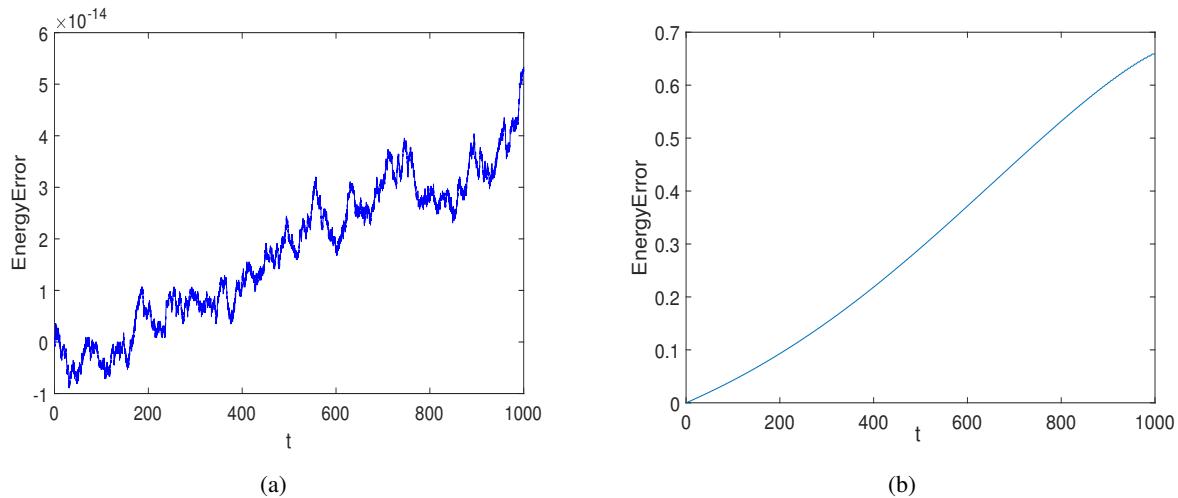


Figure 6. Energy error of Eq (21) at $t \in [0, 1000]$ by (a): RKMK method and (b): RK method.

5. Conclusions

In conclusion, we put forward energy invariant explicit RKMK formula to solve the pendulum problem and the Hénon Heiles system. Numerical results indicate that the new explicit formulas can well simulate the evolution of the solution of these systems and preserve the discrete energy invariant of these systems. Compared to the explicit scheme of the reformulated system of energy conservation differential equations based on the project method, the new method is rather simple and does not need to change the real value of the numerical solution at every computation step. Compared to the classical explicit RK method, the new method can preserve the energy of the Hamiltonian system exactly. Obviously, the new energy invariant explicit RKMK method can also be adopted to solve other energy conservation Hamiltonian dynamical systems, which have the same property as the two classical dynamical systems. But the new method can not solve the general Hamiltonian systems. In the future, we will study the high order explicit energy preserving method for the general Hamiltonian systems.

Author contributions

Jianqiang Sun: Formal analysis, Investigation, Methodology, Validation, Review; Jie Chen: Conceptualization, Data curation, Methodology, Software, Writing; Lijuan Zhang: Data curation, Investigation, Resources, Software, Writing. All authors have read and agreed to the published version of the manuscript.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflicts of interest.

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