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The existence of explicit symplectic ARKN methods with several stages and algebraic order greater than two[☆]

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ABSTRACT

Adapted Runge–Kutta–Nyström (ARKN) methods for solving the oscillatory problem $q''(t)+w^2q(t) = f(q(t))$ have been investigated by several authors. Recently, Shi et al. *[Comput. Phys. Comm. 183 (2012) 1250–1258]* conclude that there exist only one-stage explicit symplectic ARKN methods and the algebraic order cannot exceed two. In this paper we investigate the symplecticity of ARKN methods and present that there exist explicit symplectic ARKN methods with several stages and algebraic order greater than two. Some numerical experiments are provided to confirm the theoretical expectations.

1. Introduction

In this paper, we consider the numerical integration of a second-order initial value problem of the form

$$\begin{cases} q''(t) + w^2q(t) = f(q(t)), \quad t \in [t_0, T], \\ q(t_0) = q_0, \quad q'(t_0) = q'_0, \end{cases} \tag{1}$$

where the main frequency w may be known or accurately estimated, $q \in R^d$ and $f(q)$: $R^d \to R^d$. For this kind of oscillatory second-order initial value problems, adapted Runge–Kutta–Nyström methods (ARKN methods) were investigated by several authors [1–3]. When the function $f(q)$ satisfies $f(q) - Mq = -\nabla V(q)$ for some smooth function $V(q)$, the problem (1) is equivalent to the separable Hamiltonian system of the following form:

$$\begin{cases} q' = p, \quad q(t_0) = q_0, \\ p' = -\nabla V(q), \quad p(t_0) = p_0, \end{cases} \tag{2}$$

where $q : R \to R^d$ and $p : R \to R^d$ are generalized position and generalized momenta, respectively. The Hamiltonian of (2) is

$$H(p, q) = \frac{1}{2}p^Tp + V(q). \tag{3}$$

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As one of the important qualitative properties of Hamiltonian systems, symplecticity has been receiving more and more attention. The symplecticity conditions of ARKN methods are investigated in [4,5]. However, the symplecticity conditions in [4,5] are only sufficient but not necessary. Based on these conditions, the author concludes that there exist only one-stage explicit symplectic ARKN methods and the algebraic order cannot exceed two. The innovation of this paper is to show that there exist explicit symplectic ARKN methods with several stages and algebraic order greater than two.

2. ARKN methods and symplectic conditions

From [1], adapted Runge–Kutta–Nyström (ARKN) methods for solving the problem (1) have the following form

$$\begin{cases} Q_i = q_n + c_i h q_n' + h^2 \sum\limits_{j=1}^{s} \bar{a}_{ij}(-w^2 Q_j + f(Q_j)), \quad i = 1, 2, \ldots, s, \\ q_{n+1} = \phi_0(v) q_n + h\phi_1(v) q_n' + h^2 \sum\limits_{i=1}^{s} \bar{b}_i(v) f(Q_i), \\ q_{n+1}' = -wv\phi_1(v) q_n + \phi_0(v) q_n' + h \sum\limits_{i=1}^{s} b_i(v) f(Q_i), \end{cases} \tag{4}$$

where $\bar{b}_i(v)$ and $b_i(v)$ with $i = 1, \ldots, s$ are all functions of $v = wh$ whereas $\bar{a}_{ij}$, $i, j = 1, \ldots, s$ are constants. Here the matrix-valued ϕ-functions are defined as $\phi_0(v) = \cos v, \quad \phi_1(v) = \frac{\sin v}{v}$. The order conditions for ARKN methods were given in [1].

In order to derive the symplectic conditions for ARKN methods (4), firstly we recall the modified RKN scheme for the system (1) considered in [6]:

$$\begin{cases} Q_i = C_i(v) q_n + D_i(v) h q_n' + h^2 \sum\limits_{j=1}^{s} a_{ij}^*(v) f(Q_j), \quad i = 1, \ldots, s, \\ q_{n+1} = C(v) q_n + hD(v) q_n' + h^2 \sum\limits_{i=1}^{s} \bar{b}_i(v) f(Q_i), \\ q_{n+1}' = h^{-1} B(v) q_n + A(v) q_n' + h \sum\limits_{i=1}^{s} b_i(v) f(Q_i), \end{cases} \tag{5}$$

where $A(v)$, $B(v)$, $C(v)$, $D(v)$, $C_i(v)$ and $D_i(v)$, $i = 1, \ldots, s$ are functions of $v = hw$. The authors of [6] present the symplectic conditions of the method (5) as follows

Theorem 2.1 (*See [6]*). *An s-stage modified RKN method (5) is symplectic if and only if its coefficients satisfy*

$$\begin{aligned} & A(v)C(v) - B(v)D(v) = 1, \\ & \bar{b}_i(v)\left(A(v) - B(v)\frac{D_i(v)}{C_i(v)}\right) = b_i(v)\left(D(v) - C(v)\frac{D_i(v)}{C_i(v)}\right), \\ & b_i(v)\left(\bar{b}_j(v) - a_{ij}^*(v)\frac{C(v)}{C_i(v)}\right) + \bar{b}_i(v) a_{ij}^*(v)\frac{B(v)}{C_i(v)} \\ & \qquad = b_j(v)\left(\bar{b}_i(v) - a_{ji}^*(v)\frac{C(v)}{C_j(v)}\right) + \bar{b}_j(v) a_{ji}^*(v)\frac{B(v)}{C_j(v)}. \end{aligned} \tag{6}$$

where $i, j = 1, \ldots, s$.

In the rest of this paper, we denote the ith row and jth column element of the matrix M as $[M]_{ij}$ for convenience. By using the necessary tensor signs, the internal stage vector of the method (4) can be expressed as

$$Q = e \otimes q_n + c \otimes h q_n' + h^2(\bar{A} \otimes I_d)(-w^2 Q + f(Q)), \tag{7}$$

where

$$\begin{aligned} & e = (1, \ldots, 1)^T, \qquad c = (c_1, \ldots, c_s)^T, \\ & Q = (Q_1^T, \ldots, Q_s^T)^T, \qquad f(Q) = (f(Q_1)^T, \ldots, f(Q_s)^T)^T, \end{aligned} \tag{8}$$

and I_d is $d \times d$ identity matrix. From (7), we obtain

$$Q = \left(I_{sd} + v^2(\bar{A} \otimes I_d)\right)^{-1}\left(e \otimes q_n + c \otimes h q_n' + h^2(\bar{A} \otimes I_d) f(Q)\right).$$

With $I_{sd} + v^2(\bar{A} \otimes I_d) = I_s \otimes I_d + v^2(\bar{A} \otimes I_d) = (I_s + v^2\bar{A}) \otimes I_d$, we obtain

$$Q = \Big((I_s + v^2\bar{A})^{-1} \otimes I_d\Big)\Big(e \otimes q_n + c \otimes hq_n' + h^2(\bar{A} \otimes I_d)f(Q)\Big). \tag{9}$$

From (9) and the following relation

$$\begin{aligned}
&\Big((I_s + v^2\bar{A})^{-1} \otimes I_d\Big)\Big(e \otimes q_n\Big) = \Big((I_s + v^2\bar{A})^{-1}e\Big) \otimes q_n,\\
&\Big((I_s + v^2\bar{A})^{-1} \otimes I_d\Big)\Big(c \otimes hq_n'\Big) = \Big((I_s + v^2\bar{A})^{-1}c\Big) \otimes hq_n',\\
&h^2\Big((I_s + v^2\bar{A})^{-1} \otimes I_d\Big)\Big(\bar{A} \otimes I_d\Big)f(Q) = h^2\Big(((I_s + v^2\bar{A})^{-1}\bar{A}) \otimes I_d\Big)f(Q),
\end{aligned}$$

we obtain

$$Q = \Big((I_s + v^2\bar{A})^{-1}e\Big) \otimes q_n + \Big((I_s + v^2\bar{A})^{-1}c\Big) \otimes hq_n' + h^2\Big(\Big((I_s + v^2\bar{A})^{-1}\bar{A}\Big) \otimes I_d\Big)f(Q). \tag{10}$$

Through the above expression (10), we know that the method (4) is equivalent to the following method

$$\begin{cases}
Q_i = C_i(v)q_n + D_i(v)hq_n' + h^2 \displaystyle\sum_{j=1}^{s} a_{ij}^*(v)f(Q_j), \quad i = 1, \dots, s,\\
q_{n+1} = \phi_0(v)q_n + h\phi_1(v)q_n' + h^2 \displaystyle\sum_{i=1}^{s} \bar{b}_i(v)f(Q_i),\\
q_{n+1}' = -wv\phi_1(v)q_n + \phi_0(v)q_n' + h \displaystyle\sum_{i=1}^{s} b_i(v)f(Q_i),
\end{cases} \tag{11}$$

where $C_i(v)$ and $D_i(v)$ are the ith components of $(I + v^2\bar{A})^{-1}e$ and $(I + v^2\bar{A})^{-1}c$, respectively, and $a_{ij}^*(v)$ is the ith row and jth column element of the matrix $(I + v^2\bar{A})^{-1}\bar{A}$, i.e.

$$\begin{aligned}
&C_i(v) = \Big[(I + v^2\bar{A})^{-1}e\Big]_i, \qquad D_i(v) = \Big[(I + v^2\bar{A})^{-1}c\Big]_i,\\
&a_{ij}^*(v) = \Big[(I + v^2\bar{A})^{-1}\bar{A}\Big]_{ij}.
\end{aligned} \tag{12}$$

By taking $C(v) = \phi_0(v)$, $D(v) = \phi_1(v)$, $A(v) = \phi_0(v)$ and $B(v) = -v^2\phi_1(v)$, the method (11) can be seen as a modified RKN method (5). From Theorem 2.1, we obtain the following result.

Theorem 2.2. *An s-stage ARKN method (4) is symplectic if and only if its parameters satisfy*

$$\begin{aligned}
&\bar{b}_i(v)\left(\phi_0(v) + v^2\phi_1(v)\frac{D_i(v)}{C_i(v)}\right) = b_i(v)\left(\phi_1(v) - \phi_0(v)\frac{D_i(v)}{C_i(v)}\right),\\
&b_i(v)\left(\bar{b}_j(v) - a_{ij}^*(v)\frac{\phi_0(v)}{C_i(v)}\right) - \bar{b}_i(v)a_{ij}^*(v)\frac{v^2\phi_1(v)}{C_i(v)}\\
&\qquad = b_j(v)\left(\bar{b}_i(v) - a_{ji}^*(v)\frac{\phi_0(v)}{C_j(v)}\right) - \bar{b}_j(v)a_{ji}^*(v)\frac{v^2\phi_1(v)}{C_j(v)},
\end{aligned} \tag{13}$$

where $C_i(v)$, $D_i(v)$ and $a_{ij}^*(v)$ are given by (12) with $i, j = 1, \dots, s$.

Remark 2.1. For an ARKN method, when $\bar{a}_{ij} = 0$ for $i, j = 1, \dots, s$, we obtain

$$C_i(v) = 1, \qquad D_i(v) = c_i, \qquad a_{ij}^*(v) = \bar{a}_{ij} = 0.$$

where $i, j = 1, \dots, s$. In this case, from Theorem 2.2, the sufficient condition in [4,5] is obtained.

By using the necessary and sufficient symplectic conditions in Theorem 2.2, we can construct explicit symplectic ARKN methods with several stages and algebraic order greater than two. This point will be confirmed in the next section.

3. Construction of new symplectic ARKN method

In this section, we focus on construction of three stage explicit symplectic ARKN (SARKN) methods. We consider symmetric nodes $c_2 = \frac{1}{2}$ and $c_3 = 1 - c_1$. From the symplecticity conditions (13) for three-stage ARKN methods, we obtain

$$\begin{aligned}
&\bar{b}_1(v) = \bar{b}_1(c_1, \bar{a}_{21}, \bar{a}_{31}, \bar{a}_{32}, \bar{b}_3(v)), \qquad \bar{b}_2(v) = \bar{b}_2(c_1, \bar{a}_{21}, \bar{a}_{31}, \bar{a}_{32}, \bar{b}_3(v)),\\
&b_1(v) = b_1(c_1, \bar{a}_{21}, \bar{a}_{31}, \bar{a}_{32}, \bar{b}_3(v)), \qquad b_2(v) = b_2(c_1, \bar{a}_{21}, \bar{a}_{31}, \bar{a}_{32}, \bar{b}_3(v)),\\
&b_3(v) = b_3(c_1, \bar{a}_{21}, \bar{a}_{31}, \bar{a}_{32}, \bar{b}_3(v)),
\end{aligned} \tag{14}$$

where $c_1, \bar{a}_{21}, \bar{a}_{31}, \bar{a}_{32}$ and $\bar{b}_3(v)$ are free parameters. Assume that $\bar{b}_3(v)$ does not depend on v. Letting the coefficients of (14) satisfy order conditions

$$\begin{aligned}
&\sum_{i=1}^{3} \bar{b}_i(v) = \phi_2(v) + O(h^3), \qquad \sum_{i=1}^{3} \bar{b}_i(v) c_i = \phi_3(v) + O(h^2), \qquad \sum_{i=1}^{3}\sum_{j=1}^{i-1} b_i(v)\bar{a}_{ij} = \phi_3(v) + O(h^2),\\
&\sum_{i=1}^{3}\sum_{j=1}^{i-1} b_i(v)\bar{a}_{ij} c_j = \phi_4(v) + O(h), \qquad \sum_{i=1}^{3}\sum_{j=1}^{i-1} b_i(v) c_i \bar{a}_{ij} = 3\phi_4(v) + O(h),
\end{aligned}$$

we obtain

$$\begin{aligned}
&c_1 = \frac{1}{12}(4 + 2\sqrt[3]{2} + \sqrt[3]{4}), \qquad \bar{a}_{21} = \frac{1}{12(1-2c_1)},\\
&\bar{a}_{31} = \frac{1}{6(1-2c_1)}, \qquad \bar{a}_{32} = \frac{1-6c_1+6c_1^2}{3(1-2c_1)}, \qquad \bar{b}_3 = \frac{c_1}{6(1-2c_1)^2}.
\end{aligned} \tag{15}$$

Inserting (15) into (14), we obtain

$$\begin{aligned}
&\bar{b}_1 = \frac{-c_1 v\cos(v) + \sin(v)}{6(1-2c_1)^2 v}, \qquad \bar{b}_2 = -\Big((1-6c_1+6c_1^2)(v(-6+c_1(12+v^2))\cos(v)\\
&\quad - (-12+24c_1+v^2)\sin(v))\Big)\Big/(18(-1+2c_1)^3 v),\\
&b_1 = \frac{\cos(v) + c_1 v\sin(v)}{6(1-2c_1)^2}, \qquad b_2 = \Big((1-6c_1+6c_1^2)((-12+24c_1+v^2)\cos(v)\\
&\quad + v(-6+c_1(12+v^2))\sin(v))\Big)\Big/\Big(18(-1+2c_1)^3\Big),\\
&b_3 = -\Big(\bar{b}_3 v((36 - 18v^2 + 144c_1^3 v^2 + v^4 + 6c_1^2(24 - 36v^2 + v^4)\\
&\quad - 6c_1(24 - 18v^2 + v^4))\cos(v) + v(-6(-6+v^2) + 6c_1^3(-24+12v^2+v^4)\\
&\quad - 6c_1^2(-48+16v^2+v^4) + c_1(-180+42v^2+v^4))\sin(v))\Big)\\
&\quad \Big/\Big(v(-6(-6+v^2) + 6c_1^3(-24+12v^2+v^4) - 6c_1^2(-48+16v^2+v^4)\\
&\quad + c_1(-180+42v^2+v^4))\cos(v) - (36 - 18v^2 + 144c_1^3 v^2 + v^4\\
&\quad + 6c_1^2(24-36v^2+v^4) - 6c_1(24-18v^2+v^4))\sin(v)\Big).
\end{aligned} \tag{16}$$

By expanding the previous coefficients into Taylor series, it is easy to check that this set of coefficients satisfies the conditions of order four. This method is denoted by SARKN3S4P.

4. Numerical experiments

In this section, in order to show the competence and superiority of the new method compared with other codes from the literature, we use two model problems. The integrators we select for comparison are

- SARKN3S4P: the symplectic three-stage ARKN method of order four given in this paper;
- SARKN1S2P: the one-stage symplectic ARKN method given in [4];
- SSRKN3S4P: the three-stage symmetric and symplectic RKN method of order four given in [7].

Problem 1. We consider the Duffing equation

$$\begin{cases} q'' + w^2 q = 2k^2 q^3 - k^2 q, \quad t \in [0, t_{end}],\\ q(0) = 0, \quad q'(0) = w, \end{cases} \tag{17}$$

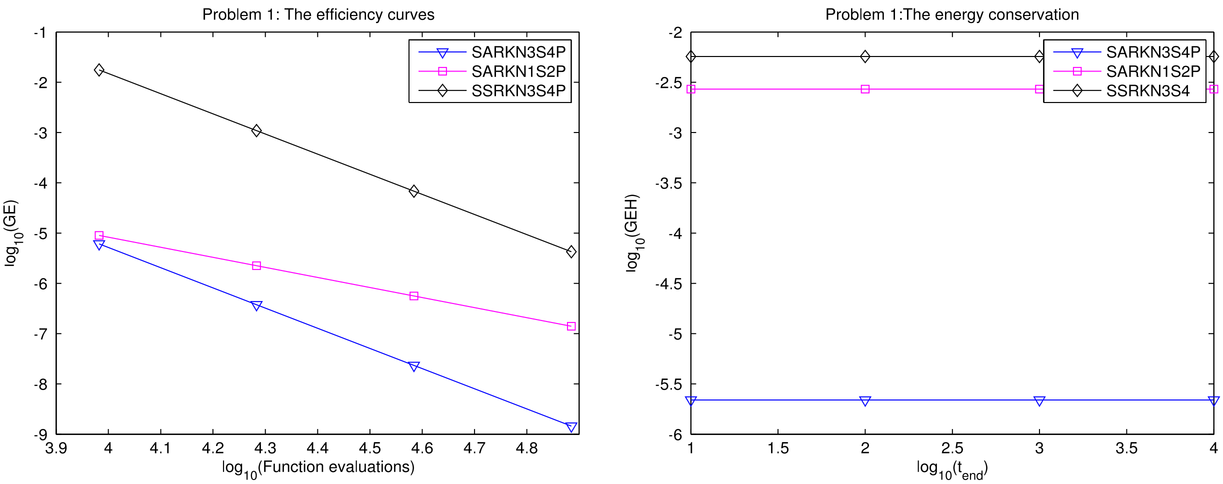

Fig. 1. Efficiency curves (left) and energy conservation (right) for Problem 1.

The Hamiltonian of this system is given by

$$H(p,q)=\frac{1}{2}p^2+\frac{1}{2}(\omega^2+k^2)q^2-\frac{k^2}{2}q^4.$$

where $k=0.03$. The exact solution of this initial-value problem is $y(t)=\mathrm{sn}(wt;\,k/w)$, the so-called Jacobian elliptic function. In this test we choose the frequency $w=5$ as fitting parameter.

This problem has been solved in the interval $[0, 100]$ with the step sizes $h=1/2^j$ for the three-stage methods, where $j=5,6,7,8$. Then we integrate the problem with a fixed step size $h=1/10$ in different length of intervals and see the preservation of the Hamiltonian by each code. The numerical results are presented in Fig. 1.

Problem 2. Two coupled oscillators with different frequencies

$$\begin{cases} q_1''+q_1=2\varepsilon q_1q_2, & q_1(0)=1, \quad q_1'(0)=0,\\ q_2''+2q_2=\varepsilon q_1^2+4\varepsilon q_2^3, & q_2(0)=1, \quad q_2'(0)=0. \end{cases}$$

The Hamiltonian of this system is given by

$$H(p,q)=\frac{1}{2}(p_1^2+p_2^2)+\frac{1}{2}(q_1^2+2q_2^2)-\varepsilon\left(q_1^2q_2+q_2^4\right).$$

In this numerical test we choose $\varepsilon=10^{-3}$. We first solve this problem in the interval $[0, 100]$ and step sizes $h=1/2^j$ for the three-stage methods, where $j=3,\dots,6$. Then we integrate the problem with a fixed step size $h=1/10$ in different length of intervals and see the preservation of the Hamiltonian by each code. The numerical results are presented in Fig. 2.

In our numerical experiments we take the numerical solution obtained by the classical four-stage RKN method of order five [8] with small step size as the exact solution.

5. Conclusions and discussions

In this paper, we study the symplecticity of ARKN methods for solving oscillatory problems (1). We derived the symplectic conditions for ARKN methods and show that there exist explicit symplectic ARKN methods with several stages and algebraic order greater than two. The results of the numerical experiments show the robustness of the new method.

How to find a suitable value for the fitting parameter w for a trigonometrically fitted method is a critical issue, because the coefficients of the method depend on w. The knowledge of an estimation to the unknown frequency is needed in order to apply the numerical method efficiently. However, for different algorithms, the way to determine the frequency is also different. For the technique of frequency choice in trigonometrically fitted methods, the reader is referred to [9]. We intend to follow this line of research in the future.

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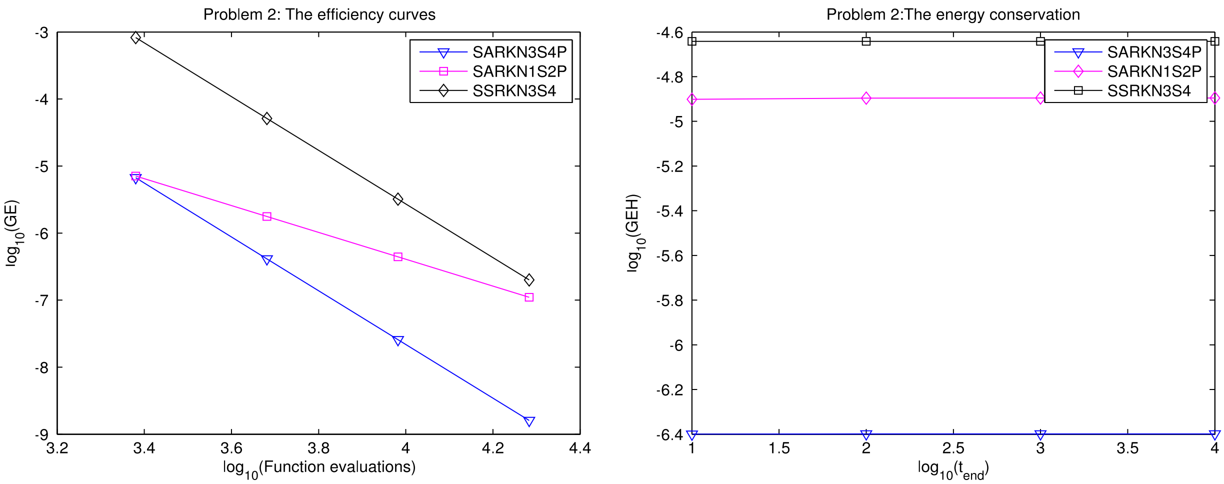

Fig. 2. Efficiency curves (left) and energy conservation (right) for Problem 2.

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