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A CLASS OF EXPLICIT RATIONAL SYMPLECTIC INTEGRATORS*

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Abstract In this paper, a class of rational explicit symplectic integrators for one-dimensional oscillatory Hamiltonian problems is presented. These methods are zero-dissipative, and of first algebraic order and high phase-lag order. By means of composition technique, we construct second and fourth order methods with high phase-lag order of this type. Based on our ideas, three applicable explicit symplectic schemes with algebraic order one, two and four are derived, respectively. We report some numerical results to illustrate the good performance of our methods.

Keywords Oscillatory Hamiltonian problems, rational explicit symplectic integrators, zero-dissipative, phase-lag order, composition methods.

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1. Introduction

The classical dynamic equations $q''(t) = f(q(t))$ can be written by the following Hamiltonian formulation

$$p' = -\frac{\partial H(p,q)}{\partial q}, \qquad q' = \frac{\partial H(p,q)}{\partial p}, \tag{1.1}$$

where $q, p \in R^d$ are the Lagrangian coordinates and the corresponding momenta respectively, d the number of degrees of freedom and the total energy function $H(p,q) = T(p) + V(q)$ with the kinetic energy $T(p) = p^T p/2$ and the potential energy $V(q)$ whose negative gradient is the force $f(q)$. It is well known that, for system (1), the symplectic structure $dp \wedge dq$ of its exact flow and the total energy $H(p,q)$ are invariant as the time evolves. When solving the system numerically, symplectic methods, which have been studied thoroughly in recent years (See [4, 8, 13]), can conserve the discrete symplecticity law $dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n$ at each time step, where p_n, q_n are the numerical approximations of $p(t_n)$ and $q(t_n)$, and for this reason, they are quite efficient for solving Hamiltonian systems over long time.

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In this paper, we are concerned on the numerical integration of autonomous second order initial value problems having oscillatory solutions

$$q''(t) = f(q(t)), \qquad q(0) = q_0, \qquad q'(0) = q_0'. \tag{1.2}$$

This kind of problems often arise in many applied scientific fields and can be integrated by some conventional numerical methods such as Partitioned Runge-Kutta, Runge-Kutta-Nyström methods or linear multi-step methods and so on. Setting $p = q'$ in problems (1.2), it may be considered as a kind of special Hamiltonian problems. Naturally, symplectic methods are considered to solve these problems. However, conventional explicit symplectic methods, say, symplectic Euler methods or Störmer-Verlet methods, can not yield the numerical results of high accuracy. Implicit symplectic methods, especially the ones of high algebraic order, can yield more precise numerical results, but a nonlinear system has to be solved at each step. Moreover, the exact solutions of problems (1.2) exhibit some pronounced periodic or oscillatory behavior, so the numerical methods employed also should also mimic the character as possible as they can.

For the above reasons, as an attempt, we turn to consider some nonconventional numerical integrators. In our previous work, we have developed some nonconventional methods of high phase-lag order for second order periodic or oscillatory problems [10, 11]. Based on the ideas, in this paper, a class of rational explicit symplectic integrators for one-dimensional Hamiltonian oscillatory problems is presented. These integrators are zero-dissipative, and of first algebraic order and high phase-lag order. By means of composition technique, we construct second and fourth order methods with high phase-lag order of this type. Some applicable rational explicit symplectic schemes are derived. We report some numerical results to illustrate the good performance of our methods.

At the end of this section, we give some preliminaries on symplectic integrators and the stability analysis of numerical methods for solving second order oscillatory problems so that our discussion can be followed easily.

Let $\Phi_{\Delta t} : (p_n, q_n) \to (p_{n+1}, q_{n+1})$ be a one-step integrator for Hamiltonian problems and Δt be the fixed step. $\Phi_{\Delta t}$ is *symplectic* if $dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n$. Denote $\partial\Phi_{\Delta t}$ as the Jacobian of $\Phi_{\Delta t}$, namely, $\partial\Phi_{\Delta t} = \partial(p_{n+1}, q_{n+1})/\partial(p_n, q_n)$, then $\Phi_{\Delta t}$ is symplectic if and only if

$$\partial\Phi_{\Delta t}^T \, J \, \partial\Phi_{\Delta t} = J, \qquad J = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}.$$

For a one-step integrator $\Phi_{\Delta t}$ for second order oscillatory problems, the stability analysis is based on the following linear model equation [5, 7]

$$\dot{q} = p, \qquad \dot{p} = -\omega^2 q, \qquad \omega > 0. \tag{1.3}$$

When $\Phi_{\Delta t}$ is applied to equation (1.3), one can obtain the difference equation of the form

$$\begin{pmatrix} q_{n+1} \\ \Delta t p_{n+1} \end{pmatrix} = S(\nu^2) \begin{pmatrix} q_n \\ \Delta t p_n \end{pmatrix},$$

where $\nu := \omega\Delta t$, $S(\nu^2)$ is a second order square matrix named *stability matrix* whose elements are only dependent on ν^2. Let λ_1 and λ_2 be the two eigenvalues of $S(\nu^2)$, the method has an *interval of periodicity* $(0, \Gamma^2)$, if λ_1 and λ_2 are conjugate complex and $|\lambda_1| = |\lambda_2| = 1$ for all $\nu^2 \in (0, \Gamma^2)$; The method is *P-stable*, if the interval of periodicity is $(0, +\infty)$. Denote $\det(S(\nu^2))$ and $\mathrm{tr}(S(\nu^2))$ as the determinant and the trace of matrix $S(\nu^2)$ respectively, then it is easily shown that $\Phi_{\Delta t}$ is P-stable if and only if for all $\nu^2 > 0$

$$\det(S) = 1, \qquad |\mathrm{tr}(S)| \le 2.$$

For the method $\Phi_{\Delta t}$, the *phase-lag error* (also called *dispersion error*) and the *dissipation error* (also called *amplification error*) are defined by respectively

$$\varphi(\nu) = \nu - \cos^{-1}\left(\frac{\mathrm{tr}(S)}{2\sqrt{\det(S)}}\right), \qquad \psi(\nu) = 1 - \sqrt{\det(S)}.$$

The method is said to be of *order p phase-lag error* and *order q dissipation error*, if

$$\varphi(\nu) = \mathcal{O}(\Delta t^{p+1}), \qquad \psi(\nu) = \mathcal{O}(\Delta t^{q+1}), \qquad \text{as} \quad \Delta t \to 0.$$

Here, if $p = +\infty$, then we call the method *phase-fitted*, while if $q = +\infty$ and there exists some interval $(0, \Gamma^2)$ such that $|\mathrm{tr}(S(\nu^2))| \le 2$ for all $\nu^2 \in (0, \Gamma^2)$, we call the method *zero-dissipative,* which means that the method has a nonempty interval of periodicity. Moreover, it can be shown that a method has phase-lag order p if

$$\mathrm{tr}(S) - 2\cos(\nu)\sqrt{\det(S)} = C\nu^{p+2} + \mathcal{O}(\nu^{p+4}),$$

where C is some constant. For details, we refer to [1, 3, 5, 6, 7].

2. The explicit symplectic integrators

We consider the numerical integration of problems (1.2) in one dimension. Consider the following method

$$q_{n+1} = q_n G(Q_n) + \Delta t p_n, \qquad p_{n+1} = q_n \frac{G(Q_n) - 1}{\Delta t} + p_n, \tag{2.1}$$

where $G(x)$ is a real analytic function defined in $\mathbb{R}$, $Q_n = \Delta t^2 f_n / q_n$, $f_n = f(q_n)$ and we always suppose that $q_n \neq 0$ for all n. Equivalently, method (2.1) can be written as

$$q_{n+1} = q_n G(Q_n) + \Delta t p_n, \qquad p_{n+1} = \frac{q_{n+1} - q_n}{\Delta t}. \tag{2.2}$$

From Taylor's expansions of q_{n+1} and p_{n+1}, we have

$$\begin{aligned} q_{n+1} &= q_n \sum_{k=0}^{+\infty} \frac{G^{(k)}(0)}{k!} \left(\frac{\Delta t^2 f_n}{q_n}\right)^k + \Delta t p_n \\ &= G(0) q_n + \Delta t p_n + G'(0) \Delta t^2 f_n + \mathcal{O}(\Delta t^4) \end{aligned}$$

and

$$\begin{aligned} p_{n+1} &= \frac{q_n}{\Delta t} \left(\sum_{k=0}^{+\infty} \frac{G^{(k)}(0)}{k!} \left(\frac{\Delta t^2 f_n}{q_n}\right)^k - 1 \right) + p_n \\ &= p_n + \frac{G(0) - 1}{\Delta t} q_n + G'(0) \Delta t f_n + \mathcal{O}(\Delta t^3). \end{aligned}$$

Therefore, if function $G(x)$ satisfies $G(0) = G'(0) = 1$, then method (2.1) has first algebraic order with the local truncation error

$$q(t_{n+1}) - q_{n+1} = -\frac{\Delta t^2}{2} f_n + \mathcal{O}(\Delta t^3), \quad p(t_{n+1}) - p_{n+1} = \frac{\Delta t^2}{2} f'_n + \mathcal{O}(\Delta t^3). \quad (2.3)$$

Note that the Jacobian of method (2.1) is

$$\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} = \begin{pmatrix} 1 & \frac{1}{\Delta t}(G(Q_n) - 1 + q_n G_{q_n}(Q_n)) \\ \Delta t & G(Q_n) + q_n G_{q_n}(Q_n) \end{pmatrix},$$

so we have

$$\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}^T J \frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} = J, \qquad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

and method (2.1) is symplectic.

As examples, if we take respectively function

- $G(x) = 1 + x$, then method (2.1) becomes a linear method as follows

$$q_{n+1} = q_n + \Delta t p_n + \Delta t^2 f_n, \qquad p_{n+1} = \frac{q_{n+1} - q_n}{\Delta t}; \quad (2.4)$$

- $G(x) = 1/(1 - x)$, then we obtain the following rational method

$$q_{n+1} = \frac{q_n^2}{q_n - \Delta t^2 f_n} + \Delta t p_n, \qquad p_{n+1} = \frac{q_{n+1} - q_n}{\Delta t}. \quad (2.5)$$

Consider the linear stability and phase-lag order of method (2.1). When applying the method to the model equation (1.3), we have $Q_n = -(\omega \Delta t)^2 =: -\nu^2$ and

$$\begin{pmatrix} q_{n+1} \\ \Delta t p_{n+1} \end{pmatrix} = \begin{pmatrix} G(-\nu^2) & 1 \\ G(-\nu^2) - 1 & 1 \end{pmatrix} \begin{pmatrix} q_n \\ \Delta t p_n \end{pmatrix} := S(\nu^2) \begin{pmatrix} q_n \\ \Delta t p_n \end{pmatrix}. \quad (2.6)$$

Obviously, $\det(S(\nu^2)) = 1$ is valid. Moreover, note that

$$\begin{aligned} \operatorname{tr}(S) - 2\cos(\nu)\sqrt{\det(S)} &= 1 + G(-\nu^2) - 2\cos(\nu) \\ &= G(0) - 1 + \sum_{n=1}^{+\infty} (-1)^n \left(\frac{G^{(n)}(0)}{n!} - \frac{2}{(2n)!} \right) \nu^{2n}, \end{aligned}$$

so method (2.1) has $2r$-th phase-lag order if there exists an integer r such that

$$G(0) = 1, \qquad G^{(n)}(0) = \frac{2n!}{(2n)!}, \qquad 1 \le n \le r. \quad (2.7)$$

Due to its low algebraic accuracy, the method (2.1) is not competitive in practice. To improve its algebraic order, we will employ the composition technique to construct some high order methods of this type. Indeed, it is well-known that in the theory of numerical solutions of ODEs, composition is an important and useful technique that a high order method can be obtained from some low order methods. For details, we refer to [4, 8].

In method (2.2), if exchange $\Delta t \leftrightarrow -\Delta t$, $q_n \leftrightarrow q_{n+1}$ and $p_n \leftrightarrow p_{n+1}$, then we have

$$q_{n+1} = q_n + \Delta t p_n, \qquad p_{n+1} = \frac{q_{n+1}G(Q_{n+1}) - q_n}{\Delta t}, \tag{2.8}$$

where $Q_{n+1} = \Delta t^2 f_{n+1}/q_{n+1}$. Method (2.8) is the adjoint method of (2.2) and clearly, it is also explicit. For the sake of convenience, we denote methods (2.2) and (2.8) by $\Phi_{\Delta t}$ and $\Phi^*_{\Delta t}$ respectively.

Theorem 2.1. *For the rational integrators $\Phi_{\Delta t}$ and $\Phi^*_{\Delta t}$, if there exist some interval $(-L, 0)$, $L > 0$ and a positive integer r such that $-3 \le G(x) \le 1$ for all $x \in (-L, 0)$ and*

$$G(0) = 1, \qquad G^{(n)}(0) = \frac{2n!}{(2n)!}, \qquad 1 \le n \le r, \tag{2.9}$$

then the two integrators are both zero-dissipative, symplectic and have algebraic order one and phase-lag order $2r$.

Proof. From the above analysis, we have shown that the assertion is true to $\Phi_{\Delta t}$. For $\Phi^*_{\Delta t}$, we have $q_{n+1} - q(t_{n+1}) = -f(q_n)\Delta t^2/2 + \mathcal{O}(\Delta t^3)$ and

$$\begin{aligned} p_{n+1} &= \frac{1}{\Delta t}\left(q_{n+1} \sum_{n=0}^{+\infty} \frac{G^{(n)}(0)}{n!} \left(\frac{\Delta t^2 f_{n+1}}{q_{n+1}} \right)^n - q_n \right) \\ &= p_n + \Delta t f(q_n + \Delta t p_n) + \mathcal{O}(\Delta t^3) \\ &= p_n + \Delta t f_n + \Delta t^2 f'_q(q_n) p_n + \mathcal{O}(\Delta t^3), \end{aligned}$$

so $\Phi^*_{\Delta t}$ is also a first order method. The symplecticity of $\Phi^*_{\Delta t}$ is obvious. Moreover, the stability matrix of $\Phi^*_{\Delta t}$ is

$$S^*(\nu^2) = \begin{pmatrix} 1 & 1 \\ G(-\nu^2) - 1 & G(-\nu^2) \end{pmatrix},$$

as a result, $\det(S^*(\nu^2)) = \det(S(\nu^2)) = 1$ and $\mathrm{tr}(S^*(\nu^2)) = \mathrm{tr}(S(\nu^2)) = 1 + G(-\nu^2)$. The proof is completed here. □

Next, based on methods $\Phi_{\Delta t}$ and $\Phi^*_{\Delta t}$, we have the following composition method of second order under condition $G(0) = G'(0) = 1$

$$\Psi_{\Delta t} := \Phi_{\Delta t/2} \circ \Phi^*_{\Delta t/2},$$

that is,

$$\begin{aligned} &q_{n+1/2} = q_n + \frac{\Delta t}{2} p_n, \qquad Q_{n+1/2} = \frac{\Delta t^2 f(q_{n+1/2})}{4 q_{n+1/2}}, \\ &q_{n+1} = 2 q_{n+1/2} G(Q_{n+1/2}) - q_n, \\ &p_{n+1} = \frac{2}{\Delta t}(q_{n+1} - q_{n+1/2}). \end{aligned}$$

Consider the stability and phase-lag properties of $\Psi_{\Delta t}$. Applying $\Psi_{\Delta t}$ to the model equation (1.3), we obtain the stability matrix of $\Psi_{\Delta t}$ as follows

$$S_{\Psi_{\Delta t}}(\nu^2) = \begin{pmatrix} 2G(-\nu^2/4) - 1 & G(-\nu^2/4) \\ 4G(-\nu^2/4) - 4 & 2G(-\nu^2/4) - 1 \end{pmatrix}.$$

Clearly,

$$\det(S_{\Psi_{\Delta t}}(\nu^2)) = 1, \qquad \operatorname{tr}(S_{\Psi_{\Delta t}}(\nu^2)) = 4G\left(-\nu^2/4\right) - 2,$$

therefore, method Ψ_h is zero-dissipative provided that $0 \le G\left(-\nu^2/4\right) \le 1$. Moreover, note that

$$\begin{aligned}(S_{\Psi_{\Delta t}}) - 2\cos(\nu)\sqrt{\det(S_{\Psi_{\Delta t}})} &= 4G(-\nu^2/4) - 2 - 2\cos(\nu)\\ &= 4(G(0)-1) + \sum_{n=1}^{+\infty}(-1)^n\left(\frac{4G^{(n)}(0)}{n!4^n} - \frac{2}{(2n)!}\right)\nu^{2n},\end{aligned}$$

so method $\Psi_{\Delta t}$ has $2r$-th phase-lag order if there exists an integer r such that

$$G(0) = 1, \qquad G^{(n)}(0) = \frac{n!2^{2n-1}}{(2n)!}, \qquad 1 \le n \le r. \tag{2.10}$$

then method has $2r$-th phase-lag order.

Theorem 2.2. *For the integrator $\Psi_{\Delta t}$, if there exist some interval $(-M, 0)$, $M > 0$ and an positive integer r such that $0 \le G(x) \le 1$ for all $x \in (-M, 0)$ and the conditions (2.10) are satisfied, then the integrator is zero-dissipative, symmetric, symplectic and of algebraic order two and phase-lag order $2r$.*

Note that $\Psi_{\Delta t}$ is a symmetric and symplectic method of second algebraic order, so we go on to consider the following composition method

$$\Xi_{\Delta t} := \Psi_{\sigma_1\Delta t} \circ \Psi_{\sigma_2\Delta t} \circ \Psi_{\sigma_1\Delta t}, \tag{2.11}$$

namely,

$$\begin{aligned}
&q_{n+\sigma_1/2} = q_n + \frac{\sigma_1\Delta t}{2}p_n, \quad Q_{n+\sigma_1/2} = \frac{\sigma_1^2\Delta t^2 f(q_{n+\sigma_1/2})}{4q_{n+\sigma_1/2}},\\
&q_{n+\sigma_1} = 2q_{n+\sigma_1/2}G(Q_{n+\sigma_1/2}) - q_n,\\
&p_{n+\sigma_1} = \frac{2}{\sigma_1\Delta t}(q_{n+\sigma_1} - q_{n+\sigma_1/2}),\\
&q_{n+\sigma_1+\sigma_2/2} = q_{n+\sigma_1} + \frac{\sigma_2\Delta t}{2}p_{n+\sigma_1}, \quad Q_{n+\sigma_1+\sigma_2/2} = \frac{\sigma_2^2\Delta t^2 f(q_{n+\sigma_1+\sigma_2/2})}{4q_{n+\sigma_1+\sigma_2/2}},\\
&q_{n+\sigma_1+\sigma_2} = 2q_{n+\sigma_1+\sigma_2/2}G(Q_{n+\sigma_1+\sigma_2/2}) - q_{n+\sigma_1},\\
&p_{n+\sigma_1+\sigma_2} = \frac{2}{\sigma_2\Delta t}(q_{n+\sigma_1+\sigma_2} - q_{n+\sigma_1+\sigma_2/2}),\\
&q_{n+\sigma_2+3\sigma_1/2} = q_{n+\sigma_1+\sigma_2} + \frac{\sigma_1\Delta t}{2}p_{n+\sigma_1+\sigma_2}, \ Q_{n+\sigma_2+3\sigma_1/2} = \frac{\sigma_1^2\Delta t^2 f(q_{n+\sigma_2+3\sigma_1/2})}{4q_{n+\sigma_2+3\sigma_1/2}},\\
&q_{n+1} = 2q_{n+\sigma_2+3\sigma_1/2}G(Q_{n+\sigma_2+3\sigma_1/2}) - q_{n+\sigma_2+\sigma_1},\\
&p_{n+1} = \frac{2}{\sigma_1\Delta t}(q_{n+1} - q_{n+\sigma_2+3\sigma_1/2}),
\end{aligned}$$

where $\sigma_1 = 1/(2 - 2^{1/3})$, $\sigma_2 = -2^{1/3}/(2 - 2^{1/3})$. Obviously, method $\Xi_{\Delta t}$ has algebraic order four since method (2.11) is a symmetric composition one [12]. Applying $\Xi_{\Delta t}$ to the model equation (1.3), we have

$$\begin{pmatrix} q_{n+1}\\ p_{n+1}\end{pmatrix} = A_1A_2A_1\begin{pmatrix} q_n\\ p_n\end{pmatrix}, \tag{2.12}$$

where

$$A_i := \begin{pmatrix} 2G(-\sigma_i^2\nu^2/4) - 1 & G(-\sigma_i^2\nu^2/4)\sigma_i\Delta t \\ 4(G(-\sigma_i^2\nu^2/4) - 1)/(\sigma_i\Delta t) & 2G(-\sigma_i^2\nu^2/4) - 1 \end{pmatrix}, \qquad i = 1, 2.$$

As a result, the stability matrix is

$$S_{\Xi_{\Delta t}}(\nu^2) = \text{diag}\{1, \Delta t\} A_1 A_2 A_1 \text{diag}\{1, 1/\Delta t\}.$$

Since $\det(A_i) = 1$, we have

$$\det(S_{\Xi_{\Delta t}}(\nu^2)) = 1.$$

Moreover, if $G(0) = G'(0) = 1$, the estimation

$$\text{tr}(S_{\Xi_{\Delta t}}(\nu^2)) - 2\cos(\nu) = C\nu^6 + \mathcal{O}(\Delta t^8) \tag{2.13}$$

holds and it follows that method $\Xi_{\Delta t}$ has phase-lag order four at least.

Theorem 2.3. *If function $G(x)$ satisfies $G(0) = G'(0) = 1$, then method $\Xi_{\Delta t}$ is symmetric, symplectic and of phase-lag order four at least.*

3. Some rational symplectic schemes

In this section, based on the ideas presented in Section 2, we will derive three applicable rational symplectic schemes with algebraic order one, two and four, by taking function $G(x)$ as a polynomial function, respectively.

3.1. First order schemes

In method (2.1), take $G(x) = 1 + x + \sum_{n=2}^{r} \alpha_n x^n$ with real coefficients α_n. By condition (2.9), we have $\alpha_n = 2/(2n)!,\ n = 2, \ldots, r$. Without loss of generality, set $r = 5$ and the coefficients are

$$\alpha_2 = \frac{1}{12}, \quad \alpha_3 = \frac{1}{360}, \quad \alpha_4 = \frac{1}{20160}, \quad \alpha_5 = \frac{1}{1814400}.$$

The scheme has phase-lag order ten and its interval of periodicity is $\Omega \approx (0, 1.04719^2)$ since for all $\nu^2 \in \Omega$, we have $-3 \le G(-\nu^2) \le 1$, that is, $|\text{tr}(S)| \le 2$.

3.2. Second order schemes

In method $\Psi_{\Delta t}$, take $G(x) = 1 + x + \sum_{n=2}^{r} \gamma_n x^n$. By condition (2.10), we have $\gamma_n = 2^{2n-1}/(2n)!,\ n = 2, \ldots, r$. Again, if set $r = 5$, then the coefficients are

$$\gamma_2 = \frac{1}{3}, \quad \gamma_3 = \frac{2}{45}, \quad \gamma_4 = \frac{1}{315}, \quad \gamma_5 = \frac{2}{14175}$$

and the scheme has phase-lag order ten with the interval of periodicity $\Omega \approx (0, 3.08708^2)$.

3.3. Fourth order schemes

From Theorem 2.3, we know that method $\Xi_{\Delta t}$ has fourth phase-lag order at least provided that $G(0) = G'(0) = 1$ fulfills. Indeed, we can improve the phase-lag order of $\Xi_{\Delta t}$ to arbitrary even order. For instance, consider the following estimation

$$\mathrm{tr}(S_{\Xi_{\Delta t}}(\nu^2)) - 2\cos(\nu) = \sum_{n=3}^{5} C_n \nu^{2n} + \mathcal{O}(\nu^{12}).$$

Solving equations $C_n = 0, n = 3, 4, 5$, we have

$$G^{(3)}(0) = \frac{3}{5}\left(5\theta - 4\right), \tag{3.1}$$

$$G^{(4)}(0) = \frac{12\left(44\sqrt[3]{2} - 92 + 35\theta(3 - 2\sqrt[3]{2}) + 35\theta^2(\sqrt[3]{2} - 1)\right)}{35\left(2\sqrt[3]{2} - 1\right)}, \tag{3.2}$$

$$\begin{aligned} G^{(5)}(0) = & \frac{4\left(31324\sqrt[3]{4} - 31256 - 14260\sqrt[3]{2}\right)}{105\left(\sqrt[3]{2} - 2\right)\left(2\sqrt[3]{2} - 1\right)} \\ & + \frac{4\theta\left(358 + 141\sqrt[3]{2} - 334\sqrt[3]{4} - 105\theta - 40\sqrt[3]{2}\theta + 95\sqrt[3]{4}\theta\right)}{\left(\sqrt[3]{2} - 2\right)\left(2\sqrt[3]{2} - 1\right)}, \end{aligned} \tag{3.3}$$

where $\theta := G''(0)$ is free parameter. Under these conditions, method $\Xi_{\Delta t}$ has phase-lag order ten.

In $\Xi_{\Delta t}$, take $G(x) = 1 + x + \sum_{n=2}^{5} \zeta_n x^n$ and $G^{(n)}(0) = n!\zeta_n$. For simplicity, set $\theta = 0$, that is, $\zeta_2 = 0$, and by conditions (3.1-3.3), we have

$$\zeta_3 = -\frac{2}{5}, \qquad \zeta_4 = \frac{22\sqrt[3]{2} - 46}{35\left(2\sqrt[3]{2} - 1\right)}, \qquad \zeta_5 = \frac{31324\sqrt[3]{4} - 14260\sqrt[3]{2} - 31256}{3150\left(\sqrt[3]{2} - 2\right)\left(2\sqrt[3]{2} - 1\right)}.$$

Moreover, the interval of periodicity of the scheme is $\Omega \approx (0, 1.50382^2)$.

4. Numerical experiments

To illustrate the performance of our methods, we use the three schemes given in Section 3, denoted by **SI, SII, SIII**, with relatively large time steps to solve the cubic oscillatory problem and compare the numerical results with the ones given by the following three conventional explicit symplectic integrators

- Symplectic Euler method (SEM):

$$p_{n+1} = p_n + \Delta t f_n, \qquad q_{n+1} = q_n + \Delta t p_{n+1};$$

- Störmer-Verlet method (SVM) :

$$p_{n+1/2} = p_n + \Delta t f_n/2, \quad q_{n+1} = q_n + \Delta t p_{n+1/2}, \quad p_{n+1} = p_{n+1/2} + \Delta t f_{n+1}/2;$$

- Symmetric composition method based on Störmer-Verlet method (SCM), namely,

$$\Phi^{SCM}_{\Delta t} = \Phi^{SVM}_{\sigma_1 \Delta t} \circ \Phi^{SVM}_{\sigma_2 \Delta t} \circ \Phi^{SVM}_{\sigma_1 \Delta t},$$

  where $\Phi^{SVM}_{\Delta t}$ is Störmer-Verlet method and σ_i defined as in method (2.11).

Consider the problem of the cubic oscillator given by problem [2, 9]

$$q'' = -q + \varepsilon q^3, \qquad q(0) = 1, \qquad p(0) = 0.$$

Its exact solution is

$$q(t) = \tau + \left(\frac{1}{8}\varepsilon + \frac{25}{256}\varepsilon^2 + \frac{161}{2048}\varepsilon^3\right)\tau - \left(\frac{1}{8}\varepsilon + \frac{29}{256}\varepsilon^2 + \frac{212}{2048}\varepsilon^3\right)\tau^3 + \left(\frac{4}{256}\varepsilon^2 + \frac{55}{2048}\varepsilon^3\right)\tau^5 - \frac{\varepsilon^3}{512}\tau^7,$$

where $\tau = \cos(\mu t)$ and

$$\mu = 1 - \left(\frac{3}{8}\varepsilon + \frac{21}{256}\varepsilon^2 + \frac{81}{2048}\varepsilon^3 + \frac{6549}{262144}\varepsilon^4\right).$$

For this problem, the quotient $Q_n = \Delta t^2 f_n/q_n = \Delta t^2(\varepsilon q_n^2 - 1)$. In the experiment, we take $\varepsilon = 10^{-3}$ and the endpoint $T = 1000$. We give the relative errors of numerical solutions

$$\max_{t_n \in [0,T]} \frac{\|(p(t_n), q(t_n)) - (p_n, q_n)\|_\infty}{\|(p(t_n), q(t_n))\|_\infty}$$

and the relative errors of the Hamiltonian

$$\left\| \frac{H(p(0), q(0)) - H(p_n, q_n)}{H(p(0), q(0))} \right\|_\infty$$

with $H(p_n, q_n) = p_n^2/2 + q_n^2/2 - \varepsilon q_n^4/4$ and the CPU time of our schemes as well as the three conventional explicit symplectic integrators with the fixed steps $\Delta t = 1/2^j,\ j = 2:6$, respectively (See Tables 1, 2 and 3).

Table 1. The relative errors of the six methods.

h	1/4	1/8	1/16	1/32	1/64
SI	1.2565e-1	6.2580e-2	3.1260e-2	1.5626e-2	7.8126e-3
SEM	2.4102e+0	8.8161e-1	2.0948e-1	5.7455e-2	1.8054e-2
SII	1.0938e-2	2.7426e-3	6.8686e-4	1.7164e-4	4.2917e-5
SVM	2.3987e+0	8.0606e-1	1.7498e-1	4.1498e-2	1.0226e-2
SIII	1.1191e-3	7.0122e-5	4.3832e-6	2.7532e-7	1.6547e-8
SCM	2.8722e-1	1.6217e-2	1.0060e-3	6.2824e-5	3.9259e-6

Table 2. The relative errors of the Hamiltonian of the six methods.

h	1/4	1/8	1/16	1/32	1/64
SI	1.3942e-1	6.5901e-2	3.2072e-2	1.5825e-2	7.8607e-3
SEM	1.4278e-1	6.6637e-2	3.2245e-2	1.5867e-2	7.8710e-3
SII	1.0496e-2	2.6067e-3	6.5059e-4	1.6258e-4	4.0641e-5
SVM	1.5617e-2	3.9043e-3	9.7607e-4	2.4402e-4	6.1005e-5
SIII	2.2113e-4	1.3810e-5	8.6288e-7	5.3928e-8	3.3717e-9
SCM	3.1141e-4	1.8805e-5	1.1652e-6	7.2668e-8	4.5393e-9

Table 3. The CPU time (s) of the six methods.

h	1/4	1/8	1/16	1/32	1/64
SI	0.005750	0.012202	0.023295	0.045214	0.084023
SEM	0.001151	0.002375	0.006872	0.009402	0.018058
SII	0.006024	0.011258	0.023645	0.043160	0.085954
SVM	0.002260	0.007037	0.010444	0.018020	0.037968
SIII	0.017912	0.032643	0.062616	0.118922	0.245064
SCM	0.007282	0.015386	0.027154	0.053852	0.107558

From the numerical results, we can find that our schemes are more accurate than the conventional methods of same algebraic order and the behavior of the Hamiltonian persevering is almost same for these methods of same algebraic order. However, the computational work of our methods are a bit larger than that of the conventional methods.

At the end of this section, we have two remarks on our schemes:

- The singular case that q_n *varnishes* at some step, which means the quotient $Q_n = \Delta t^2 f_n/q_n$ may be infinite and then our schemes will be not applicable, does not arise all along in our numerical experiments. Indeed, once the singularity arises at some computational step, we can adopt the following remedial strategy, that is, if $\lim_{q_n \to 0} f(q_n)/q_n$ exists, then we set $Q_n = \Delta t^2 \lim_{q_n \to 0} f_n/q_n$, else, we may employ a higher accurate conventional symplectic method to *jump* the step.
- Since our schemes are rational, they only can be applicable for one-dimensional problems. It need to go on discussing how to apply these rational methods to multi-dimensional problems. The problem that how to make our methods applicable for multi-dimensional Hamiltonian oscillatory problems will be considered in future work.

5. Conclusions

In this paper, a class of rational explicit symplectic integrators for one-dimensional Hamiltonian oscillatory problems are presented. These methods are zero-dissipative, and of first algebraic order and high phase-lag order. By means of composition technique, we construct second and fourth order methods with high phase-lag order of this type. Based on our ideas, some applicable explicit symplectic schemes are derived. We report some numerical results to illustrate the good performance of our methods.

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