A general symplectic integrator for canonical Hamiltonian systems

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Abstract

The focus of this paper is to recommend a novel symplectic scheme for canonical Hamiltonian systems. The new scheme contains a real parameter which makes the symplectic Euler methods and implicit midpoint rule as its special cases. The validity of the symplecticity of this scheme is well explained from the perspectives of the generating function and partitioned Runge-Kutta methods. The generating function of the new symplectic scheme with new coordinates is studied, and these coordinates include the three typical coordinates. Employing the generating function method and symmetric composition methods, two new classes of symplectic schemes of any high order are devised, respectively. Furthermore, based on these symplectic schemes, two energy-preserving schemes and the feasibility of constructing higher order energy-preserving schemes are presented by the parameter serving for clever tuning. The solvability of all the schemes mentioned is proved, and the numerical performances of these schemes are demonstrated with numerical experiments.

Keywords: Hamiltonian systems; Symplectic schemes; Generating function; Hamilton-Jacobi equation; Symmetric composition methods; Energy-preserving schemes

1. Introduction

All real physical processes with negligible dissipation could be represented in the appropriate Hamiltonian form. The canonical Hamiltonian system has the following form

\[
\dot{p} = -H_q(p, q), \quad \dot{q} = H_p(p, q),
\]

where \(H_p\) and \(H_q\) denote the column vectors of partial derivatives of the Hamiltonian. As a first integral of the system, the Hamiltonian represents the physical meaning of the total energy. The system (1.1) serving as the basic mathematical formalism often appears in the relevant areas of analytical dynamics, geometrical optics, particle accelerators, plasma physics, control theory and hydrodynamics, etc. The most characteristic property of (1.1) is the symplecticity and energy conservation along any exact flows. These facts motivate to search for numerical methods that preserve one or more properties of the system. Numerical methods conserving the symplecticity are called symplectic integrators and were first introduced in the pioneering work of De Vogelaere [1]. Here, the symplectic Euler methods and implicit midpoint rule with \(h\) as the time step can be written in relatively simple forms as follows:

\[
\begin{align*}
p_{n+1} &= p_n - hH_q(p_n, q_n), \\
q_{n+1} &= q_n + hH_p(p_n, q_n),
\end{align*}
\]

\[\text{or } \begin{align*}
p_{n+1} &= p_n - hH_q(p_n, q_{n+1}), \\
q_{n+1} &= q_n + hH_p(p_n, q_{n+1}).
\end{align*}\]

\[
\begin{align*}
p_{n+1} &= p_n - hH_q\left(\frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2}\right), \\
q_{n+1} &= q_n + hH_p\left(\frac{p_n + p_{n+1}}{2}, \frac{q_n + q_{n+1}}{2}\right).
\end{align*}
\]

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The milestone-style works of symplectic integrators were developed in [2,7]. Feng [4] has obtained symplectic integrators by verifying that the one-step map associated with a numerical method is symplectic, and thus proved the symplectic properties of methods (1.2) and (1.3). It is worth noting that Hairer et al. [7] presented a symplectic method called the Störmer-Verlet method by the composition of (1.2). The symplectic members of Runge-Kutta (RK) methods have been studied in [8]. Sanz-Serna [5] has given the RK symplecticity condition for the first time and confirmed the existence of symplectic integrators of any high order. Another general and simple way to construct symplectic RK methods was derived in [8] with the help of symplecticity condition [7, 9] of partitioned RK methods. Symplectic partitioned RK methods which are extensions of symplectic RK methods have been investigated in [6,11]. Gan et al. [11] has defined the symplectic adjoint method and given an approach for constructing symplectic partitioned RK methods. The numerical performance of symplectic integrators that always has excellent long-time behaviour and stability was demonstrated in [7, 12]. There are currently many ways to construct symplectic integrators, but of the methods obtained, only the methods (1.2) and (1.3) have the simplest form, and the application of these two methods in some practical problems [13] is very friendly.

In this paper, we propose a novel symplectic scheme with a real parameter $\lambda$ as follows:

$$
\begin{align*}
    p_{n+1} &= p_n - hH_q(\lambda p_{n+1} + (1 - \lambda) p_n, \lambda q_n + (1 - \lambda) q_{n+1}), \\
    q_{n+1} &= q_n + hH_p(\lambda p_{n+1} + (1 - \lambda) p_n, \lambda q_n + (1 - \lambda) q_{n+1}).
\end{align*}
$$

(1.4)

We denote the above scheme as Scheme I. For the case where $\lambda = 0, 1, \frac{1}{2}$, respectively, we recognize the symplectic Euler methods (1.2) and implicit midpoint rule (1.3). For any $\lambda$, the symplecticity of Scheme I is proved in the next section. It is note that the correct pairing of variables of the Hamiltonian plays a key role in the symplecticity of Scheme I. Furthermore, when $\lambda \neq \frac{1}{2}$ Scheme I is a one-stage symplectic partitioned RK method of order 1. Substituting $1 - \lambda$ for $\lambda$ yields the adjoint method of Scheme I, and the resulting method is still symplectic.

A fundamental approach devised for constructing symplectic schemes is based on generating functions, the theory of which has been completely established in [1, 7, 14, 15]. The generating function is a solution of Hamilton-Jacobi equation that can generate arbitrary symplectic mappings. It is theoretically possible to find such a function to generate a given symplectic transformation. Actually, for symplectic RK and partitioned RK methods, Hairer et al. [7] have presented the explicit expression of the generating functions. According to the relationship between generating functions and the exact flows of Hamiltonian systems, the generating function method was first proposed in [15], where Feng and Qin chosen the suitable coordinates of generating functions and their explicit power series of time $t$. Symplectic integrators of any high order can be generated by truncating this series to approximate the solution of the Hamilton-Jacobi equation. Following this research route, we first introduce a generating function with new coordinates and the associated Hamilton-Jacobi equation. Then the connection between Scheme I and the solution of this Hamilton-Jacobi equation is obtained. In order to avoid the calculation of higher derivatives of the Hamiltonian in the generating function method, we derive an approach to obtain the symmetric symplectic scheme of any high order without higher derivatives of the Hamiltonian by symmetric composition methods [16] and the symplecticity of the adjoint method of Scheme I.

At present, the research on energy-preserving schemes of the system (1.1) is also a prominent route. Although symplectic integrators are superior in long-time behavior, they fail to conserve non-quadratic first integrals. It is natural to think about whether such a discretization scheme can be found to share both the symplecticity and energy conservation of the exact flow of (1.1). It is verified in [17, 18] that the constant time stepping scheme cannot inherit both features for general Hamiltonian systems. The only symplectic method (as B-series) that conserves the Hamiltonian for arbitrary $H$ is the exact flow of the differential equation. This difficulty has been solved in a weaker sense to obtain symplectic-energy-momentum integrators [19], where time step adaption is used to impose energy conservation. A new family of methods was introduced in [20], known as averaged vector field (AVF) method, which can exactly preserve the energy for Hamiltonian systems. With the advent of partitioned AVF methods [21], the computational efficiency of such methods has been greatly improved. The Hamiltonian boundary value methods were discussed in [22], which can be energy-preserving when the Hamiltonian is a polynomial. For more details on energy-preserving schemes, please refer to [7, 23, 25]. In particular, Hairer et al. presented a one-parameter integrator called modified midpoint rule [7] suitable for separable Hamiltonian systems, where the parameter was suitably tuned to
enforce energy conservation. In this paper, we propose an energy-preserving scheme by adjusting the real parameter \( \lambda \) in Scheme I, which reads

\[
\begin{cases}
p_{n+1} = p_n - hH_q(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_{n} + (1 - \lambda)q_{n+1}), \\
q_{n+1} = q_n + hH_p(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_{n} + (1 - \lambda)q_{n+1}), \\
H(p_{n+1}, q_{n+1}) = H(p_n, q_n).
\end{cases}
\]

(1.5)

In the subsequent content, it will be clear that this scheme accurately maintains all quadratic first integrals associated with the system \((1.1)\). The feasibility of constructing high order energy-preserving schemes is also mentioned, and the solvability of all the schemes reported in this paper is confirmed in the later section. It is worth mentioning that in such a way the Hamiltonian in the last equation of \((1.5)\) can be replaced with any non-quadratic first integral of \((1.1)\) to achieve other invariant conservation.

The rest of this paper is organized as follows. In Section 2, a direct proof of the symplecticity of Scheme I is deduced. In Section 3, the symplecticity of Scheme I is illustrated from two different perspectives of the generating function method and partitioned RK methods. We introduce the generating function with new coordinates and derive the corresponding Hamilton-Jacobi equation. It will be seen that the generating function with new coordinates generates the exact flow of the Hamiltonian system \((1.1)\). In addition, we provide three symplectic schemes, two of which are symmetric. In Section 4, two energy-preserving schemes are devised and the theoretical proof of the existence of the solution for all the schemes is presented. Numerical experiments in Section 5 support our theoretical analysis. Finally, some concluding remarks are given in Section 6.

2. Direct proof of the symplecticity of Scheme I

In this section, a simple proof of the symplecticity of Scheme I is presented. We denote the exact flow of the system \((1.1)\) by \( \varphi_t \) that advances the solution by time \( t \), i.e., \( \varphi_t(p_0, q_0) = (p(t, p_0, q_0), q(t, p_0, q_0)) \), where \( p(t, p_0, q_0), q(t, p_0, q_0) \) is a solution of the system corresponding to initial values \( p(0) = p_0, q(0) = q_0 \). Then the symplectic conservation law \([20]\) is equivalent to

\[
\left( \frac{\partial \varphi_t(p_0, q_0)}{\partial (p_0, q_0)} \right)^T J \left( \frac{\partial \varphi_t(p_0, q_0)}{\partial (p_0, q_0)} \right) = J,
\]

(2.1)

where \( J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \) and \( I \) is an identity matrix with appropriate dimensions.

**Theorem 2.1.** Scheme I is symplectic for any \( \lambda \).

**Proof.** In order to prove that Scheme I is symplectic, we only need to verify the validity of \((2.1)\) \([4]\), i.e.,

\[
\left( \frac{\partial (p_{n+1}, q_{n+1})}{\partial (p_n, q_n)} \right)^T J \left( \frac{\partial (p_{n+1}, q_{n+1})}{\partial (p_n, q_n)} \right) = J.
\]

(2.2)

Differentiating the two equations of Scheme I with respect to \( p_n \) and \( q_n \) yields

\[
\begin{pmatrix} I + \lambda hH_{qp} - \lambda hH_{pp} \\ -\lambda hH_{qp} - \lambda hH_{pp} \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} I & I \\ 0 & 0 \end{pmatrix}.
\]

It is apparent that the coefficient matrix is diagonally dominant. Let the notations

\[
A = I + \lambda hH_{qp}, \quad B = I - (1 - \lambda)hH_{pp}, \quad C = hH_{qq}, \quad D = hH_{pp},
\]

then the matrixes \( A, B \) and \( E \triangleq B + \lambda(1 - \lambda)DA^{-1}C \) are non-singular. This allows us to compute the Jacobian matrix \( \frac{\partial (p_{n+1}, q_{n+1})}{\partial (p_n, q_n)} \) as

\[
\begin{pmatrix} A^{-1}B^T - (1 - \lambda)A^{-1}CE^{-1}D((1 - \lambda)I + \lambda A^{-1}B^T) & A^{-1}C((1 - \lambda)E^{-1}(\lambda^2DA^{-1}C - A^T) - \lambda I) \\ E^{-1}D((1 - \lambda)I + \lambda A^{-1}B^T) & -E^{-1}(\lambda^2DA^{-1}C - A^T) \end{pmatrix}.
\]

Inserting it into the left-hand side of \((2.2)\) and taking a simple matrix multiplication, we get the relation \((2.2)\). The proof is completed. \( \square \)
Remark 2.1. When $\lambda = \frac{1}{2}$, Scheme I is of order 2, otherwise it is of order 1. It is noted that when $\lambda = \frac{1}{2}$, Scheme I is the implicit midpoint rule, which is known to be of order 2. The accuracy of Scheme I can be obtained by computing the Taylor expansion to approximate the exact solution of (1.1), and we omit the detail proof.

Remark 2.2. The examples of Scheme I with four choices of $\lambda$ are applied to (1.1) as follows:

$$
\begin{align*}
\lambda &= -1 : \\
&\begin{cases}
p_{n+1} = p_n - hH_q(2p_n - p_{n+1}, 2q_{n+1} - q_n), \\
q_{n+1} = q_n + hH_p(2p_n - p_{n+1}, 2q_{n+1} - q_n);
\end{cases}
\end{align*}
$$

$$
\begin{align*}
\lambda &= \frac{1}{3} : \\
&\begin{cases}
p_{n+1} = p_n - hH_q\left(\frac{2p_n + p_{n+1}}{3}, \frac{2q_{n+1} + q_n}{3}\right), \\
q_{n+1} = q_n + hH_p\left(\frac{2p_n + p_{n+1}}{3}, \frac{2q_{n+1} + q_n}{3}\right);
\end{cases}
\end{align*}
$$

$$
\begin{align*}
\lambda &= \frac{3}{2} : \\
&\begin{cases}
p_{n+1} = p_n - hH_q\left(\frac{3p_{n+1} - p_n}{2}, \frac{3q_{n} - q_{n+1}}{2}\right), \\
q_{n+1} = q_n + hH_p\left(\frac{3p_{n+1} - p_n}{2}, \frac{3q_{n} - q_{n+1}}{2}\right);
\end{cases}
\end{align*}
$$

$$
\begin{align*}
\lambda &= 2 : \\
&\begin{cases}
p_{n+1} = p_n - hH_q(2p_{n+1} - p_n, 2q_n - q_{n+1}), \\
q_{n+1} = q_n + hH_p(2p_{n+1} - p_n, 2q_n - q_{n+1}).
\end{cases}
\end{align*}
$$

Notice that we show the three cases where $\lambda$ is outside the range of 0 to 1. Their symplecticity is confirmed by Theorem 2.1 and will be demonstrated in the numerical experiments.

Remark 2.3. Assume that we have a Hamiltonian system with separable Hamiltonian $H(p, q) = T(p) + U(q)$, where the expressions $T$ and $U$ represent the kinetic energy and potential energy of the system (1.1). Scheme I applied to separable systems has the following form

$$
\begin{align*}
&\begin{cases}
p_{n+1} = p_n - hU_q(\lambda q_n + (1 - \lambda)q_{n+1}), \\
q_{n+1} = q_n + hT_p(\lambda p_{n+1} + (1 - \lambda)p_n).
\end{cases}
\end{align*}
$$

It is explicit if and only if $\lambda = 0$ or 1, which is the classic symplectic Euler methods for separable systems.

3. Reconstruction of Scheme I based on two different frameworks and some other results

In this section, we interpret the symplecticity of Scheme I based on the generating function method and partitioned RK methods. The generating function method [15] plays a central role in the construction of symplectic schemes. Any symplectic transformations can be generated with various generating functions. We bring in the generating function with new coordinates and establish the relevant Hamilton-Jacobi equation theory. Furthermore, three symplectic schemes are given, including Scheme I proposed in this paper.

3.1. Generating function with new coordinates

The construction of generating functions is dependent on the different choices of coordinates. And a given symplectic transformation can theoretically be obtained from a generating function. We first give the following lemma which, as we know, is called the integrability lemma [7]. In order to facilitate the expression, some notations are introduced. We consider a Hamiltonian system with $d$ degrees of freedom and a fixed time interval $[t_0, t_1]$, and denote by $p, q \in \mathbb{R}^d$ the initial values $p_1, \cdots, p_d$ and $q_1, \cdots, q_d$ at $t_0$, respectively. Likewise, the exact solution of the system at $t_1$ is represented by $P, Q \in \mathbb{R}^d$. This implies that the mapping $(p, q) \mapsto (P, Q)$ is symplectic.
Lemma 3.1. Let $D \subset \mathbb{R}^n$ be an open set and $f : D \to \mathbb{R}^n$ be continuously differentiable, and assume that the Jacobian $f'(y)$ is symmetric for all $y \in D$. Then, for every $y_0 \in D$ there exists a neighbourhood and a function $H(y)$ such that the differential form
\[ f_1(y)dy_1 + \cdots + f_n(y)dy_n = dH \]
is a total differential on this neighbourhood.

Theorem 3.1. Let $\lambda$ be a real number and the mapping $\varphi : (p, q) \mapsto (P, Q)$ be smooth, close to the identity. It is symplectic if and only if a function $S(\lambda P + (1 - \lambda)p, \lambda q + (1 - \lambda)Q)$ exists locally such that
\[ (Q - q)^T d(\lambda P + (1 - \lambda)p) - (P - p)^T d(\lambda q + (1 - \lambda)Q) = dS. \quad (3.1) \]

Proof. Applying the smoothness of the mapping $\varphi$, we write the Jacobian matrix of $\varphi$ as a block matrix
\[ \frac{\partial(P, Q)}{\partial(p, q)} = \begin{pmatrix} p & q \\ q & p \end{pmatrix}. \]
Inserting this into (2.1) and taking a simple calculation, the symplecticity is equivalent to the following conditions
\[ P_p Q_p = Q_p^T P_p, \quad Q_q^T P_q = Q_p^T Q_q, \quad Q_p^T P_q + I = P_p^T Q_q. \quad (3.2) \]
Substituting $dP = P_p dp + P_q dq$, $dQ = Q_p dp + Q_q dq$ into the left-hand side of (3.1), we obtain
\[ \left( \lambda P_p^T (Q - q) - (1 - \lambda)Q_p^T (P - p) + (1 - \lambda)(Q - q) \right)^T \begin{pmatrix} dp \\ dq \end{pmatrix}. \quad (3.3) \]

In order to use Lemma 3.1, one would like to expect the symmetry of the Jacobian matrix of the coefficient vector of (3.3). With this idea, we get the Jacobian matrix
\[ \lambda \begin{pmatrix} P_p^T Q_p & P_p^T Q_q \cr P_q^T Q_p & P_q^T Q_q \end{pmatrix} - \begin{pmatrix} Q_p^T P_p & Q_p^T P_q + I \\ Q_q^T P_p & Q_q^T P_q \end{pmatrix} + \lambda \sum_{i=1}^d (Q_i - q_i) \frac{\partial^2 P_i}{\partial(p, q)^2} \]
\[ + \begin{pmatrix} (1 - \lambda)(Q_p + Q_q^T) & -\lambda P_p^T + (1 - \lambda)Q_q^T \\ -\lambda P_p + (1 - \lambda)Q_q \end{pmatrix} - (1 - \lambda) \sum_{i=1}^d (P_i - p_i) \frac{\partial^2 Q_i}{\partial(p, q)^2}. \quad (3.4) \]

Since the Hessian matrixes of $P_i$ and $Q_i$ are symmetric, it is obvious that the symmetry of (3.4) is equivalent to the symplecticity conditions (3.2). Hence there exists locally a function $\hat{S}(p, q)$ such that
\[ (Q - q)^T d(\lambda P + (1 - \lambda)p) - (P - p)^T d(\lambda q + (1 - \lambda)Q) = d\hat{S}. \]
In order to simplify, we introduce the following notations
\[ u = \lambda P + (1 - \lambda)p, \quad v = \lambda q + (1 - \lambda)Q \]
in the subsequent section. Moreover, we define an implicit function group
\[ \left\{ \begin{array}{l} F_1(u, v, p, q) \triangleq \lambda P(p, q) + (1 - \lambda)p - u = 0, \\
F_2(u, v, p, q) \triangleq (1 - \lambda)Q(p, q) + \lambda q - v = 0. \end{array} \right. \quad (3.5) \]
The Jacobi matrix of (3.5) is obtained as follows:
\[ \frac{\partial(F_1, F_2)}{\partial(p, q)} = \begin{pmatrix} I + \lambda(\frac{\partial P}{\partial p} - I) \\ (1 - \lambda)\frac{\partial Q}{\partial p} - \lambda(\frac{\partial Q}{\partial q} - I) \end{pmatrix}. \quad (3.6) \]
Since the mapping $\varphi$ is close to the identity, the matrix (3.6) is always nonsingular. The implicit function theorem thus proves that $p$ and $q$ are both functions of the new coordinates $u$ and $v$. Setting
\[ S(u, v) \triangleq \hat{S}(p(u, v), q(u, v)), \]
this completes the proof.
Comparing the coefficient functions of $dS = \partial_u S du + \partial_v S dv$ with the left-hand side of (3.1), we derive the system

$$
\begin{align*}
P &= p - \partial_v S(\lambda P + (1 - \lambda)p, \lambda q + (1 - \lambda)Q), \\
Q &= q + \partial_u S(\lambda P + (1 - \lambda)p, \lambda q + (1 - \lambda)Q).
\end{align*}
$$

(3.7)

Theorem 3.1 tells us that whatever the scalar function $S$ is, the system (3.7) defines a symplectic transformation $(p, q) \mapsto (P, Q)$ for any fixed parameter $\lambda$. It is once again noticed that the correct pairing of variables of the Hamiltonian plays a key role in the symplecticity of (3.7).

**Remark 3.1.** Theorem 3.1 gives a more general form of generating functions. In particular, when $\lambda = 0, 1, \frac{1}{2}$, respectively, we reproduce the generating functions with the three typical coordinates [7] as follows:

1. $(Q - q)^T dp - (P - p)^T dq = dS_1$ for some function $S_1(p, Q)$;
2. $(Q - q)^T dP - (P - p)^T dq = dS_2$ for some function $S_2(P, q)$;
3. $(Q - q)^T d(P + p) - (P - p)^T d(Q + q) = 2dS_3$ for some function $S_3(\frac{P + p}{2}, \frac{Q + q}{2})$.

Similar to (3.7), we get the next systems with respect to the above three points that can be written as

$$
\begin{align*}
\lambda = 0 : \quad & \begin{cases} 
P = p - \partial_q S_1(p, Q), \\
Q = q + \partial_p S_1(p, Q);
\end{cases} \\
\lambda = 1 : \quad & \begin{cases} 
P = p - \partial_q S_2(P, q), \\
Q = q + \partial_p S_2(P, q);
\end{cases} \\
\lambda = \frac{1}{2} : \quad & \begin{cases} 
P = p - \partial_v S_3(\frac{P + p}{2}, \frac{Q + q}{2}), \\
Q = q + \partial_u S_3(\frac{P + p}{2}, \frac{Q + q}{2}).
\end{cases}
\end{align*}
$$

(3.8), (3.9), (3.10)

Setting $S_1 = hH(p, Q), S_2 = hH(P, q)$ and $S_3 = hH(\frac{P + p}{2}, \frac{Q + q}{2})$ in turn, we recognize the symplectic Euler methods and implicit midpoint rule applied to a Hamiltonian system.

### 3.2. The Hamilton-Jacobi equation with new variables

We now continue the above construction of $S$ for a symplectic mapping $(p, q) \mapsto (P, Q)$. The Hamilton-Jacobi equations corresponding to the three typical variables were discussed in [7, 15]. The Hamilton-Jacobi theory for a new time-dependent generating function $S(u, v, t)$ will be presented in this subsection. Assuming the point $(P(t), Q(t))$ to move along the exact flow of the Hamiltonian system (1.1), it is found that a smooth generating function $S(u, v, t)$ generates via (3.7) the exact flow of the Hamiltonian system.

**Theorem 3.2.** Let $\lambda$ be a real number. If $S(u, v, t)$ is a smooth solution of the partial differential equation

$$
\frac{\partial S}{\partial t}(u, v, t) = H(u - (1 - \lambda) \frac{\partial S}{\partial v}(u, v, t), v + \lambda \frac{\partial S}{\partial u}(u, v, t))
$$

(3.11)

with initial condition $S(u, v, 0) = 0$, then the mapping $(p, q) \mapsto (P, Q)$, defined by (3.7), is the exact flow of the Hamiltonian system (1.1).

**Proof.** From the hypothesis, the mapping $(p, q) \mapsto (P, Q)$ is the transformation given by (3.7). Differentiating the first relation of (3.7) with respect to time $t$ yields

$$
\frac{\partial^2 S}{\partial v^2}(u, v, t) = -(I + \lambda \frac{\partial^2 S}{\partial u \partial v}(u, v, t)) \dot{P} - (1 - \lambda) \frac{\partial^2 S}{\partial v^2}(u, v, t) \dot{Q}.
$$

(3.12)

Differentiating both sides of the Hamilton-Jacobi equation (3.11) about the variable $v$ reads

$$
\frac{\partial^2 S}{\partial t \partial v}(u, v, t) = -(1 - \lambda) \frac{\partial^2 S}{\partial v^2}(u, v, t) H_P(P, Q) + (I + \lambda \frac{\partial^2 S}{\partial u \partial v}(u, v, t)) H_Q(P, Q).
$$

(3.13)
Subtracting (3.13) from (3.12), we obtain

\[(I + \lambda \frac{\partial^2 S}{\partial u \partial v}(u,v,t))(\dot{P} + H_Q(P,Q)) + (1 - \lambda) \frac{\partial^2 S}{\partial v^2}(u,v,t)(\dot{Q} - H_P(P,Q)) = 0.\]  

(3.14)

Similarly, differentiating the second relation of (3.7) and using (3.11) lead to

\[-\lambda \frac{\partial^2 S}{\partial u^2}(u,v,t)(\dot{P} + H_Q(P,Q)) + (I - (1 - \lambda) \frac{\partial^2 S}{\partial u \partial v}(u,v,t))(\dot{Q} - H_P(P,Q)) = 0.\]  

(3.15)

Combining equations (3.14) and (3.15), we get the following matrix equation

\[
\begin{pmatrix}
I + \lambda \frac{\partial^2 S}{\partial u \partial v}(u,v,t)
& (1 - \lambda) \frac{\partial^2 S}{\partial v^2}(u,v,t)

-\lambda \frac{\partial^2 S}{\partial u^2}(u,v,t)
& I - (1 - \lambda) \frac{\partial^2 S}{\partial u \partial v}(u,v,t)
\end{pmatrix}
\begin{pmatrix}
\dot{P} + H_Q(P,Q)

\dot{Q} - H_P(P,Q)
\end{pmatrix} = 0.
\]

(3.16)

Owing to the mapping \((p,q) \mapsto (P,Q)\) defined by (3.7), close to the identity, the coefficient matrix of the equation (3.16) is invertible. This proves the validity of the first and second equations of the Hamiltonian system (1.1), i.e.,

\[\dot{P} = -H_Q(P,Q), \quad \dot{Q} = H_P(P,Q).\]

With the system (3.7), the initial condition \(S(u,v,0) = 0\) ensures that

\[P(0) = p, \quad Q(0) = q.\]

This completes the proof.

\(\square\)

**Remark 3.2.** Based on Theorem 3.2, we can obtain the Hamilton-Jacobi equations under the three typical variables [7, 15]. That is, when \(\lambda = 0, 1, \frac{1}{2}\), respectively, the following three items hold as

(1) Suppose that \(S_1(p,Q,t)\) is a smooth solution of

\[\frac{\partial S_1}{\partial t}(p,Q,t) = H(p - \frac{\partial S_1}{\partial Q}(p,Q,t),Q), \quad S_1(p,Q,0) = 0,\]  

(3.17)

then the exact flow of the Hamiltonian system (1.1) satisfies the system (3.8);

(2) Suppose that \(S_2(P,q,t)\) is a smooth solution of

\[\frac{\partial S_2}{\partial t}(P,q,t) = H(P,p + \frac{\partial S_2}{\partial P}(P,q,t)), \quad S_2(P,q,0) = 0,\]  

(3.18)

then the exact flow of the Hamiltonian system (1.1) satisfies the system (3.9);

(3) Suppose that \(S_3(\xi,\eta,t)\) is a smooth solution of

\[\frac{\partial S_3}{\partial t}(\xi,\eta,t) = H(\xi - \frac{1}{2} \frac{\partial S_3}{\partial \eta}(\xi,\eta,t),\eta + \frac{1}{2} \frac{\partial S_3}{\partial \xi}(\xi,\eta,t)), \quad S_3(\xi,\eta,0) = 0,\]  

(3.19)

then the exact flow of the Hamiltonian system (1.1) satisfies the system (3.10), where the notations \(\xi = \frac{P + p}{2}, \eta = \frac{Q + q}{2}\).

3.3. Symplectic schemes based on generating functions

It is well-known that a series of symplectic schemes with arbitrary order of accuracy based on the above generating functions (3.8)–(3.10) and the Hamilton-Jacobi equations (3.17)–(3.19) can be constructed [15]. The generating function with new coordinates is introduced in this paper. We still consider gaining an approximate solution of the Hamilton-Jacobi equation (3.11) to construct symplectic schemes of any high order. For this purpose, we consider a convergent power series about \(t\) as follows:

\[S(u,v,t) = \sum_{i=1}^{\infty} K_i(u,v)t^i,\]  

(3.20)
which is an explicit expression of the generating function $S$ with undetermined coefficients $K_i$, and automatically satisfies the initial condition $S(u, v, 0) = 0$. Inserting this series into (3.21) and comparing like powers of $t$ follow

\[
K_1(u, v) = H(u, v),
\]

\[
K_2(u, v) = (\lambda - \frac{1}{2}) \left( \frac{\partial H}{\partial u} \right)^T \frac{\partial H}{\partial v}(u, v),
\]

\[
K_3(u, v) = \frac{1}{2} (\lambda^2 - \lambda + \frac{1}{3}) \left( \frac{\partial H}{\partial u} \right)^T \frac{\partial^2 H}{\partial v^2} \frac{\partial H}{\partial u} + \left( \frac{\partial H}{\partial v} \right)^T \frac{\partial^2 H}{\partial u^2} \frac{\partial H}{\partial v} \right)(u, v)
+ (\lambda^2 - \lambda + \frac{1}{6}) \left( \frac{\partial H}{\partial v} \right) \frac{\partial^2 H}{\partial u \partial v} \frac{\partial H}{\partial u} \right)(u, v),
\]

and further $K_i(u, v), i \geq 4$ can be obtained by computing the Taylor expansion in (3.11). A natural way to approximate $S$ is to truncate the series (3.20) as

\[
\tilde{S}(u, v) = \sum_{i=1}^{r} K_i(u, v) h^i,
\]

and insert it into (3.7). Then we get a symplectic scheme of order $r$. Symplecticity follows at once from Theorem 3.1 and order $r$ is a consequence of the fact that the series (3.21) is the $r$-th order approximation to (3.20). Next, three symplectic schemes for (1.1) are devised, which contain a real parameter $\lambda$. For all the following schemes, we use the notations

\[
\tilde{u} = \lambda p_{n+1} + (1 - \lambda) p_n, \quad \tilde{v} = \lambda q_n + (1 - \lambda) q_{n+1}.
\]

The following two schemes can be obtained by taking $r = 1, 2$ in (3.21), respectively.

\[
\begin{cases}
p_{n+1} = p_n - h \partial_{\tilde{u}} H(\tilde{u}, \tilde{v}), \\
q_{n+1} = q_n + h \partial_{\tilde{v}} H(\tilde{u}, \tilde{v}).
\end{cases}
\]

\[
\begin{cases}
p_{n+1} = p_n - h \partial_{\tilde{u}} H(\tilde{u}, \tilde{v}) - (\lambda - \frac{1}{2}) h^2 \frac{\partial^2 H}{\partial \tilde{v}^2} \frac{\partial H}{\partial \tilde{u}} + \frac{\partial^2 H}{\partial \tilde{v} \partial \tilde{u}} \frac{\partial H}{\partial \tilde{v}} \right)(\tilde{u}, \tilde{v}), \\
q_{n+1} = q_n + h \partial_{\tilde{v}} H(\tilde{u}, \tilde{v}) + (\lambda - \frac{1}{2}) h^2 \left( \frac{\partial^2 H}{\partial \tilde{u}^2} \frac{\partial H}{\partial \tilde{v}} + \frac{\partial^2 H}{\partial \tilde{u} \partial \tilde{v}} \frac{\partial H}{\partial \tilde{u}} \right)(\tilde{u}, \tilde{v}).
\end{cases}
\]

Note that the former is indeed Scheme I, and we name the latter Scheme II. According to the above discussion, it is obtained that Schemes I–II are symplectic schemes of order 1, 2, respectively. Similarly, keeping the coefficient function $K_3(u, v)$, a symplectic scheme of order 3 can be gained. This procedure can be repeated to obtain symplectic schemes of any high order. It is unfortunately noted that for $r \geq 2$, the schemes require the computation of higher derivatives of the Hamiltonian.

### 3.4. Symplectic schemes based on symmetric composition methods

With the purpose of avoiding higher derivatives of the Hamiltonian, we consider the symmetric composition methods [7, 16]. Scheme I represents a mapping

\[
\Phi_h^\lambda : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}),
\]

which is called the numerical flow. By a straightforward check, the adjoint method of scheme I is

\[
(\Phi_h^\lambda)^* = \Phi_h^{1-\lambda}.
\]

It is surprising to note that $\Phi_h^{1-\lambda}$ is also symplectic. Hence the symmetry requirement for order 2 leads to a new symplectic numerical flow, denoted by

\[
\Psi_h \triangleq \Phi_h^\lambda \circ (\Phi_h^\lambda)^* = \Phi_h^\lambda \circ \Phi_h^{1-\lambda} : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}),
\]

\[
(3.24)
\]

\[
8
\]
which is named Scheme III. The symplecticity of Scheme III follows from the fact that the composition of symplectic schemes is still symplectic. Symmetric schemes applied to a Hamiltonian system also have advantages with regards to excellent long-time behaviour and stability.

Using the idea of composition methods, we can continue to drive a symmetric symplectic scheme of order 4 by the symmetric composition of Scheme III. Just as the Triple Jump and Suzuki’s Fractals [7, 27], this procedure can also be repeated to construct higher order symmetric symplectic schemes without higher derivatives of the Hamiltonian. Here, we only present Scheme III as an example of this class of symmetric symplectic schemes.

3.5. Derivation of Scheme I based on partitioned RK methods

In view of the special form of Scheme I and the system (1.1) given in the partitioned form, we attempt to give another derivation of Scheme I by the formula of partitioned RK methods. Applying partitioned RK methods [6, 7] to (1.1), we can get the next relations

\[
\begin{align*}
    k_i &= -H_q(p_n + h \sum_{j=1}^{s} a_{ij}k_j, q_n + h \sum_{j=1}^{s} \hat{a}_{ij}l_j), \\
    l_i &= H_p(p_n + h \sum_{j=1}^{s} a_{ij}k_j, q_n + h \sum_{j=1}^{s} \hat{a}_{ij}l_j), \\
    p_{n+1} &= p_n + h \sum_{i=1}^{s} b_{i1}k_i, 
     q_{n+1} = q_n + h \sum_{i=1}^{s} \hat{b}_{i1}l_i,
\end{align*}
\]

where \(b_i, a_{ij}\) and \(\hat{b}_i, \hat{a}_{ij}\) \((i, j = 1, \ldots, s)\) are the coefficients of two different RK methods with \(s\) stages. It is known that if the identities below

\[
\begin{align*}
    b_i \hat{a}_{ij} + \hat{b}_j a_{ji} &= b_i \hat{b}_j \quad \text{for } i, j = 1, \ldots, s, \\
    b_i &= \hat{b}_i \quad \text{for } i = 1, \ldots, s,
\end{align*}
\]

are satisfied with a given partitioned RK method, then it is symplectic [7, 9]. Next, we present a one-stage partitioned RK method by setting \(a_{11} = \lambda, \hat{a}_{11} = 1 - \lambda\) and \(b_1 = \hat{b}_1 = 1\). The Butcher tableau of such a method is thus of the form as

\[
\begin{array}{c|c|c|c|c|c}
& & & & & \\
\lambda & \lambda & 1 - \lambda & 1 - \lambda & 1 \\
\hline
1 & 1 & 1 & & \\
\end{array}
\]

with arbitrary parameter \(\lambda\). Furthermore, this method applied to (1.1) can be written as

\[
\begin{align*}
    k_1 &= -H_q(p_n + \lambda h k_1, q_n + (1 - \lambda) h l_1), \\
    l_1 &= H_p(p_n + \lambda h k_1, q_n + (1 - \lambda) h l_1), \\
    p_{n+1} &= p_n + h k_1, 
     q_{n+1} = q_n + h l_1.
\end{align*}
\]

Notice that such a method is exactly Scheme I through a simple substitution process.

**Remark 3.3.** Scheme I fulfills the partitioned RK symplecticity condition (3.25) such that it is proved again as a symplectic scheme for any \(\lambda\).

**Remark 3.4.** For a separable Hamiltonian system with the kinetic energy \(T(p) = \frac{1}{2} p^T M^{-1} p\) in some practical situations, where \(M\) is a constant non-degenerate matrix, the dynamics obeys the differential equations

\[
\dot{p} = -U_q(q), \quad \dot{q} = M^{-1} p,
\]

which are equivalent to the second-order system \(\ddot{q} = -M^{-1} U_q(q)\). We can further get a one-stage symplectic Nyström method by applying Scheme I to the second-order system as follows

\[
\begin{align*}
    k_1 &= -M^{-1} U_q(q_n + (1 - \lambda) h q_n + \lambda(1 - \lambda) h^2 k_1), \\
    q_{n+1} &= q_n + h \dot{q} n + \lambda h^2 k_1, 
     \dot{q}_{n+1} = \dot{q}_n + h k_1.
\end{align*}
\]

This is the version of the Nyström method corresponding to Scheme I.
4. The construction and solvability of energy-preserving schemes

Energy conservation is also an outstanding property of Hamiltonian systems. Multiplying $-\dot{q}$, $\dot{p}$ on both equations of (1.1) respectively, and summing the two equalities, we get the energy conservation law

$$\frac{d}{dt} H(p, q) = 0. \quad (4.1)$$

Just as Schemes I–III, such symplectic schemes only conserve the quadratic invariants of (1.1). Here, we concentrate on the case that the Hamiltonian is not in a quadratic form, and wish to provide energy-preserving schemes.

4.1. Energy-preserving schemes

The next two energy-preserving schemes are devised by using the above symplectic schemes and the parameter $\lambda$ therein. The parameter is used to enforce an energy conservation constraint. Based on Scheme I, we get the next energy-preserving symplectic scheme, which we called Scheme IV in the following discussion. The notations $\bar{u}$, $\bar{v}$ and $\Phi^\lambda_h$ are introduced in (3.22) and (3.23).

$$\begin{cases} 
  p_{n+1} = p_n - h \partial_p H(\bar{u}, \bar{v}), \\
  q_{n+1} = q_n + h \partial_q H(\bar{u}, \bar{v}), \\
  H(p_{n+1}, q_{n+1}) = H(p_n, q_n).
\end{cases} \quad (4.2)$$

**Remark 4.1.** If a real value $\lambda_1$ can be found such that the constraint condition $H(p_{n+1}, q_{n+1}) = H(p_n, q_n)$ is satisfied, we get a one-step scheme at the current step

$$\Phi^\lambda_h : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}) \quad (4.2)$$

which ensures energy conservation. According to the previous theory, it is also known that for a fixed $\lambda_1$, the scheme (4.2) is symplectic. The important implication of the symplecticity of (4.2) is the conservation of all quadratic invariants of (1.1). If the existence of the parameter $\lambda$ in Scheme IV is verified, there exists a real sequence $\{\lambda_i\}$ as the following diagram

$$\begin{aligned}
  (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}) \mapsto (p_{n+2}, q_{n+2}) \mapsto (p_{n+3}, q_{n+3}) \mapsto \cdots \quad (4.3)
\end{aligned}$$

such that the numerical solution $(p_{n+i}, q_{n+i})$ defined by $\Phi^\lambda_h$ satisfies $H(p_{n+i}, q_{n+i}) = H(p_n, q_n)$, $i = 1, 2, \ldots$. The existence of the sequence $\{\lambda_i\}$ will be proved in the next subsection. It is noted that in (4.3), symplectic schemes with different fixed parameters are used at each step to obtain energy conservation. In summary, Scheme IV is an energy and quadratic invariants preserving scheme, and its performance will be reported in numerical experiments.

Similarly, the next energy and quadratic invariants preserving scheme called Scheme V is obtained based on Scheme III, where the notation $\Psi_h$ is introduced in (3.24).

$$\begin{cases} 
  (p_{n+1}, q_{n+1}) = \Psi_h(p_n, q_n), \\
  H(p_{n+1}, q_{n+1}) = H(p_n, q_n).
\end{cases} \quad (4.2)$$

For Schemes IV–V, we need to seek a fixed value of parameter $\lambda$ at each step such that $H(p_{n+1}, q_{n+1}) = H(p_n, q_n)$. Scheme IV is an energy-preserving scheme of order 1. And Scheme V is a second order energy-preserving symmetric scheme. Based on high-order symmetric symplectic schemes mentioned, a serier of higher order energy-preserving symmetric schemes can be derived by using $\lambda$ to add an energy conservation constraint, and all the schemes obtained accurately conserve the quadratic invariants of (1.1). In terms of computational complexity, we do not consider the construction of the energy-preserving scheme by Scheme II. As conveyed in the introduction, the Hamiltonian in the last equation of these schemes can be replaced with any non-quadratic invariant of mechanical systems.
4.2. The solvability of the proposed schemes

The solvability of all the schemes reported in this paper is an urgent problem to be solved, and it is related to whether these schemes applied to solve the system \([\mathcal{L}]\) will be effective. For the given initial points \((p_n, q_n)\), we first consider the question about the existence of the solution to two new classes of symplectic schemes in Section 3. The implicit function theorem is used as a primary tool to verify that these schemes are solvable. We define the following vector function

\[
F(p_{n+1}, q_{n+1}, \lambda, h) \triangleq \left( \begin{array}{c}
p_{n+1} - p_n + hH_q(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_n + (1 - \lambda)q_{n+1}) \\
q_{n+1} - q_n - hH_p(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_n + (1 - \lambda)q_{n+1})
\end{array} \right)
\]

(4.4)

with initial conditions \(M(p_n, q_n, \lambda_0, 0) = N(p_n, q_n, \lambda_0, 0) = 0\), where \(\lambda_0\) is any predetermined real number. It is noted that Scheme I is equivalent to \(M(p_n, q_n, \lambda, 0, 0) = 0\). The Jacobi matrix of (4.4) with respect to \(p_{n+1}\) and \(q_{n+1}\) is

\[
\frac{\partial F}{\partial (p_{n+1}, q_{n+1})} = \left( \begin{array}{cc}
I + \lambda hH_{qp} & (1 - \lambda)hH_{qq} \\
-\lambda hH_{qp} & I - (1 - \lambda)hH_{pq}
\end{array} \right).
\]

(4.5)

Therefore, the determinant of (4.5) calculated at \((p_n, q_n, \lambda, 0, 0)\) is equal to 1. This proves the existence and uniqueness of the solution of Scheme I with any \(\lambda_0\) when \(h\) is small. The conclusion that the high-order symplectic schemes are uniquely solvable can be obtained similarly, whether this scheme is based on the generating function method or the symmetric composition method.

In the following content, we address the problem of the existence of the solution of the energy-preserving schemes designed in this section. Following the classical formulation of the implicit function theorem, we define the vector equation

\[
G(p_{n+1}, q_{n+1}, \lambda, p_n, q_n, h) \triangleq \left( \begin{array}{c}
p_{n+1} - p_n + hH_q(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_n + (1 - \lambda)q_{n+1}) \\
q_{n+1} - q_n - hH_p(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_n + (1 - \lambda)q_{n+1}) \\
H(p_{n+1}, q_{n+1}) - H(p_n, q_n)
\end{array} \right) = 0
\]

which is equivalent to Scheme IV. The function \(G\) vanishes at point \((p_n, q_n, \frac{1}{2}, p_n, q_n, 0)\). The Jacobi matrix of \(G\) at this point is obtained as

\[
\left. \frac{\partial G}{\partial (p_{n+1}, q_{n+1}, \lambda)} \right|_{(p_n, q_n, \frac{1}{2}, p_n, q_n, 0)} = \left( \begin{array}{ccc}
I & 0 & 0 \\
0 & I & 0 \\
H_p(p_n, q_n) & H_q(p_n, q_n) & 0
\end{array} \right).
\]

(4.6)

Since the matrix (4.6) is degenerate anyway, it is immediately clear that the traditional steps does not help to acquire the solvability of Scheme IV. For this reason, the next nonlinear function

\[
E(\lambda, h) = H(p_{n+1}(\lambda, h), q_{n+1}(\lambda, h)) - H(p_n, q_n)
\]

(4.7)

is introduced as an error function of the numerical Hamiltonian, where \(p_{n+1}(\lambda, h)\) and \(q_{n+1}(\lambda, h)\) are defined by the first two equations of Scheme IV. It is apparent that the solvability of Scheme IV is equivalent to the existence of a solution in the form \(\lambda = \lambda(h)\) of \(E(\lambda, h) = 0\), in particular \(E(\frac{1}{2}, 0) = 0\) as the initial condition. Through a series of calculations, the following derivatives of (4.7) vanish at \((\frac{1}{2}, 0)\), i.e.,

\[
E_{\lambda}(\frac{1}{2}, 0) = E_h(\frac{1}{2}, 0) = E_{\lambda\lambda}(\frac{1}{2}, 0) = E_{\lambda h}(\frac{1}{2}, 0) = E_{hh}(\frac{1}{2}, 0) = 0.
\]

(4.8)

This is an unfortunate result making the calculations more difficult, but (4.8) will prompt us to continue the following derivation. The Taylor expansion of \(E\) at \((\frac{1}{2}, 0)\) is calculated as

\[
E(\lambda, h) = \frac{1}{6}E_{hhh}(\frac{1}{2}, 0)h^3 + \frac{1}{2}E_{\lambda hh}(\frac{1}{2}, 0)(\lambda - \frac{1}{2})h^2 + O((\lambda - \frac{1}{2})^3) + O((\lambda - \frac{1}{2})^2 h) + O((\lambda - \frac{1}{2}) h^3) + O(h^4).
\]

(4.9)

Inspired by the equation (4.9), we attempt to prove the existence of a solution of the form \(\lambda(h) = \frac{1}{2} + \varepsilon(h)h\), where \(\varepsilon(h)\) is a real-valued function of \(h\). For this purpose, the following expansion

\[
\tilde{E}(\varepsilon, h) = \frac{1}{6}E_{hhh}(\frac{1}{2}, 0)h^3 + \frac{1}{2}E_{\lambda hh}(\frac{1}{2}, 0)\varepsilon h^2 + O(\varepsilon^2 h^3) + O(h^4),
\]
is shown by substituting the variable transformation $\lambda = \frac{1}{2} + \varepsilon h$ into (4.9). It is seen that when $h \neq 0$, $E(\lambda, h) = 0$ is equivalent to $\tilde{E}(\varepsilon, h) = 0$, where

$$\tilde{E}(\varepsilon, h) = \frac{1}{6}E_{hh}h\left(\frac{1}{2}, 0\right) + \frac{1}{2}E_{\lambda hh}h\left(\frac{1}{2}, 0\right)\varepsilon + O(\varepsilon^2) + O(h).$$

Calculating the third-order derivatives of $E$ to the two variables $\lambda$ and $h$, we state that as long as

$$\frac{1}{2}E_{\lambda hh}\left(\frac{1}{2}, 0\right) = \frac{d}{dt}(H^T H_q)\bigg|_{(p_n, q_n)} \neq 0,$$

then the implicit function theorem guarantees the existence and uniqueness of a function $\varepsilon = \varepsilon(h)$ as

$$\varepsilon(h) = -\frac{1}{3}E_{h hh}\left(\frac{1}{2}, 0\right) / E_{\lambda hh}\left(\frac{1}{2}, 0\right) + O(h)$$

such that $\tilde{E}(\varepsilon(h), h) = 0$ holds. Therefore, when $h$ is small, the existence of $\lambda(h) = \frac{1}{2} + \varepsilon(h)h$ around $\frac{1}{2}$ is confirmed to make Scheme IV solvable. Similarly, we can also derive the same conclusions about the solvability of higher order energy-preserving symmetric schemes. It is worth mentioning that the requirement (4.10) is a fairly weak condition, and we find that this condition is always satisfied for all the numerical tests we have considered.

5. Numerical experiments

In this section, we consider two numerical examples to confirm our theoretical analysis and the effectiveness of the proposed scheme. The numerical performance of Schemes I–III about the four choices of $\lambda$ is presented. For comparison, we also calculate numerical solutions by an energy-preserving scheme based on the AVF method [20]. The time step size is always set to $h = 0.02$. The convergence rates of all schemes in these experiments are calculated by

$$order = \log_2 \frac{error_h}{error_\frac{1}{2}}, \quad error_h = ||y_h(1) - y_\frac{1}{2}(1)||_\infty,$$

where $y_h(1)$ represents the numerical solution of corresponding schemes at time $t = 1$.

5.1. The Hénon-Heiles model

Our first experiment is the Hénon-Heiles model that originates from a problem in celestial mechanics describing stellar motion under the action of a gravitational potential $U$ of a galaxy. After a reduction of the dimension, this model is equivalent to the motion of a test particle with unit mass subject to an arbitrary potential $U(q_1, q_2)$ in the $(q_1, q_2)$-plane. The dynamics is described by a Hamiltonian of the form

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) + U(q_1, q_2).$$

The potential $U$ is chosen for this experiment as follows

$$U(q_1, q_2) = \frac{1}{2}(q_1^2 + q_2^2 + 2q_1q_2 - \frac{2}{3}q_2^3).$$

The particular potential $U = \frac{1}{2}$ serving as the critical energy of this model consists of three straight lines forming an equilateral triangle, whose vertices are saddle points of $U$ as plotted in Fig. [1]. For values of energy $H < \frac{1}{6}$, the equipotential curves of the system are close thus making escape impossible. However, for larger energy levels ($H > \frac{1}{6}$), the equipotential curves open and three exit channels appear through which the test particles may escape to infinity [28]. The two classical orbits of the Hénon-Heiles model will be illustrated with two kinds of initial values as (1) box orbits (see the first row of Fig. [1]):

$$H_0 = 0.02, \quad p_2(0) = 0, \quad q_1(0) = 0, \quad q_2(0) = -0.082;$$
(2) chaotic orbits (see the second row of Fig. 1):

\[ H_0 = \frac{1}{6}, \quad p_2(0) = 0, \quad q_1(0) = 0, \quad q_2(0) = 0.82. \]

The values of \( p_1(0) \) are found from the Hamiltonian \((5.1)\).

![Fig. 1. Box orbits (first row, till \( t = 1000 \)) and chaotic orbits (second row, till \( t = 2000 \)) of Scheme I for the Hénon-Heiles model.](image)

![Fig. 2. Energy conservation of three symplectic schemes for the Hénon-Heiles model with box orbits (first row) and chaotic orbits (second row).](image)

The box orbits emerging with the internal shape of an equilateral triangle are presented in the first row of Fig. 1. Under the critical energy, Schemes I–III depict that the numerical trajectories never escapes to the
outside of the equilateral triangle at any time \( t \). The numerical trajectories of three symplectic schemes are similar, so we only show the numerical curves of Scheme I. The symplecticity of all schemes ensures that the energy error remains bounded and small over long times in Fig. 2. The convergence rates of Schemes I–III are reported in Tab. 1. The three energy-preserving schemes also give the box orbits and chaotic orbits we are looking forward to in Fig. 3. Fig. 4 presents the corresponding energy error and the value distribution of \( \lambda \) in Schemes IV–V. This tells us that \( \lambda \) will fluctuate around \( \frac{1}{2} \) to achieve energy conservation, which confirm the theoretical analysis in Section 4. The energy errors of Schemes IV–V are smaller than the AVF method on the order of magnitude and remain bounded over long times. Tab. 2 exhibits the convergence rates for three energy-preserving schemes.

**Tab. 1.** Convergence tests of Schemes I–III for the Hénon-Heiles model with chaotic orbits.

| Scheme | \( h \) | \( \lambda = -1 \) | \( \lambda = \frac{1}{2} \) | \( \lambda = \frac{3}{2} \) | \( \lambda = 2 \) |
|--------|--------|-----------------|-----------------|-----------------|-----------------|
|        | error  | order           | error           | order           | error           | order           |
| I      | 0.02/2 | 4.3102e-03 -    | 4.3799e-04 -    | 2.6258e-03 -    | 3.8521e-03 -    |
|        | 0.02/4 | 2.0947e-03 1.0410 | 2.2263e-04 0.9762 | 1.3350e-03 0.9760 | 1.9803e-03 0.9599 |
|        | 0.02/8 | 1.0326e-03 1.0204 | 1.1223e-04 0.9883 | 6.7312e-04 0.9879 | 1.0041e-03 0.9799 |
|        | 0.02/16 | 5.1270e-04 1.0102 | 5.6341e-05 0.9942 | 3.3798e-04 0.9939 | 5.0556e-04 0.9899 |
| II     | 0.02/2 | 5.0853e-04 -    | 2.3500e-05 -    | 2.2429e-04 -    | 4.7743e-04 -    |
|        | 0.02/4 | 1.2522e-04 2.0218 | 5.8734e-06 2.0004 | 5.6662e-05 1.9849 | 1.2134e-04 1.9763 |
|        | 0.02/8 | 3.1065e-05 2.0111 | 1.4681e-06 2.0003 | 1.4238e-05 1.9926 | 3.0579e-05 1.9884 |
|        | 0.02/16 | 7.7361e-06 2.0056 | 3.6698e-07 2.0001 | 3.5687e-06 1.9963 | 7.6753e-06 1.9943 |
| III    | 0.02/2 | 1.1158e-04 -    | 3.5351e-06 -    | 5.0447e-05 -    | 1.1757e-04 -    |
|        | 0.02/4 | 2.7880e-05 2.0008 | 8.8370e-07 2.0001 | 1.2608e-05 2.0004 | 2.9374e-05 2.0008 |
|        | 0.02/8 | 6.9689e-06 2.0002 | 2.2092e-07 2.0000 | 3.1519e-06 2.0001 | 7.3425e-06 2.0002 |
|        | 0.02/16 | 1.7422e-06 2.0001 | 5.5230e-08 2.0000 | 7.8795e-07 2.0000 | 1.8356e-06 2.0001 |

**Tab. 2.** Convergence tests of three energy-preserving schemes for the Hénon-Heiles model with chaotic orbits.

| \( h \) | AVF | Scheme IV | Scheme V |
|---------|-----|-----------|----------|
|         | error | order | error | order | error | order | error | order |
| 0.02/2  | 1.7818e-05 | - | 2.4999e-03 | - | 4.2338e-06 | - |
| 0.02/4  | 4.4552e-06 | 1.9998 | 1.2375e-03 | 1.0145 | 1.0569e-06 | 2.0021 |
| 0.02/8  | 1.1139e-06 | 1.9999 | 6.2182e-04 | 0.9928 | 2.6411e-07 | 2.0007 |
| 0.02/16 | 2.7847e-07 | 2.0000 | 3.1014e-04 | 1.0036 | 6.6019e-08 | 2.0002 |

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Fig. 3. Box orbits (first row) and chaotic orbits (second row) of three energy-preserving schemes for the Hénon-Heiles model till \( t = 1000 \).

Fig. 4. Energy conservation (left) of three energy-preserving schemes for the Hénon-Heiles model; value distribution (right) of \( \lambda \) in Schemes IV-V with box orbits (first row) and chaotic orbits (second row).
5.2. The perturbed Kepler problem

Our second experiment is the motion of a planet in the Schwarzschild potential for Einstein’s general relativity theory with unitary masses and gravitational constant. The Hamiltonian of the dynamics reads

\[
H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{\mu}{3\sqrt{(q_1^2 + q_2^2)^3}},
\]

where \(\mu\) is a positive or negative small number. Moreover, the angular momentum of this system

\[
L(p_1, p_2, q_1, q_2) = q_1 p_2 - q_2 p_1
\]

is a quadratic first integral. We choose the initial points as

\[
p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1 + e}{1 - e}}, \quad q_1(0) = 1 - e, \quad q_2(0) = 0,
\]

which confers an eccentricity \(e\) on the orbit. We set \(e = 0.6\) and \(\mu = 0.0075\) in this experiment. Then \(H(p, q) = H_0 \approx -0.5391, L(p, q) = L_0 = 0.8\). The system \([5.2]\) represents approximately an ellipse orbit with eccentricity \(e\) for \(H_0 < 0\). Due to the relatively complex form of the Hamiltonian \([5.2]\), and Scheme II contains the calculation of higher derivatives of the Hamiltonian, we do not consider this scheme. We will investigate the numerical behaviours of Schemes I and III–V with respect to the angular momentum \([5.3]\).

![Fig. 5. Numerical solutions of Scheme I for the perturbed Kepler problem till \(t = 1000\).](image-url)
Schemes I and III plot satisfactory orbits similar to those of the original problem. Since the trajectories drawn by the two schemes are similar, we give the numerical solutions of Scheme I in Fig. 5. The main observation is that error in the energy remains bounded and small in the long-time simulation, and the angular momentum is preserved in Fig. 6. These benefit from the symplecticity of both schemes. The performance of three energy-preserving schemes is presented in Fig. 7 and Fig. 8. All three schemes present an expected orbit. It is clear that the energy error grows linearly for the AVF method, and those of Schemes IV–V are bounded over longer time intervals with smaller order of magnitude. The angular momentum is conserved by Schemes IV–V as explained in Remark 4.1. We also give the numerical performance of the AVF method with respect to the angular momentum. The values of $\lambda$ still fluctuate around $\frac{1}{2}$, which is consistent with the theoretical existence of the parameter. In summary, Schemes IV–V, over long times, are much superior to the AVF method.

Fig. 6. Energy (left) and angular momentum (right) conservation of Schemes I (first row) and III (second row) for the perturbed Kepler problem.

Fig. 7. Numerical solutions of three energy-preserving schemes for the perturbed Kepler problem till $t = 1000$. 
6. Concluding remarks

We have introduced a general symplectic integrator for canonical Hamiltonian systems and given the direct proof of the symplecticity of the new scheme. Two different explanations of the symplecticity are presented by the frameworks of the generating function method and partitioned RK methods. The generating function of the new scheme has been defined by the new coordinates, which contain the three typical coordinates of the generating function method. Furthermore, we have established the connection between the Hamilton-Jacobi equation with new variables and the Hamiltonian systems, and obtained two new classes of symplectic schemes with arbitrary order of accuracy by using the generating function method and symmetric composition methods. We have devised the energy-preserving schemes by adjusting the real parameter in the above symplectic schemes and proved the theoretical existence of the solution of all schemes. The excellent long-time performances of all proposed schemes are demonstrated by the Hénon-Heiles model and the perturbed Kepler problem. The numerical results show that the proposed energy-preserving schemes are more advantageous than the AVF method over long times, especially in the ability to preserve the Hamiltonian and the quadratic invariant of the system.

We remark on some going works. The stability analysis [29] of the new schemes needs to be completed. The classes of symplectic integrators and variational integrators [26, 30] are identical. It is thus meaningful to discuss the new symplectic schemes and their properties based on a discretization of Hamilton’s principle. Besides, we wish to construct the volume-preserving algorithms of source-free dynamical systems [31] by using the parameter of the new symplectic schemes. We will further generalize these results to non-canonical Hamiltonian systems and Hamiltonian PDEs. Last but not least, as we know, the conditions of partitioned RK methods to be symplectic and to preserve quadratic invariants are same, and quadratic invariants are precisely conserved by these energy-preserving schemes derived in this paper. Whether these schemes are symplectic and their connection to existing symplectic-energy-momentum integrators [19] will be the subject of future investigations.

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