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Structure-preserving algorithms for the Duffing equation*

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In this paper, the dissipative and the forced terms of the Duffing equation are considered as the perturbations of nonlinear Hamiltonian equations and the perturbational effect is indicated by parameter ε. Firstly, based on the gradient-Hamiltonian decomposition theory of vector fields, by using splitting methods, this paper constructs structure-preserving algorithms (SPAs) for the Duffing equation. Then, according to the Liouville formula, it proves that the Jacobian matrix determinants of the SPAs are equal to that of the exact flow of the Duffing equation. However, considering the explicit Runge–Kutta methods, this paper finds that there is an error term of order p+1 for the Jacobian matrix determinants. The volume evolution law of a given region in phase space is discussed for different algorithms, respectively. As a result, the sum of Lyapunov exponents is exactly invariable for the SPAs proposed in this paper. Finally, through numerical experiments, relative norm errors and absolute energy errors of phase trajectories of the SPAs and the Heun method (a second-order Runge–Kutta method) are compared. Computational results illustrate that the SPAs are evidently better than the Heun method when ε is small or equal to zero.

Keywords: structure-preserving algorithm, Duffing equation, gradient-Hamiltonian decomposition, Runge–Kutta method

PACC: 0547, 0260, 4630M

1. Introduction

In 1918, Duffing introduced a nonlinear oscillator with a cubic stiffness. Since then, the study of its phase portraits becomes one of the most famous problems in the field of nonlinear oscillations.[1] Moon and Holmes[2,3] gave the modified Duffing equation as

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \delta\frac{\mathrm{d}x}{\mathrm{d}t} - x + x^3 = F\cos(\omega t). \tag{1}$$

This equation is known as the double-welled forced Duffing equation, where the damping coefficient is $\delta \geq 0$, $x - x^3$ denotes a restore force and $F\cos(\omega t)$ is a forced term. Through the application of variable substitution and the multiplication of small parameter ε before the dissipative and the forced terms, Eq.(1) can be transformed into first-order autonomous equations in a normal form, i.e.

$$\begin{aligned} &\mathrm{d}x/\mathrm{d}t = y, \\ &\mathrm{d}y/\mathrm{d}t = x - x^3 + \varepsilon(-\delta y + F\cos(\omega z)), \\ &\mathrm{d}z/\mathrm{d}t = 1. \end{aligned} \tag{2}$$

After this transformation, Eq.(2) can be considered as the perturbation system of the following nonlinear Hamiltonian system,

$$\begin{aligned} &\mathrm{d}x/\mathrm{d}t = y = \partial H/\partial y, \\ &\mathrm{d}y/\mathrm{d}t = x - x^3 = -\partial H/\partial x, \end{aligned} \tag{3}$$

where $H = (-x^2 + y^2)/2 + x^4/4$.

The Duffing equation is a simple and classic equation of mathematical physics. Researchers have been carrying out a lot of studies on it. Guckenheimer and Holmes[1] performed systemically qualitative and quantitative analysis on the Duffing equation. Ding[4] gave proper mathematical analysis and proof on the nonresonance properties of different forms of the Duffing equation. Based on one-dimensional map, Zhu *et al* [5] discussed the scaling property of bifurcation regions. By using Taylor transformation, Su *et al* [6] computed the chaos and periodic properties of the Duffing equation. In Ref.[7], Ma *et al* employed Laguerre polynomial approximation method to study the bifurcation and chaotic behaviour of the Duffing equation with a random parameter.

Since the appearance of symplectic algorithms,[8] researchers attach more and more importance to structure-preserving algorithms (SPAs). Hairer *et*

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al,[9] Feng and Qin[10] make descriptions of SPAs in detail. It is feasible and easy to construct SPAs by using splitting methods and order conditions can be easily given by the Baker–Campbell–Hausdorff formula.

In this paper, splitting methods are adopted to construct SPAs for the Duffing equation with small dissipation. The SPAs and Runge–Kutta methods are compared through qualitative analysis and numerical experiments.

2. The gradient-Hamiltonian decomposition (GHD) theory of vector fields

A vector field $\boldsymbol{f}$ can be expressed as the sum of a gradient vector field $\boldsymbol{f}_{\rm G}:\mathbf{R}^n\to\mathbf{R}^n$ and a source-free vector field $\boldsymbol{f}_{\rm H}:\mathbf{R}^n\to\mathbf{R}^n$, i.e. $\boldsymbol{f}=\boldsymbol{f}_G+\boldsymbol{f}_{\rm H}$.[11] $\boldsymbol{f}_{\rm G}$ can be expressed as a negative gradient of a scalar function, i.e. $\boldsymbol{f}_{\rm G}=-I\nabla G(\boldsymbol{u})$ where I is a unit matrix and $G\in C^\infty(\mathbf{R}^n,\mathbf{R})$. $\boldsymbol{f}_{\rm H}$ can be decomposed into the sum of Hamiltonian vector fields, namely $\boldsymbol{f}_{\rm H}=\sum J_i\nabla H_i\ (1\leq i\leq n)$, where J_i is a skew-symmetric matrix and H_i is the Hamiltonian function. In a two-dimensional case, $\boldsymbol{f}_{\rm H}$ is simply a Hamiltonian vector field.

Let $\boldsymbol{u}=[x,y,z]^{\rm T}$, according to the GHD theory of vector fields, Eq.(2) can be decomposed into a gradient system and a source-free system, i.e.

$$\boldsymbol{f}_{\rm G}=\boldsymbol{f}^{(1)}=-I\nabla G, \tag{4a}$$

$$\boldsymbol{f}_{\rm H}=J_1\nabla H_1+J_2\nabla H_2, \tag{4b}$$

where $G=\varepsilon\delta y^2/2$, $H_1=H=(-x^2+y^2)/2+x^4/4$, $H_2=(\varepsilon F\sin(\omega z))/\omega-y$, $J_1=\begin{bmatrix}0&1&0\\-1&0&0\\0&0&0\end{bmatrix}$ and $J_2=\begin{bmatrix}0&0&0\\0&0&1\\0&-1&0\end{bmatrix}$.

The source-free system expressed by Eq.(4b) can be further decomposed into three exact integrable vector fields: $\boldsymbol{f}^{(2)}=[y,\ 0,\ 0]^{\rm T}$, $\boldsymbol{f}^{(3)}=\big[0,\ x-x^3,\ 0\big]^{\rm T}$ and $\boldsymbol{f}^{(4)}=[0,\ F\cos(\omega z),\ 1]^{\rm T}$. Thus, Eq.(2) can be rewritten as

$$\dot{\boldsymbol{u}}=\boldsymbol{f}(\boldsymbol{u})=\sum_{i=1}^{4}\boldsymbol{f}^{(i)}(\boldsymbol{u}). \tag{5}$$

3. Construction of SPAs by using splitting methods

For an open set U in a 3-dimensional Euclidean space $\boldsymbol{R}^3$, we use $\varphi_t:\mathbf{R}^3\to\mathbf{R}^3$ to denote the exact flow mapping of $\dot{\boldsymbol{u}}=\boldsymbol{f}(\boldsymbol{u})$. Record the corresponding exact flow mapping of $\boldsymbol{f}^{(1)}(\boldsymbol{u})$, $\boldsymbol{f}^{(2)}(\boldsymbol{u})$, $\boldsymbol{f}^{(3)}(\boldsymbol{u})$ and $\boldsymbol{f}^{(4)}(\boldsymbol{u})$ as $\varphi_t^{(1)}$, $\varphi_t^{(2)}$, $\varphi_t^{(3)}$ and $\varphi_t^{(4)}$, respectively. In terms of splitting methods of ordinary differential equations,[9] a first-order one-step algorithm can be constructed to approximate φ_t and we have

$$\psi_h^1=\varphi_h^{(1)}\circ\varphi_h^{(2)}\circ\varphi_h^{(3)}\circ\varphi_h^{(4)}, \tag{6}$$

where h denotes the step size. The adjoint algorithm of ψ_h^1 is $(\psi_h^1)^*=\varphi_h^{(4)}\circ\varphi_h^{(3)}\circ\varphi_h^{(2)}\circ\varphi_h^{(1)}$. Composing ψ_h^1 and $(\psi_h^1)^*$, we can obtain a second-order symmetric algorithm $\psi_h^2=\psi_{h/2}^1\circ(\psi_{h/2}^1)^*$. Based on ψ_h^2, by using composition methods, a higher-order symmetric SPA can be constructed.[9] We adopt $\psi_{h,{\rm SPA}}^p$ to represent the unified form of the above SPAs ψ_h^1, $(\psi_h^1)^*$ and ψ_h^2. Since the first-order explicit Euler method and the Heun method are both explicit Runge–Kutta methods, we use $\psi_{h,{\rm RK}}^p$ to denote the corresponding unified form.

4. Propositions

In this section, two propositions are proposed and proved. We discuss whether the algorithms preserve the volume evolution law of a region in phase space. For the proof of propositions, it is necessary to introduce the Liouville formula first.

Theorem (Liouville formula).[12] For differential equations $\dot{\boldsymbol{u}}=\boldsymbol{f}(\boldsymbol{u})$ in $\mathbf{R}^n$, let $\boldsymbol{R}^n$ and $\partial f_i(\boldsymbol{u})/\partial u_j$ are continuous on $\boldsymbol{u}$ for an open set $\boldsymbol{U}\subset\mathbf{R}^n$, then the determinant of Jacobian matrix of the flow is equal to the exponent of the vector field divergence integral along the trajectory, i.e.

$$\det(D\varphi_t)=\exp\bigg(\int_0^t\nabla\cdot\boldsymbol{f}(\boldsymbol{u})\mathrm{d}s\bigg).$$

Proposition 1 For the Duffing equation, the Jacobian matrix determinant of the SPA $\psi_{h,{\rm SPA}}^p$ is equal to that of the exact flow φ_h, i.e.

$$\det(D\psi_{h,{\rm SPA}}^p(\boldsymbol{u}))=\det(D\varphi_h(\boldsymbol{u})).$$

For the explicit Runge–Kutta method $\psi^p_{h,\mathrm{RK}}$, the Jacobian matrix determinant contains an error term of order p+1, i.e.

$$\det(D\psi^p_{h,\mathrm{RK}}(\boldsymbol{u})) = \det(D\varphi_h(\boldsymbol{u})) + \mathcal{O}(h^{p+1}).$$

Proof For the first-order SPA ψ^1_h, we have

$$\det(D\psi^1_h(\boldsymbol{u})) = \det(D\varphi^{(1)}_h \circ \varphi^{(2)}_h \circ \varphi^{(3)}_h \circ \varphi^{(4)}_h(\boldsymbol{u})).$$

According to the chain rule and the Liouville formula, we can obtain

$$\begin{aligned}\det(D\psi^1_h(\boldsymbol{u})) =& \prod_{i=1}^{4} \det(D\varphi^{[i]}_h(\boldsymbol{u}))\\ =& \prod_{i=1}^{4} \exp\Big(\int_0^h \nabla \cdot f^{[i]}(\boldsymbol{u})\mathrm{d}s\Big)\\ =& \exp\Big(\sum_{i=1}^{4}\int_0^h \nabla \cdot f^{[i]}(\boldsymbol{u})\mathrm{d}s\Big)\\ =& \exp(-\varepsilon\delta h)\\ =& \det(D\varphi_h(\boldsymbol{u})).\end{aligned}$$

Similarly, we can prove that

$$\det(D(\psi^1_h)^*(\boldsymbol{u})) = \det(D\psi^2_h(\boldsymbol{u})) = \det(D\varphi_h(\boldsymbol{u})).$$

For the Runge–Kutta method, we get

$$\begin{aligned}\det(D\psi^p_{h,\mathrm{RK}}(\boldsymbol{u})) =& \det(D(\varphi_h(u) + \mathcal{O}(h^{p+1})))\\ =& \exp(-\varepsilon\delta h) + \mathcal{O}(h^{p+1})\\ =& \det(D(\varphi_h(\boldsymbol{u})) + \mathcal{O}(h^{p+1}).\end{aligned}$$

Suppose that D is a region in $\mathbf{R}^3$ with a limited volume and a smooth boundary. Let $D(t)$ be the region formed by the exact flow φ_t for time t, i.e. $D(t) = \varphi_t(D)$. It is obvious that $D(0)$=D. Let $V(t)$ be the volume of $D(t)$. Similarly, we have $D_{\mathrm{SPA}}(t)$ and $V_{\mathrm{SPA}}(t)$ for the SPAs, and $D_{\mathrm{RK}}(t)$ and $V_{\mathrm{RK}}(t)$ for the Runge–Kutta methods. When t=0, we can obtain that $D_{\mathrm{SPA}}(0) = D_{\mathrm{RK}}(0) = D(0)$ and $V_{\mathrm{SPA}}(0) = V_{\mathrm{RK}}(0) = V(0)$.

Proposition 2 For SPAs and Runge–Kutta methods, there exist the following two formulas, respectively:

$$V_{\mathrm{SPA}}(t) = V(t),$$
$$V_{\mathrm{RK}}(t) = V(0)(\exp(-\varepsilon\delta h) + \mathcal{O}(h^{p+1}))^n.$$

Proof

$$\begin{aligned}V_{\mathrm{SPA}}(h) =& \int_{D(h)} \mathrm{d}V\\ =& \int_{D(0)} \det(D\psi^p_{h,\mathrm{SPA}}(\boldsymbol{u}))\mathrm{d}V\\ =& V(0)\exp(-\varepsilon\delta h),\end{aligned}$$

$$\begin{aligned}V_{\mathrm{SPA}}(t) =& V_{\mathrm{SPA}}(nh)\\ =& V(0)\exp(-\varepsilon\delta nh)\\ =& V(0)\exp(-\varepsilon\delta t)\\ =& V(t).\end{aligned}$$

$$\begin{aligned}V_{\mathrm{RK}}(h) =& \int_{D(h)} \mathrm{d}V\\ =& \int_{D(0)} \det(D\psi^p_{h,\mathrm{RK}}(u))\mathrm{d}V\\ =& V(0)(\exp(-\varepsilon\delta h) + \mathcal{O}(h^{p+1})),\end{aligned}$$

$$\begin{aligned}V_{\mathrm{RK}}(t) =& V_{\mathrm{RK}}(nh)\\ =& V(0)(\exp(-\varepsilon\delta h) + \mathcal{O}(h^{p+1}))^n.\end{aligned}$$

Remark When $t = nh \to +\infty$, $V_{\mathrm{SPA}}(t)$ will certainly decrease monotonically to zero in accordance with an exponent law $V(0)\exp(-\varepsilon\delta t)$. This is completely the same as the evolution law of $V(t)$ formed by the exact flow. Although, for $V_{\mathrm{RK}}(t)$, at each iterative step, there is an error term $\mathcal{O}(h^{p+1})$ in comparison with the evolution law of the exact flow, this does not contradict with the fact that $V_{\mathrm{RK}}(t)$ will be eventually contracted to zero. Thus, the sequence $\{V_{\mathrm{RK}}(0)$,V_{RK}(h),$V_{\mathrm{RK}}(2h)\ldots\}$ produced by Runge–Kutta methods is still convergent. It can be concluded that there exists $0 < \eta < 1$ such that if $0 < h < \eta$, we have the inequality $0 < \exp(-\varepsilon\delta h) + \mathcal{O}(h^{p+1}) < 1$. Hence, there is

$$\begin{aligned}\lim_{t\to+\infty} V_{\mathrm{RK}}(t) =& \lim_{n\to+\infty} V_{\mathrm{RK}}(nh)\\ =& \lim_{t\to+\infty} V(t)\\ =& 0.\end{aligned}$$

In addition, the SPAs exactly preserve the divergence of the system expressed by Eq.(2), which is $-\varepsilon\delta$. Therefore, the sum of Lyapunov exponents is exactly invariable for the SPAs constructed in this paper.[12]

5. Numerical experiments

In this section, numerical experiments are performed by using the SPAs proposed above and Runge–Kutta methods. Considering conditions of zero perturbation ($\varepsilon = 0$) and small perturbation ($\varepsilon = 0.01 << 1$), we compare relative norm errors and absolute energy errors of phase trajectories of the SPAs and Runge–Kutta methods, respectively. For

the comparison results between the first-order methods and those between the second-order ones are completely similar, we only take comparisons between the second-order SPA ψ_h^2 and the Heun method for an example. Since there are no exact solutions for the Duffing equation, we can use results of the dverk78 method in Maple (a computer algebra language) as the exact solutions. The dverk78 can find a numerical solution using a seventh-eighth order continuous Runge–Kutta method. It is capable of working in arbitrary precision based on the setting of Maple and can be used to obtain high accuracy solutions, but it takes more time than other methods. The relative norm errors of phase trajectories are defined as $TE = ||\boldsymbol{u}_{\text{dverk78}} - \boldsymbol{u}_n||/||\boldsymbol{u}_{\text{dverk78}}||$ and the absolute energy errors of phase trajectories defined as $EE = H_{\text{dverk78}} - H_n$.

For numerical computations under the condition of zero perturbation ($\varepsilon = 0$), let the initial point be P and the corresponding coordinates be $x(0) = 0.2$ and $y(0) = z(0) = 0$, $t \in [0, 200]$ and the step size be h=0.1. Phase trajectories obtained by ψ_h^2 and the Heun method are shown in Figs.1 and 2.

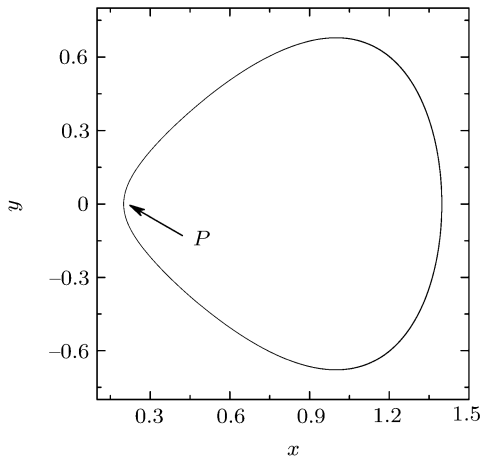


Fig.1. The phase trajectory of ψ_h^2 (h=0.1).

For $\varepsilon = 0$, Eq.(2) can be simplified as Eq.(3). In this case, the level set $H = 0$ is composed of a pair of homoclinic trajectories and a saddle point. For the given initial point P, the level set $H_P < 0$ and $x = 0.01 > 0$. Hence, from the point of qualitative analysis, the computational result should be a closed trajectory in the right half xy-plane (as shown in Fig.1). From Fig.2, the qualitative behaviour derived by the Heun method is wrong. The trajectory obtained by the Heun method is developed spirally outward and run from the right closed branch into the left one. For this case, only by further reducing step size can the Heun method give a correct qualitative behaviour (as shown in Fig.3 when h=0.01).

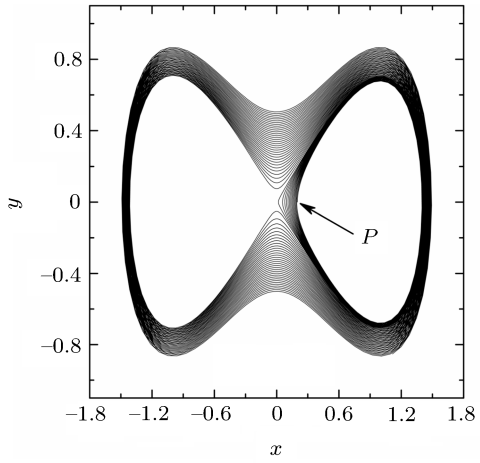


Fig.2. The phase trajectory of the Heun method (h=0.1).

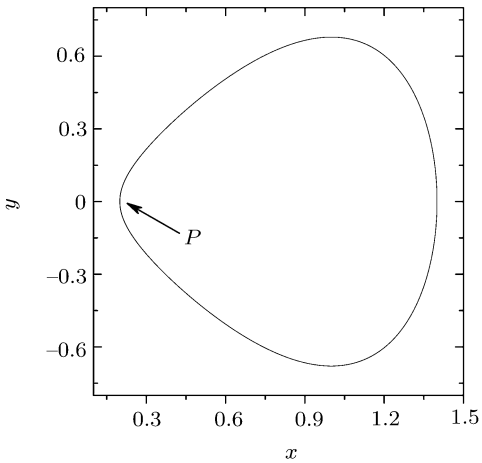


Fig.3. The phase trajectory of the Heun method (h=0.01).

For h=0.01, the relative norm errors and the absolute energy errors of the phase trajectories are shown in Figs.4 and 5. From these figures, the errors of the SPA are varying periodically about a fixed value, which is of great significance for the numerical simulation of long-time qualitative properties. It is clear that numerical results by the SPA are better than those of the Heun method.

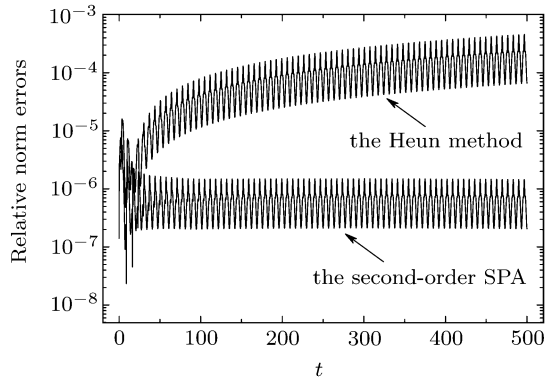


Fig.4. Relative norm errors of phase trajectories ($\varepsilon = 0$).

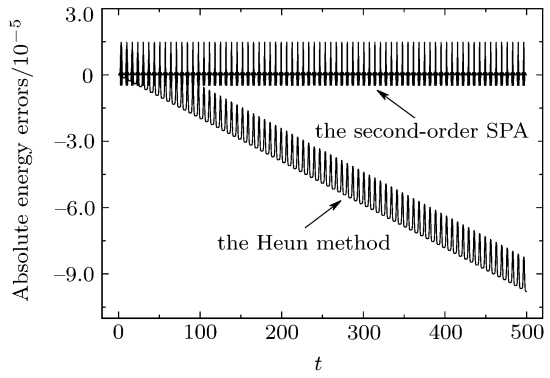


Fig.5. Absolute energy errors ($\varepsilon = 0$).

Under small perturbation condition ($\varepsilon = 0.01 << 1$), we take $h = 0.01$, $\delta = 0.25$, $F = 0.4$ and $\omega = 1$ for numerical computations. The computational results are similar with those for $\varepsilon = 0$. The corresponding relative norm errors and the absolute energy errors of the phase trajectories are shown in Figs.6 and 7. The errors vibration amplitudes of the SPA are evidently smaller than those of the Heun method.

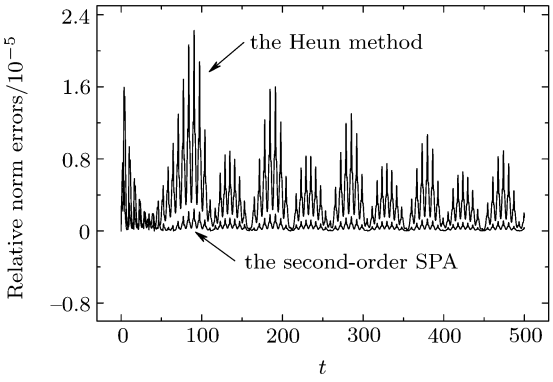


Fig.6. Relative norm errors of phase trajectories ($\varepsilon = 0.01$).

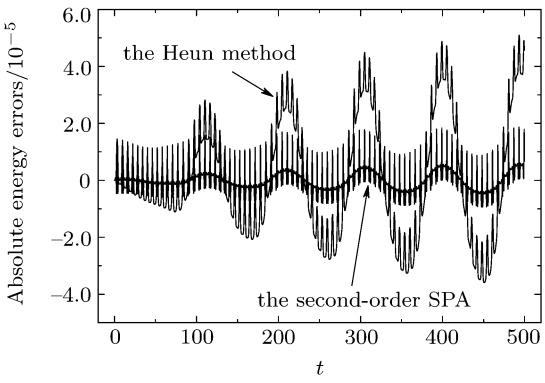


Fig.7. Absolute energy errors ($\varepsilon = 0.01$).

When $\varepsilon = 1$, Eq.(2) shows a very complex dynamic behaviour, which is first observed by Ueda and called chaos. It is well known that when a nonlinear oscillation system shows a chaotic phenomenon, the solution in the chaotic set is very sensitive to initial values of parameters and consequently sensitive to the accuracy and the step size of numerical algorithms. When the initial values are given within the chaotic set, there is no sense to discuss solution errors. Even so, it is necessary to mention that for the SPAs of the Duffing equation constructed in this paper, there is a very important invariant, i.e. the sum of Lyapunov exponents is exactly invariable.

6. Conclusions

In this paper, for the Duffing equation, the SPAs are constructed based on splitting methods, and two important propositions are proposed and proved. Correspondingly, we perform some numerical experiments by using different methods. The computational results illustrate that the SPAs can exactly preserve global qualitative behaviour properties of a system, i.e. $\det(D\psi^p_{h,\mathrm{SPK}}(\boldsymbol{u})) = \det(D\varphi_h(\boldsymbol{u}))$ and $V_{\mathrm{SPA}}(t) = V(t)$. For small or zero perturbation, computational results by the SPAs are evidently better than those of the Heun method. When chaotic phenomenon appears for a system, the sum of Lyapunov exponents of the SPAs can be exactly preserved, which is expected to show superiority for the simulation of chaotic phenomenon.

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