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ORIGINAL PAPER

Energy-preserving trigonometrically fitted continuous stage Runge-Kutta-Nyström methods for oscillatory Hamiltonian systems

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Abstract

Recently, continuous-stage Runge-Kutta-Nyström (CSRKN) methods for solving numerically second-order initial value problem $q'' = f(q)$ have been proposed and developed by Tang and Zhang (Appl. Math. Comput. **323**, 204–219, 2018). This problem is equivalent to a separable Hamiltonian system when $f(q) = -\nabla U(q)$ with smooth function $U(q)$. Symplecticity-preserving discretizations of this system were studied in that paper. However, as an important representation of the Hamiltonian system, energy preservation has not been studied. In addition, many Hamiltonian systems in practical applications often have oscillatory characteristics so we should design special algorithms adapted to this feature. In this paper, we propose and study energy-preserving trigonometrically fitted CSRKN methods for oscillatory Hamiltonian systems. We extend the theory of trigonometrical fitting to CSRKN methods and derive sufficient conditions for energy preservation. We also study the symmetry and stability of the methods. Two symmetric and energy-preserving trigonometrically fitted schemes of order two and four, respectively, are constructed. Some numerical experiments are provided to confirm the theoretical expectations.

Keywords Trigonometrically fitted methods · Continuous-stage Runge-Kutta–Nyström methods · Order conditions · Energy-preserving · Oscillatory Hamiltonian systems

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1 Introduction

In this paper, we consider numerical integration of second-order ordinary differential equations of the form

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

whose solution has an oscillatory character, where $q \in R^d$, $f : R^d \to R^d$ is sufficiently differentiable. This problem usually arises in mechanics, theoretical physics, quantum dynamics, molecular biology, etc. Regarding the oscillatory feature of the problem (1), researchers have proposed to develop special integrators by some techniques like trigonometrical/exponential fitting (see [1]). All of these methods integrate exactly the oscillatory system $q''(t) = -w^2 q(t)$ where w is the approximate value of the main frequency. Early presentations of these techniques are due to Gautschi [2] and Lyche [3]. Since then, a lot of exponentially (or trigonometrically) fitted linear multi-step methods and RKN methods have been developed [4–10]. In the past 10 years, the technology of trigonometrical/exponential fitting has been applied to more methods such as multi-step hybrid methods [11–16] and to high dimensional problem [17, 18].

When the function $f(q)$ satisfies $f(q) = -\nabla U(q)$ for some smooth function $U(q)$, problem (1) is equivalent to a separable Hamiltonian system of the following form:

$$\begin{cases} q'(t) = p(t) \\ p'(t) = -\nabla U(q(t)), \quad t \in [t_0, T], \\ q(t_0) = q_0, \quad p(t_0) = p_0 \end{cases} \tag{2}$$

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

$$H(q, p) = \frac{1}{2} p^T p + U(q), \tag{3}$$

which is also referred to as the energy. It is well known that the exact flow of Hamiltonian systems is symplectic for every t. Another important property of the flow is that it preserves energy $H(q, p)$, i.e., $H(q(t), p(t)) \equiv H(q_0, p_0)$ for all $t \in [t_0, T]$. From a viewpoint of geometric numerical integration, an integrator that inherits such geometric properties as much as possible would be preferable. But since a numerical integrator cannot inherit both symplecticity and energy preservation [19, 20], the methods satisfying one of these properties have been developed in the last decades.We call such methods symplectic or energy-preserving methods, respectively. It is widely accepted that such methods produce qualitatively nice numerical solutions over a long time [21]. Although there are already a lot of symplecitic RKN methods, energy-preserving methods are not RKN methods in general [22].

For first-order ordinary differential equations of the form

$$\begin{cases} y'(t) = F(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{4}$$

Hairer [23] proposed a family of continuous-stage Runge-Kutta (CSRK) methods which exactly preserve energy when this problem is an Hamiltonian system. Miyatake et al. [24] proved a sufficient and necessary energy-preserving condition of CSRK methods and presented high-order energy-preserving methods. For further work, we see [25, 26]. Recently, Tang et al. [27] developed continuous-stage Runge-Kutta-Nyström (CSRKN) methods for numerical integration of second-order ordinary differential equations (1) and studied symplecticity-preserving algorithms. However, the authors of [27] did not study the nature of energy preservation, which is also very important in practical applications. In addition, many Hamiltonian systems in practical applications often have oscillatory characteristics so we should design special algorithms adapted to this feature.

In this paper, we will extend the idea of trigonometrical fitting to CSRKN methods and study their energy preservation. The rest of this paper is organized as follows: In Section 2, we restate the RKN methods and their trigonometrical version for the problem (1). In Section 3, trigonometrically fitted CSRKN (TFCSRKN) methods are presented and then the energy-preserving conditions and symmetric conditions are studied. In Section 4, the stability properties are analyzed. With these conditions, two new energy-preserving and symmetric TFCSRKN methods of order two and four, respectively, are constructed in Section 5. In Section 6, numerical experiments are carried out and the numerical results show the robustness of the new methods. Section 7 is concerned with conclusions and discussions.

2 Trigonometrically fitted Runge-Kutta-Nyström methods

As we all know, an s-stage Runge-Kutta-Nyström (RKN) method for the numerical integration of problem (1) is given as

$$\begin{cases} Q_i = q_n + hc_i q_n' + h^2 \sum_{j=1}^{s} a_{ij} f\left(Q_j\right), \quad i = 1, \cdots, s, \\ q_{n+1} = q_n + hq_n' + h^2 \sum_{i=1}^{s} \bar{b}_i f\left(Q_i\right), \\ q_{n+1}' = q_n' + h \sum_{i=1}^{s} b_i f\left(Q_i\right) \end{cases} \tag{5}$$

where c_i, a_{ij}, $\bar{b}_i$, and b_i with $i, j = 1, \cdots, s$ are all real coefficients. Method (5) can also be expressed briefly in the Butcher-type tableau as

$$\begin{array}{c|c} c & A \\ \hline & \bar{b}^T \\ \hline & b^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_s \\ \hline & b_1 & \cdots & b_s \end{array}$$

or equivalently by the four-elements group $(c, A, \bar{b}, b)$. The conditions for an RKN method (5) to have algebraic order of accuracy p have been given in [28] by using the theory of B-series [29]. It is well known that the theory of B-series provides an essential tool to analyze the properties of numerical methods for ordinary differential equations. The theory is attributed to a smart intuition of J. C. Butcher [30]. For second-order differential equations, the related theory has been given in [31]. Here, we restate the conditions for a RKN method having order p as follows.

Theorem 1 *The RKN method (5) is convergent of order p if and only if*

$$\begin{aligned}
\sum_{i=1}^{s} \bar{b}_i \Phi_i(t) &= \frac{1}{(\rho(t)+1)\gamma(t)}, \quad \rho(t) \le p-1, \\
\sum_{i=1}^{s} b_i \Phi_i(t) &= \frac{1}{\gamma(t)}, \quad \rho(t) \le p,
\end{aligned} \tag{6}$$

where the rooted trees t (no confusion with the time variable t shall arise) and functions $\rho(t)$, $\gamma(t)$, and $\Phi_i(t)$ are defined in [28].

In order to let method (5) behave better in integrating oscillatory problems (1), some authors [32] modified method (5) by introducing frequency-depending coefficients and proposed the following modified RKN methods:

$$\begin{cases}
Q_i = \beta_i(v) q_n + h\gamma_i(v) c_i q_n' + h^2 \sum_{j=1}^{s} a_{ij}(v) f\left(Q_j\right), \quad i = 1, \cdots, s, \\
q_{n+1} = \beta_{s+1}(v) q_n + h\gamma_{s+1}(v) q_n' + h^2 \sum_{i=1}^{s} \bar{b}_i(v) f\left(Q_i\right), \\
q_{n+1}' = \alpha_{s+1}(v) q_n' + h \sum_{i=1}^{s} b_i(v) f\left(Q_i\right).
\end{cases} \tag{7}$$

The idea of constructing methods which integrate exactly a set of linearly independent functions different of the polynomials has been proposed by several authors. The corresponding technique is often called functional fitting and the methods are called functionally fitted methods. This idea consists of selecting the available parameters of modified RKN method (7) in order to make the method exact for a linear space of functions with basis

$$\mathcal{F} = \langle\, \varphi_1(t), \varphi_2(t), \cdots, \varphi_r(t) \,\rangle, \quad r \le s+1.$$

The bases can be given in different ways and some examples of bases have been listed in [33]. When $\mathcal{F}$ contains only polynomial functions up to a certain degree ($\varphi_m(t) = t^{m+1}$), the corresponding methods are the standard RKN methods. Here, we consider the following exponential functions as reference set of functions:

$$\mathcal{F}_1 = \langle\, \exp(\mathrm{i}wt), \exp(-\mathrm{i}wt) \,\rangle, \quad \text{with} \quad \mathrm{i}^2 = -1,$$

where w is an approximate value of the main frequency. This leads to the following equations:

$$\begin{aligned}
&\exp(\pm \mathrm{i} c_i v) = \beta_i(v) \pm \mathrm{i} v \gamma_i(v) c_i \mp v^2 \sum_{j=1}^{s} a_{ij}(v) \exp(\pm \mathrm{i} c_j v),\\
&\exp(\pm \mathrm{i} v) = \beta_{s+1}(v) \pm \mathrm{i} v \gamma_{s+1}(v) \mp v^2 \sum_{i=1}^{s} \bar{b}_i(v) \exp(\pm \mathrm{i} c_i v),\\
&\exp(\pm \mathrm{i} v) = \alpha_{s+1}(v) \pm \mathrm{i} v \sum_{i=1}^{s} b_i(v) \exp(\pm \mathrm{i} c_i v), \quad v = wh.
\end{aligned} \tag{8}$$

With the Euler formula $\exp(\pm \mathrm{i} v) = \cos(v) \pm \mathrm{i} \sin(v)$, (8) is equivalent to the following trigonometrical fitting (TF) conditions:

$$\begin{aligned}
&\sin(c_i v) = \gamma_i(v) c_i v - v^2 \sum_{j=1}^{s} a_{ij}(v) \sin(c_j v),\\
&\cos(c_i v) = \beta_i(v) - v^2 \sum_{j=1}^{s} a_{ij}(v) \cos(c_j v),\\
&\sin(v) = \gamma_{s+1}(v) v - v^2 \sum_{i=1}^{s} \bar{b}_i(v) \sin(c_i v),\\
&\cos(v) = \beta_{s+1}(v) - v^2 \sum_{i=1}^{s} \bar{b}_i(v) \cos(c_i v),\\
&\cos(v) = \alpha_{s+1}(v) - v \sum_{i=1}^{s} b_i(v) \sin(c_i v), \quad \sin(v) = v \sum_{i=1}^{s} b_i(v) \cos(c_i v).
\end{aligned} \tag{9}$$

A modified RKN method (7) satisfying the TF conditions (9) will be called a trigonometrically fitted RKN (TFRKN) method. As shown in [32], the local truncation errors in the approximation of the solution and of its derivative can be expressed as

$$\begin{aligned}
q(t_n + h) - q_{n+1} &= \sum_{j=1}^{p-1} h^{j+1} \left(\sum_{i=1}^{k_j} d_i^{j+1} F^{(j)}(q_n) \right) + O(h^{p+1}),\\
q'(t_n + h) - q'_{n+1} &= \sum_{j=1}^{p} h^{j} \left(\sum_{i=1}^{\dot{k}_j} \dot{d}_i^{j} F^{(j)}(q_n) \right) + O(h^{p+1}),
\end{aligned} \tag{10}$$

where $F^{(j)}(q_n)$ denotes an elementary differential and the terms d_i^{j+1} and $\dot{d}_i^{j}$ depend on the coefficients of the method. For more detailed analysis, we see [32]. So an TFRKN method is of order p if

$$q(t_n + h) - q_{n+1} = O(h^{p+1}), \quad q'(t_n + h) - q'_{n+1} = O(h^{p+1}). \tag{11}$$

Using these assumptions and computing the terms d_i^{j+1} and $\dot{d}_i^j$ associated to the local truncation errors, the order conditions for an TFRKN method (up to fourth order) are listed in [32].

In recent years, some symplectic TFRKN methods have been proposed for the oscillatory problem (1). It is worth noting that all the methods approximately rather than exactly preserve the energy $H(p, q)$ determined by (3). In practical applications, high-precision energy preservation is often required and energy-preserving algorithms are becoming more and more popular.

3 Continuous-stage RKN methods and energy preserving

An s-degree continuous-stage Runge-Kutta (CSRK) method for problem (4) is defined by

$$\begin{cases} Y_\tau = y_n + h\int_0^1 A_{\tau\sigma} F(Y_\sigma)\,\mathrm{d}\sigma, \\ y_{n+1} = y_n + h\int_0^1 \bar{B}_\tau F(Y_\tau)\,\mathrm{d}\tau, \end{cases} \tag{12}$$

where Y_τ is a polynomial of degree s with respect to τ satisfying $Y_0 = y_n$, $A_{\tau\sigma}$ be a function of variables $\tau, \sigma \in [0, 1]$ and B_τ be a function of $\tau \in [0, 1]$. The CSRK methods were proposed firstly in [23]. Following [23] is [24], in which a sufficient and necessary energy-preserving condition of CSRK methods is proved. Recently, similarly as the CSRK method, Tang et al. [27] proposed the continuous-stage Runge-Kutta-Nyström (CSRKN) method as follows.

Definition 1 Let $A_{\tau\sigma}$ be a function of variables $\tau, \sigma \in [0, 1]$ and $\bar{B}_\tau$, B_τ, and C_τ be functions of $\tau \in [0, 1]$. An s-degree continuous-stage Runge-Kutta-Nyström (CSRKN) method for the numerical integration of problem (1) is defined as

$$\begin{cases} Q_\tau = q_n + hC_\tau q_n' + h^2\int_0^1 A_{\tau\sigma} f(Q_\sigma)\,\mathrm{d}\sigma, \\ q_{n+1} = q_n + hq_n' + h^2\int_0^1 \bar{B}_\tau f(Q_\tau)\,\mathrm{d}\tau, \\ q_{n+1}' = q_n' + h\int_0^1 B_\tau f(Q_\tau)\,\mathrm{d}\tau, \end{cases} \tag{13}$$

where Q_τ is a polynomial of degree s with respect to τ satisfying $Q_0 = q_n$. The method (13) can be characterized by the following Butcher tableau:

$$\begin{array}{c|c} C_\tau & A_{\tau\sigma} \\ \hline & \bar{B}_\tau \\ \hline & B_\tau \end{array} \tag{14}$$

As stated in the paper [27], in general, a CSRKN method (13) directly solving the problem (1) is not necessarily equivalent to the method induced by converting (1) to a first-order differential equation (4) and then using the method a CSRK scheme (12) to solve it. This fact is similar to the classical case (see [28]).

The conditions for CSRKN methods having order p can be given as order conditions for classical RKN methods with $\sum, c_i, a_{ij}, \bar{b}_i$, and b_i replaced by $\int_0^1, C_\tau, A_{\tau\sigma}, \bar{B}_\tau$, and B_τ, respectively. For a more detailed description of the order conditions of the CSRKN methods, we see [27].

In order to integrate oscillatory problems (1) more accurately, we modify the method (13) by introducing frequency-depending coefficients and introduce a modification of the CSRKN method.

Definition 2 Let $A_{\tau\sigma}(v)$ be a function of variables $\tau, \sigma \in [0, 1]$ and $v \in [0, +\infty)$, $\bar{B}_\tau(v)$ and $B_\tau(v)$ be functions of $\tau \in [0, 1]$ and $v \in [0, +\infty)$, and C_τ be a function of $\tau \in [0, 1]$. An s-degree-modified continuous-stage Runge-Kutta-Nyström (MCSRKN) method for the numerical integration of the oscillatory problem (1) is defined as

$$\begin{cases} Q_\tau = \beta_\tau(v) q_n + h\gamma_\tau(v) C_\tau q_n' + h^2 \int_0^1 A_{\tau\sigma}(v) f\left(Q_\sigma\right) \mathrm{d}\sigma, \\ q_{n+1} = \beta_{s+1}(v) q_n + h\gamma_{s+1}(v) q_n' + h^2 \int_0^1 \bar{B}_\tau(v) f\left(Q_\tau\right) \mathrm{d}\tau, \\ q_{n+1}' = \alpha_{s+1}(v) q_n' + h \int_0^1 B_\tau(v) f\left(Q_\tau\right) \mathrm{d}\tau, \end{cases} \tag{15}$$

where Q_τ is a polynomial of degree s with respect to τ satisfying $Q_0 = q_n$, the coefficients $\beta_\tau(v)$, $\gamma_\tau(v)$, $A_{\tau\sigma}(v)$, $\beta_{s+1}(v)$, $\gamma_{s+1}(v)$, $\bar{B}_\tau(v)$, $\alpha_{s+1}(v)$, and $B_\tau(v)$ are even functions of $v = wh$.

Actually, given s distinct values c_i, $i = 1, \cdots, s$ with $c_0 = 0$ and $c_s = 1$, we always can write Q_τ as a linear combination of Q_{c_i} with $i = 1, \cdots, s$, $Q_{c_0} = q_n$ and $Q_{c_s} = q_{n+1}$.

$$Q_\tau = \sum_{i=0}^{s} L_i(\tau) Q_{c_i}.$$

where Lagrange interpolation function

$$L_i(\tau) = \prod_{j=0, j\neq i}^{s} \frac{\tau - c_j}{c_i - c_j}, \quad i = 0, \cdots, s.$$

Let methods integrate exactly linearly independent functions from the reference set

$$\mathcal{F}_1 = \langle \exp(\mathrm{i}wt), \exp(-\mathrm{i}wt) \rangle, \quad \text{with} \quad \mathrm{i}^2 = -1.$$

This leads to the following equations:

$$\sum_{i=0}^{s} \exp(\pm \mathrm{i}c_i v) L_i(\tau) = \beta_\tau(v) \pm \mathrm{i}v\gamma_\tau(v) C_\tau \mp v^2 \int_0^1 A_{\tau\sigma}(v) \sum_{i=0}^{s} \exp(\pm \mathrm{i}c_i v) L_i(\sigma) \mathrm{d}\sigma,$$

$$\exp(\pm \mathrm{i}v) = \beta_{s+1}(v) \pm \mathrm{i}v\gamma_{s+1}(v) \mp v^2 \int_0^1 \bar{B}_\tau(v) \sum_{i=0}^{s} \exp(\pm \mathrm{i}c_i v) L_i(\tau) \mathrm{d}\tau,$$

$$\exp(\pm \mathrm{i}v) = \alpha_{s+1}(v) \pm \mathrm{i}v \int_0^1 B_\tau(v) \sum_{i=0}^{s} \exp(\pm \mathrm{i}c_i v) L_i(\tau) \mathrm{d}\tau, \quad v = wh. \tag{16}$$

With the Euler formula $\exp(\pm \mathrm{i}v) = \cos(v) \pm \mathrm{i}\sin(v)$, (16) is equivalent to the following trigonometrical fitting (TF) conditions:

$$\sum_{i=0}^{s} L_i(\tau) \sin(c_i v) = \gamma_\tau(v) C_\tau v - v^2 \int_0^1 A_{\tau\sigma}(v) \sum_{i=0}^{s} L_i(\sigma) \sin(c_i v) \mathrm{d}\sigma,$$

$$\sum_{i=0}^{s} L_i(\tau) \cos(c_i v) = \beta_\tau(v) - v^2 \int_0^1 A_{\tau\sigma}(v) \sum_{i=0}^{s} L_i(\sigma) \cos(c_i v) \mathrm{d}\sigma,$$

$$\sin(v) = \gamma_{s+1}(v) v - v^2 \int_0^1 \bar{B}_\tau(v) \sum_{i=0}^{s} L_i(\tau) \sin(c_i v) \mathrm{d}\tau$$

$$\cos(v) = \beta_{s+1}(v) - v^2 \int_0^1 \bar{B}_\tau(v) \sum_{i=0}^{s} L_i(\tau) \cos(c_i v) \mathrm{d}\tau$$

$$\cos(v) = \alpha_{s+1}(v) - v \int_0^1 B_\tau(v) \sum_{i=0}^{s} L_i(\tau) \sin(c_i v) \mathrm{d}\tau,$$

$$\sin(v) = v \int_0^1 B_\tau(v) \sum_{i=0}^{s} L_i(\tau) \cos(c_i v) \mathrm{d}\tau. \tag{17}$$

An MCSRKN method (15) satisfying the TF conditions (17) will be called a trigonometrically fitted CSRKN (TFCSRKN) method. In order to obtain the order conditions for TFCSRKN methods, we consider the following assumptions:

$$\begin{aligned}
&\beta_\tau(v)=\sum_{k=0}^{\infty}\beta_\tau^{(2k)}v^{2k},\quad \gamma_\tau(v)=\sum_{k=0}^{\infty}\gamma_\tau^{(2k)}v^{2k},\quad A_{\tau\sigma}(v)=\sum_{k=0}^{\infty}A_{\tau\sigma}^{(2k)}v^{2k},\\
&\beta_{s+1}(v)=\sum_{k=0}^{\infty}\beta_{s+1}^{(2k)}v^{2k},\quad \gamma_{s+1}(v)=\sum_{k=0}^{\infty}\gamma_{s+1}^{(2k)}v^{2k},\quad \bar{B}_\tau(v)=\sum_{k=0}^{\infty}\bar{B}_\tau^{(2k)}v^{2k},\\
&\alpha_{s+1}(v)=\sum_{k=0}^{\infty}\alpha_{s+1}^{(2k)}v^{2k},\quad B_\tau(v)=\sum_{k=0}^{\infty}B_\tau^{(2k)}v^{2k}.
\end{aligned}\tag{18}$$

The conditions for a TFCSRKN method (15) having order p can be given as order conditions for TFRKN methods (7) in [32] with $\sum$, $\beta_i^{(2k)}$, $\gamma_i^{(2k)}$, $a_{ij}^{(2k)}$, $\bar{b}_i^{(2k)}$, and $b_i^{(2k)}$ replaced by $\int_0^1$, $\beta_\tau^{(2k)}$, $\gamma_\tau^{(2k)}$, $A_{\tau\sigma}^{(2k)}$, $\bar{B}_\tau^{(2k)}$, and $B_\tau^{(2k)}$, respectively. Now, we list the p-th order conditions with $p\le 4$.

- Order 1 requires:
$$\int_0^1 B_\tau^{(0)}\mathrm{d}\tau=1.$$
- Order 2 requires in addition:
$$\int_0^1 B_\tau^{(0)}C_\tau\mathrm{d}\tau=\tfrac{1}{2},\quad \alpha_{s+1}^{(2)}=0,$$
$$\int_0^1 \bar{B}_\tau^{(0)}\mathrm{d}\tau=\tfrac{1}{2},\quad \beta_{s+1}^{(2)}=0.$$
- Order 3 requires in addition:
$$\int_0^1 B_\tau^{(0)}C_\tau^2\mathrm{d}\tau=\tfrac{1}{3},\quad \int_0^1\int_0^1 B_\tau^{(0)}A_{\tau\sigma}^{(0)}\mathrm{d}\tau\mathrm{d}\sigma=\tfrac{1}{6},\quad \int_0^1 B_\tau^{(0)}\beta_\tau^{(2)}\mathrm{d}\tau=0,$$
$$\int_0^1 B_\tau^{(2)}\mathrm{d}\tau=0,\quad \int_0^1 \bar{B}_\tau^{(0)}C_\tau\mathrm{d}\tau=\tfrac{1}{6},\quad \gamma_{s+1}^{(2)}=0.$$
- Order 4 requires in addition:
$$\int_0^1 B_\tau^{(0)}C_\tau^3\mathrm{d}\tau=\tfrac{1}{4},\quad \int_0^1\int_0^1 B_\tau^{(0)}C_\tau A_{\tau\sigma}^{(0)}\mathrm{d}\tau\mathrm{d}\sigma=\tfrac{1}{8},$$
$$\int_0^1\int_0^1 B_\tau^{(0)}A_{\tau\sigma}^{(0)}C_\sigma\mathrm{d}\tau\mathrm{d}\sigma=\tfrac{1}{24},\quad \int_0^1 B_\tau^{(0)}C_\tau\beta_\tau^{(2)}\mathrm{d}\tau=0,$$
$$\int_0^1 B_\tau^{(0)}C_\tau\gamma_\tau^{(2)}\mathrm{d}\tau=0,\quad \int_0^1 B_\tau^{(2)}C_\tau\mathrm{d}\tau=0,$$
$$\alpha_{s+1}^{(4)}=0,\quad \int_0^1 \bar{B}_\tau^{(0)}C_\tau^2\mathrm{d}\tau=\tfrac{1}{12},$$
$$\int_0^1\int_0^1 \bar{B}_\tau^{(0)}A_{\tau\sigma}^{(0)}\mathrm{d}\tau\mathrm{d}\sigma=\tfrac{1}{24},\quad \int_0^1 \bar{B}_\tau^{(0)}\beta_\tau^{(2)}\mathrm{d}\tau=0,$$

$$\int_0^1 \bar{B}_\tau^{(2)} \mathrm{d}\tau = 0, \quad \beta_{s+1}^{(4)} = 0.$$

We note that the conditions of orders higher than four can be obtained following the approach of this paper. The following proposition is helpful for further studying the TFCSRKN methods.

Proposition 1 *If $C_\tau = \tau$ and the coefficients satisfy*

$$\begin{aligned} &\beta_\tau(v) - 1 = O(v^5), \quad \gamma_\tau(v) - 1 = O(v^5), \quad \beta(v) - 1 = O(v^5), \\ &\gamma(v) - 1 = O(v^5), \quad \alpha(v) - 1 = O(v^5), \end{aligned}$$

with $v \to 0$, then the TFCSRKN method satisfies the following relations:

$$\begin{aligned} &\int_0^1 \bar{B}_\tau(v)\mathrm{d}\tau = \frac{1}{2} + O(v^2), \quad \int_0^1 \bar{B}_\tau(v) C_\tau \mathrm{d}\tau = \frac{1}{6} + O(v^2), \\ &\int_0^1 B_\tau(v)\mathrm{d}\tau = 1 + O(v^2), \quad \int_0^1 B_\tau(v) C_\tau \mathrm{d}\tau = \frac{1}{2} + O(v^2), \\ &\int_0^1 A_{\tau\sigma}(v)\mathrm{d}\sigma = \frac{C_\tau^2}{2} + O(v^2), \quad \int_0^1 A_{\tau\sigma}(v) C_\sigma \mathrm{d}\sigma = \frac{C_\tau^3}{6} + O(v^2), \end{aligned} \tag{19}$$

and therefore it has algebraic order at least two.

Proof First of all, we prove the second expression. Using the third condition given in (17) and expressing the trigonometric function, we have

$$\begin{aligned} \sum_{m=0}^{\infty} \frac{(-1)^m v^{2m+1}}{(2m+1)!} = {} & v \sum_{m=0}^{\infty} \gamma_{s+1}^{(2m)} v^{2m} \\ & - v^2 \int_0^1 \sum_{i=0}^{s} L_i(\tau) \bar{B}_\tau(v) \sum_{m=0}^{\infty} \frac{(-1)^m c_i^{2m+1} v^{2m+1}}{(2m+1)!} \mathrm{d}\tau \end{aligned}$$

In a more detailed manner, the above formula can be expressed as

$$\begin{aligned} v - \frac{v^3}{3!} + \sum_{m=2}^{\infty} \frac{(-1)^m v^{2m+1}}{(2m+1)!} = {} & v\gamma_{s+1}^{(0)} + \gamma_{s+1}^{(2)} v^3 + v \sum_{m=2}^{\infty} \gamma_{s+1}^{(2m)} v^{2m} \\ & - v^3 \int_0^1 \sum_{i=0}^{s} L_i(\tau) \bar{B}_\tau(v) c_i \mathrm{d}\tau \end{aligned}$$

$$-v^2\int_0^1\sum_{i=0}^{s}L_i(\tau)\bar{B}_\tau(v)\sum_{m=1}^{\infty}\frac{(-1)^m c_\tau^{2m+1}v^{2m+1}}{(2m+1)!}\mathrm{d}\tau$$

which implies that

$$-\frac{v^3}{3!}+O(v^5)=-v^3\int_0^1\bar{B}_\tau(v)C_\tau\mathrm{d}\tau+O(v^5).$$

Therefore, we obtain

$$\int_0^1\bar{B}_\tau(v)C_\tau d\tau=\frac{1}{6}+O(v^2).$$

The other expressions can be proved in a similar way. From the first, third, and fourth conditions of (19), the order conditions are satisfied for $p=2$ and the TFCSRKN method has algebraic order at least 2. □

The following theorem gives the sufficient conditions for energy preservation.

Theorem 2 *A TFCSRKN method* (15) *solving Hamiltonian systems is energy-preserving if the coefficients satisfy*

$$\begin{aligned}&\alpha_{s+1}(v)=1,\quad \beta_\tau(v)=C(v),\quad (\gamma_\tau(v)C_\tau)'=B_\tau(v),\\&B_\tau(v)B_\sigma(v)=A'_{\tau\sigma}(v)+A'_{\sigma\tau}(v),\end{aligned}\tag{20}$$

where $A'_{\tau\sigma}(v)=\frac{\mathrm{d}}{\mathrm{d}\tau}A_{\tau\sigma}(v)$, $(\gamma_\tau(v)C_\tau)'=\frac{\mathrm{d}}{\mathrm{d}\tau}(\gamma_\tau(v)C_\tau)$, *and* $C(v)$ *depends only on* v *but not on* τ.

Proof For Hamiltonian or energy, having $p_n=q'_n$ in mind, we have

$$\begin{aligned}&H(q_{n+1},p_{n+1})-H(q_n,p_n)\\&=\frac{1}{2}p_{n+1}^Tp_{n+1}+U(q_{n+1})-\frac{1}{2}p_n^Tp_n-U(q_n)\\&=\frac{1}{2}\left(\alpha_{s+1}(v)p_n+h\int_0^1B_\tau(v)f\left(Q_\tau\right)\mathrm{d}\tau\right)^T\left(\alpha_{s+1}(v)p_n+h\int_0^1B_\tau(v)f\left(Q_\tau\right)\mathrm{d}\tau\right)\\&\quad+\int_0^1\left(\nabla U\left(Q_\tau\right)\right)^T\mathrm{d}Q_\tau-\frac{1}{2}p_n^Tp_n.\end{aligned}\tag{21}$$

Further calculation results in

$$H(q_{n+1},\, p_{n+1}) - H(q_n,\, p_n) \;=\; \frac{1}{2}\left[\alpha_{s+1}^2(v)p_n^T p_n + 2h\alpha_{s+1}(v)p_n^T \int_0^1 B_\tau(v) f\,(Q_\tau)\,\mathrm{d}\tau \right.$$
$$\left. + h^2 \left(\int_0^1 B_\tau(v) f\,(Q_\tau)\,\mathrm{d}\tau\right)^T \left(\int_0^1 B_\sigma(v) f\,(Q_\sigma)\,\mathrm{d}\sigma\right)\right] - \frac{1}{2}p_n^T p_n$$
$$+ \int_0^1 (\nabla U\,(Q_\tau))^T\,\mathrm{d}\left(\beta_\tau(v)q_n + \gamma_\tau(v)C_\tau h p_n + h^2 \int_0^1 A_{\tau\sigma} f\,(Q_\sigma)\,\mathrm{d}\sigma\right).$$

Simplifying the above formula, we obtain

$$\begin{aligned}
&H(q_{n+1},\, p_{n+1}) - H(q_n,\, p_n)\\
&= \frac{1}{2}\left(\alpha_{s+1}^2(v) - 1\right) p_n^T p_n - \beta_\tau'(v) q_n^T \int_0^1 B_\sigma(v) f\,(Q_\sigma)\,\mathrm{d}\sigma\\
&\quad + h p_n^T \int_0^1 \left(\alpha_{s+1}(v)B_\tau(v) - [\gamma_\tau(v)C_\tau]'\right) f\,(Q_\tau)\,\mathrm{d}\tau\\
&\quad + \frac{h^2}{2}\int_0^1\int_0^1 f\,(Q_\tau)^T\, B_\tau(v)B_\sigma(v) f\,(Q_\sigma)\,\mathrm{d}\tau\mathrm{d}\sigma\\
&\quad + \int_0^1 (\nabla U\,(Q_\tau))^T\,\mathrm{d}\left(h^2 \int_0^1 A_{\tau\sigma}(v) f\,(Q_\sigma)\,\mathrm{d}\sigma\right),
\end{aligned} \tag{22}$$

where $\beta_\tau'(v)$ and $[\gamma_\tau(v)C_\tau]'$ mean the derivatives with respect to τ. Using (20) and $f\,(Q_\tau) = -\nabla U\,(Q_\tau)$, we have

$$\begin{aligned}
&H(q_{n+1},\, p_{n+1}) - H(q_n,\, p_n)\\
&= \frac{h^2}{2}\int_0^1\int_0^1 f\,(Q_\tau)^T \left(B_\tau(v)B_\sigma(v) - 2A_{\tau\sigma}'(v)\right) f\,(Q_\sigma)\,\mathrm{d}\tau\mathrm{d}\sigma.
\end{aligned} \tag{23}$$

Letting $\tau \leftrightarrow \sigma$ and adding the resulting results, we have

$$\begin{aligned}
&2H(q_{n+1},\, p_{n+1}) - 2H(q_n,\, p_n)\\
&= h^2\int_0^1\int_0^1 f\,(Q_\tau)^T \left(B_\tau(v)B_\sigma(v) - A_{\tau\sigma}'(v) - A_{\sigma\tau}'(v)\right) f\,(Q_\sigma)\,\mathrm{d}\tau\mathrm{d}\sigma.
\end{aligned} \tag{24}$$

From (20), we know that $H(q_{n+1},\, p_{n+1}) - H(q_n,\, p_n) = 0$. This implies the result. □

Remark 1 We know from Theorem 2 that energy-preservation properties of TFC-SRKN methods (15) have nothing to do with $\beta_{s+1}(v)$ and $\gamma_{s+1}(v)$. However, if we regard problem (1) as an equivalent representation as a first-order system of the form (4) but with doubled dimension, and then solve it by using the trigonometrically fitted CSRK (TFCSRK) methods of [34], the coefficients of resulting method must satisfy $\beta_{s+1}(v) = 1$. This shows that the TFCSRKN method solving directly problem (1) has more flexibility of the coefficient than TFCSRK methods of [34].

A detailed investigation of the numerical integration of reversible systems has been carried out in [28]. There it is shown that symmetric integration methods often have an excellent long-term behavior on such systems. Therefore, this section turns to the discussion about the symmetry of TFCSRKN methods.

Definition 3 (See [28].) The adjoint method Φ_h^* of a method Φ_h is defined as the inverse map of the original method with reversed time step $-h$, i.e., $\Phi_h^* = \Phi_{-h}^{-1}$. A method with $\Phi_h^* = \Phi_h$ is called symmetric.

Theorem 3 *The TFCSRKN method* (15) *is symmetry if and only if the coefficients satisfy*

$$\begin{aligned}
&\beta_{s+1}(v) = 1, \quad \alpha_{s+1}(v) = 1,\\
&B_\tau(v) = B_{1-\tau}(v), \quad \gamma_{s+1}(v)B_\tau(v) - \bar{B}_\tau(v) = \bar{B}_{1-\tau}(v),\\
&\beta_\tau(v)\gamma_{s+1}(v) - \gamma_\tau(v)C_\tau = \gamma_{1-\tau}(v)C_{1-\tau},\\
&\beta_\tau(v)\left(\gamma_{s+1}(v)B_\sigma(v) - \bar{B}_\sigma(v)\right) - \gamma_\tau(v)C_\tau B_\sigma(v) + A_{\tau\sigma}(v)\\
&= A_{1-\tau,1-\sigma}(v) - \bar{B}_{1-\sigma}(v).
\end{aligned} \tag{25}$$

Proof Exchanging $q_{n+1} \leftrightarrow q_n$, $p_{n+1} \leftrightarrow p_n$ and replacing $-h$ by h in the TFCSRKN formulas (15) yield

$$\begin{cases}
\bar{Q}_\tau = \beta_\tau(v)q_{n+1} - h\gamma_\tau(v)C_\tau q'_{n+1} + h^2\displaystyle\int_0^1 A_{\tau\sigma}(v)f\left(\bar{Q}_\sigma\right)\mathrm{d}\sigma,\\
q_n = \beta_{s+1}(v)q_{n+1} - h\gamma_{s+1}(v)q'_{n+1} + h^2\displaystyle\int_0^1 \bar{B}_\tau(v)f\left(\bar{Q}_\tau\right)\mathrm{d}\tau,\\
q'_n = \alpha_{s+1}(v)q'_{n+1} - h\displaystyle\int_0^1 B_\tau(v)f\left(\bar{Q}_\tau\right)\mathrm{d}\tau.
\end{cases} \tag{26}$$

To make the method symmetric, the conditions $\beta_{s+1}(v) = 1$ and $\alpha_{s+1}(v) = 1$ are necessary. From (26), we obtain

$$q'_{n+1} = q'_n + h\int_0^1 B_\tau(v)f\left(\bar{Q}_\tau\right)\mathrm{d}\tau,$$

$$
\begin{aligned}
q_{n+1} &= q_n + h\gamma_{s+1}(v)q_n' + h^2\int_0^1 \left(\gamma_{s+1}(v)B_\tau(v) - \bar{B}_\tau(v)\right) f\left(\bar{Q}_\tau\right)\mathrm{d}\tau,\\
\bar{Q}_\tau &= \beta_\tau(v)q_n + h\left(\beta_\tau(v)\gamma_{s+1}(v) - \gamma_\tau(v)C_\tau\right)q_n'\\
&\quad + h^2\int_0^1 \left[\beta_\tau(v)\left(\gamma_{s+1}(v)B_\sigma(v) - \bar{B}_\sigma(v)\right)\right.\\
&\quad \left. - \gamma_\tau(v)C_\tau B_\sigma(v) + A_{\tau\sigma}(v)\right] f\left(\bar{Q}_\sigma\right)\mathrm{d}\sigma.
\end{aligned}
\tag{27}
$$

Replacing all indices τ and σ by $1-\tau$ and $1-\sigma$, respectively, and denoting $\bar{Q}_{1-\tau} = Q_\tau$, we know that the scheme defined by (27) coincides with the scheme (15) if and only if the coefficients satisfy the conditions (25). This proves the theorem. □

Remark 2 When $v \to 0$ ($w \to 0$), we have

$$
\beta_\tau(v) \to 1, \quad \gamma_\tau(v) \to 1, \quad \beta_{s+1}(v) \to 1, \quad \gamma_{s+1}(v) \to 1, \quad \alpha_{s+1}(v) \to 1.
$$

In this case, the TFCSRKN method (15) reduces a CSRKN method (13) and the symmetric conditions (25) reduce to

$$
\begin{aligned}
&B_\tau = B_{1-\tau}, \quad B_\tau - \bar{B}_\tau = \bar{B}_{1-\tau}, \quad 1 - C_\tau = C_{1-\tau}\\
&B_\sigma - \bar{B}_\sigma - C_\tau B_\sigma + A_{\tau\sigma} = A_{1-\tau,1-\sigma} - \bar{B}_{1-\sigma},
\end{aligned}
\tag{28}
$$

where $A_{\tau\sigma}$, $\bar{B}_\tau$, and B_τ are the limit values of $A_{\tau\sigma}(v)$, $\bar{B}_\tau(v)$, and $B_\tau(v)$ as $v \to 0$.

4 Stability

In order to analyze the stability of TFCSRKN methods in this paper, we choose to consider the following linear scalar problem:

$$
y''(t) = -\lambda^2 y(t), \tag{29}
$$

where $\lambda > 0$. Applying method (15) to problem (29) yields

$$
\begin{aligned}
Q_i &= \beta_i(v)q_n + h\gamma_i(v)C_i q_n' - H^2\int_0^1 A_{i\sigma}(v)\sum_{j=0}^{s} L_j(\sigma)Q_j\mathrm{d}\sigma,\\
q_{n+1} &= \beta_{s+1}(v)q_n + h\gamma_{s+1}(v)q_n' - H^2\int_0^1 \bar{B}_\tau(v)\sum_{i=0}^{s} L_i(\tau)Q_i\mathrm{d}\tau,\\
hq_{n+1}' &= \alpha_{s+1}(v)hq_n' - H^2\int_0^1 B_\tau(v)\sum_{i=0}^{s} L_i(\tau)Q_i\mathrm{d}\tau,
\end{aligned}
\tag{30}
$$

where $C_i = C_{c_i}$, $\beta_i(v) = \beta_{c_i}(v)$, $\gamma_i(v) = \gamma_{c_i}(v)$, $A_{i\sigma}(v) = A_{c_i\sigma}(v)$, and $H = \lambda h$. We can express (30) in a vector form

$$\begin{aligned} Q &= \beta(v)q_n + h\gamma(v)Cq'_n - H^2A(v)Q, \\ q_{n+1} &= \beta_{s+1}(v)q_n + h\gamma_{s+1}(v)q'_n - H^2\bar{B}(v)Q, \\ hq'_{n+1} &= \alpha_{s+1}hq'_n - H^2B(v)Q, \end{aligned}$$

with $\beta(v) = (\beta_0(v), \cdots, \beta_s(v))^T$, $\gamma(v)C = (\gamma_0(v)C_0, \cdots, \gamma_s(v)C_s)^T$ and

$$A(v) = \begin{pmatrix} \int_0^1 A_{0\sigma}(v)L_0(\sigma)\mathrm{d}\sigma & \cdots & \int_0^1 A_{0\sigma}(v)L_s(\sigma)\mathrm{d}\sigma \\ \vdots & \ddots & \vdots \\ \int_0^1 A_{s\sigma}(v)L_0(\sigma)\mathrm{d}\sigma & \cdots & \int_0^1 A_{s\sigma}(v)L_s(\sigma)\mathrm{d}\sigma \end{pmatrix},$$

$$\bar{B}(v) = \left(\int_0^1 \bar{B}_\sigma(v)L_0(\sigma)\mathrm{d}\sigma, \cdots, \int_0^1 \bar{B}_\sigma(v)L_s(\sigma)\mathrm{d}\sigma \right),$$

$$B(v) = \left(\int_0^1 B_\sigma(v)L_0(\sigma)\mathrm{d}\sigma, \cdots, \int_0^1 B_\sigma(v)L_s(\sigma)\mathrm{d}\sigma \right).$$

Elimination of the vector Q delivers the recursion

$$\begin{pmatrix} q_{n+1} \\ hq'_{n+1} \end{pmatrix} = M(H, v) \begin{pmatrix} q_n \\ hq'_n \end{pmatrix}, \tag{31}$$

where

$$M = \begin{pmatrix} \beta_{s+1}(v) - H^2\bar{B}(v)N^{-1}\beta(v) & \gamma_{s+1}(v) - H^2\bar{B}(v)N^{-1}\gamma(v)C \\ -H^2B(v)N^{-1}\beta(v) & \alpha_{s+1}(v) - H^2B(v)N^{-1}\gamma(v)C \end{pmatrix}, \tag{32}$$

and $N = I + H^2A(v)$. The matrix $M(H, v)$ is called stability matrix. The behavior of the numerical solution will depend on the stability matrix $M(H, v)$ of (32). Geometrically, the characterization of stability becomes a two-dimensional region in (H, v) space for a TFCSRKN method.

Definition 4 For the TFCSRKN method (15) with the stability matrix (32), the region of the two-dimensional space

$$\Omega := \{(H, v) : |M(H, v)| \leq 1\}$$

is called the region of stability. And any closed surface defined by $|M(H, v)| = 1$ is a stability boundary of the method.

Definition 5 For the TFCSRKN method with the stability matrix $M(H, v)$, the two quantities

$$\phi(H, v) = H - \arccos\left(\frac{\mathrm{tr}(M)}{2\sqrt{\det(M)}}\right), \quad d(H, v) = 1 - \sqrt{\det(M)}$$

are called the dispersion error and the dissipation error, respectively. The method is said to be dispersive of order q and dissipative of order r, if $\phi(H, v) = \mathcal{O}(H^{q+1})$ and $d(H, v) = \mathcal{O}(H^{r+1})$, respectively. If $\phi(H, v) = 0$ and $d(H, v) = 0$, then the method is said to be zero dispersive and zero dissipative. Here, the pair $H,\ v$ should be replaced by the new pair $H,\ r = H/v$.

5 Construction of energy-preserving methods

In this section, we derive second- and fourth-order symmetric and energy-preserving TFCSRKN schemes. The derivation process of higher-order methods is completely similar. In the construction of the method, we always choose $C_\tau = \tau$.

5.1 The method of order two

Let us start with a one-degree TFCSRKN formulation:

$$A_{\tau\sigma}(v) = a_{11}(v)\tau, \quad \bar{B}_\tau(v) = \bar{b}_1(v), \quad B_\tau(v) = b_1(v).$$

In this case, from the TF conditions (17), symmetric conditions (25), and energy-preserving conditions (20), we have

$$\begin{aligned}
&\alpha_{s+1}(v) = 1, \quad \beta_{s+1}(v) = 1, \quad \beta_\tau(v) = 1, \quad \gamma_{s+1}(v) = \gamma_\tau(v),\\
&A_{\tau\sigma}(v) = \frac{1}{v^2}\left(2\tau\tan^2\left(\frac{v}{2}\right)\right), \quad \bar{B}_\tau(v) = \frac{2\tan^2\left(\frac{v}{2}\right)}{v^2},\\
&B_\tau(v) = 2\sin\left(\frac{v}{2}\right)\Big/\left(v\cos\left(\frac{v}{2}\right)\right), \quad \gamma_\tau(v) = \frac{2}{v}\tan\left(\frac{v}{2}\right).
\end{aligned} \tag{33}$$

For small values $|v| \to 0$, the above formulae are subject to heavy cancellations and in that case, the following Taylor series expansions must be used:

$$\begin{aligned}
A_{\tau\sigma}(v) &= \frac{\tau}{2} + \frac{\tau v^2}{12} + \frac{17\tau v^4}{1440} + \frac{31\tau v^6}{20160} + \cdots,\\
\bar{B}_\tau(v) &= \frac{1}{2} + \frac{v^2}{12} + \frac{17v^4}{1440} + \frac{31v^6}{20160} + \cdots,\\
B_\tau(v) &= 1 + \frac{v^2}{12} + \frac{v^4}{120} + \frac{17v^6}{20160} + \cdots,\\
\gamma_\tau(v) &= 1 + \frac{v^2}{12} + \frac{v^4}{120} + \frac{17v^6}{20160} + \cdots.
\end{aligned} \tag{34}$$

It is easy to verify that the symmetric and energy-preserving TFCSRKN method defined by (33) has the accuracy of order two. We denote this method as SEPTFC-SRKN2P and for this method, we have

$$\phi(H) = -\frac{-2r^4 + \sqrt{3}r^2}{24(r^2+1)^2}H^3 + \mathcal{O}(H^5), \quad d(H) = 0,$$

which shows that the method SEPTFCSRKN2P is dispersive of order 2 and zero dissipative, respectively. The region of stability for the method SEPTFCSRKN2P is depicted in Fig. 1.

5.2 The method of order four

Now, we consider two-degree TFCSRKN method whose coefficients have the following form:

$$\begin{aligned} &A_{\tau\sigma}(v) = a_{11}(v)\tau + a_{12}(v)\tau\sigma + a_{21}(v)\tau^2 + a_{22}(v)\tau^2\sigma, \\ &\bar{B}_\tau(v) = \bar{b}_1(v) + \bar{b}_2(v)\tau, \quad B_\tau(v) = b_1(v) + b_2(v)\tau. \end{aligned} \tag{35}$$

From the TF conditions (17), symmetric conditions (25), and energy-preserving conditions (20), we have

$$\begin{aligned} &\alpha_{s+1}(v) = 1, \quad \beta_{s+1}(v) = 1, \quad \beta_\tau(v) = 1, \quad \gamma_{s+1}(v) = \gamma_\tau(v), \\ &\bar{A}_{\tau\sigma}(v) = \frac{12\tau(3 - 8\sigma + 4\tau + (3 - 4\sigma + 2\tau)\cos\left(\frac{v}{2}\right))\sin^2\left(\frac{v}{4}\right)}{v^2(2+\cos\left(\frac{v}{2}\right))^2}, \\ &\bar{B}_\tau(v) = -\frac{12(-7 + 8\tau + (-5 + 4\tau)\cos\left(\frac{v}{2}\right))\sin^2\left(\frac{v}{4}\right)}{v^2(2+\cos\left(\frac{v}{2}\right))^2}, \\ &B_\tau(v) = \frac{-6(\cos(v) - 1)}{v(4\sin\left(\frac{v}{2}\right) + \sin(v))}, \quad \gamma_\tau(v) = \frac{6\sin\left(\frac{v}{2}\right)}{2v + v\cos\left(\frac{v}{2}\right)}. \end{aligned} \tag{36}$$

Note that for the numerical computation, the following series expansions should be employed:

$$\begin{aligned} A_{\tau\sigma}(v) &= \frac{1}{2}\tau(1 - 2\sigma + \tau) + \frac{1}{96}\tau(-2\sigma + \tau)v^2 + \frac{\tau(-4 - 2\sigma + \tau)v^4}{11520} \\ &\quad - \frac{\tau(80 - 34\sigma + 17\tau)v^6}{7741440} + \cdots, \\ \bar{B}_\sigma(v) &= (1 - \sigma) + \frac{1}{96}(1 - 2\sigma)v^2 + \frac{(-3 - 2\sigma)v^4}{11520} + \frac{(-97 + 34\sigma)v^6}{7741440} + \cdots, \\ B_\sigma(v) &= 1 - \frac{v^4}{2880} - \frac{v^6}{96768} - \frac{v^8}{6635520} + \cdots, \\ \gamma_\tau(v) &= 1 - \frac{v^4}{2880} - \frac{v^6}{96768} - \frac{v^8}{6635520} + \cdots. \end{aligned} \tag{37}$$

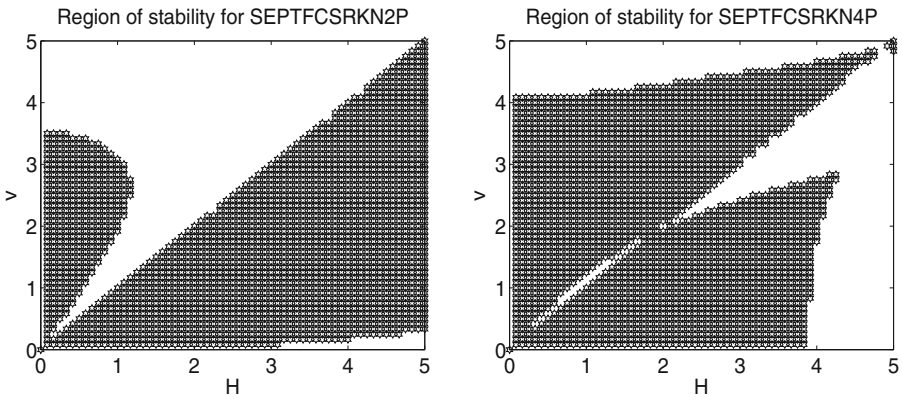

Fig. 1 The stability region for the method SEPTFCSRKN2P (left) and SEPTFCSRKN4P (right)

It is easy to verify that the coefficients of (37) satisfy the conditions of order four. We denote the symmetric and energy-preserving TFCSRKN method (15) determined by (37) as SEPTFCSRKN4P. For this method, we have

$$\phi(H) = \frac{-5r^4 + r^2}{360(r^3+1)^2} H^5 + \mathcal{O}(H^7), \quad d(H) = 0,$$

which shows that the method SEPTFCSRKN4P is dispersive of order 4 and zero dissipative, respectively. The region of stability for the method SEPTFCSRKN4P is depicted in Fig. 1.

6 Numerical experiments

In this section, in order to show the competence and superiority of the new methods compared with the well-known methods in the scientific literature, we use three model problems. Nonlinear equations were solved by fixed point iteration with tolerance 10^{-15} and the right hand side of method (15) were integrated numerically by using *quad* with tolerance 10^{-12}. The integrators we select for comparison are:

- SEPTFCSRKN2P: The symmetric and energy-preserving TFCSRKN method of order two derived in Section 5 of this paper
- SEPTFCSRKN4P: The symmetric and energy-preserving TFCSRKN method of order four derived in Section 5 of this paper
- EPCSRK2P: The energy-preserving CSRK method of order two derived in [23]
- EPCSRK4P: The energy-preserving CSRK method of order four introduced in [23]

Problem 1 We consider the Duffing equation

$$\begin{cases} q'' + 25q = 2k^2q^3 - k^2q, & t \in [0, t_{end}], \\ q(0) = 0, \quad q'(0) = w. \end{cases} \tag{38}$$

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 each method, where $j = 1, 2, 3, 4$. Then, we integrate the problem with a fixed step size $h = 1/5$ in [0, 100] and see the preservation of the Hamiltonian by each code. The numerical results are presented in Fig. 2.

Problem 2 Two coupled oscillators with different frequencies

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

The Hamiltonian of this system is given by

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

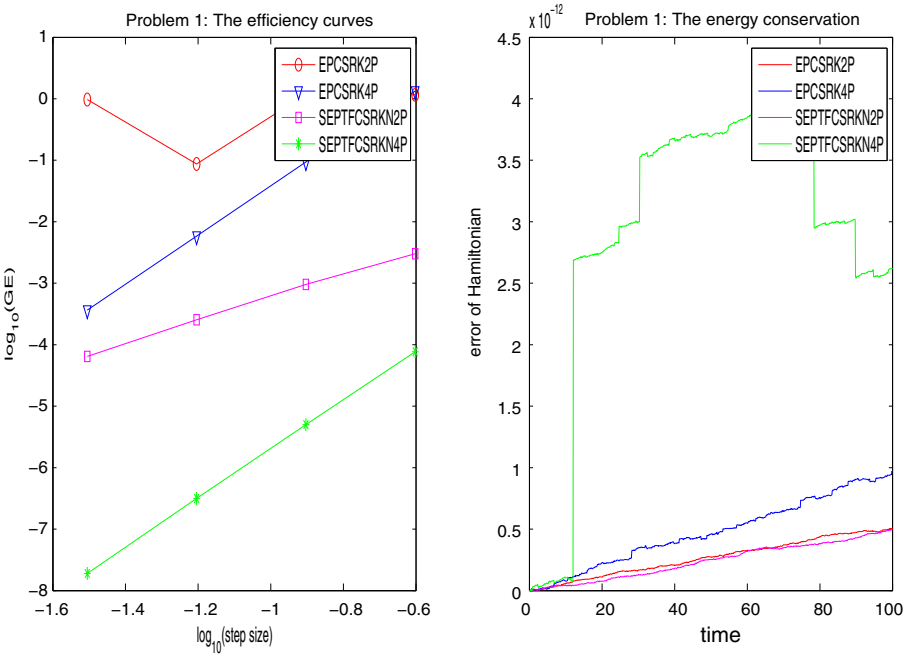

Fig. 2 Efficiency curves (left) and energy conservation (right) for problem 1

In this numerical test, we choose $\varepsilon = 10^{-3}$ and the fitting parameter $w = \sqrt{2}$. We fist solve this problem in the interval [0, 100] and step sizes $h = 1/2^j$ for all the methods, where $j = 1, \cdots, 4$. Then, we integrate the problem with a fixed step size $h = 1/2$ in [0, 100] and see the preservation of the Hamiltonian by each code. The numerical results are presented in Fig. 3.

Problem 3. Consider the pendulum system with the Hamiltonian

$$H(p, q) = \frac{1}{2}p^2 - \cos(q), \quad q(0) = 0, \quad p(0) = 1,$$

where q is the angle between the rod and a vertical, downward oriented axis. The equations of motion are

$$q'' = -\sin(q), \quad q(0) = 0, \quad q'(0) = 1.$$

In the numerical integration of this problem, the fitting frequency (a reasonable estimate of the principal frequency) is taken as $w = 1.0415$. Firstly, we integrate the problem in the interval [0, 100] with step sizes $h = 1/2^j$, $j = 1, 2, 3, 4$ for all the methods. Then, we integrate the problem with a fixed step size $h = 1/5$ in [0, 100] and see the preservation of the Hamiltonian by each code. The results are shown in Fig. 4.

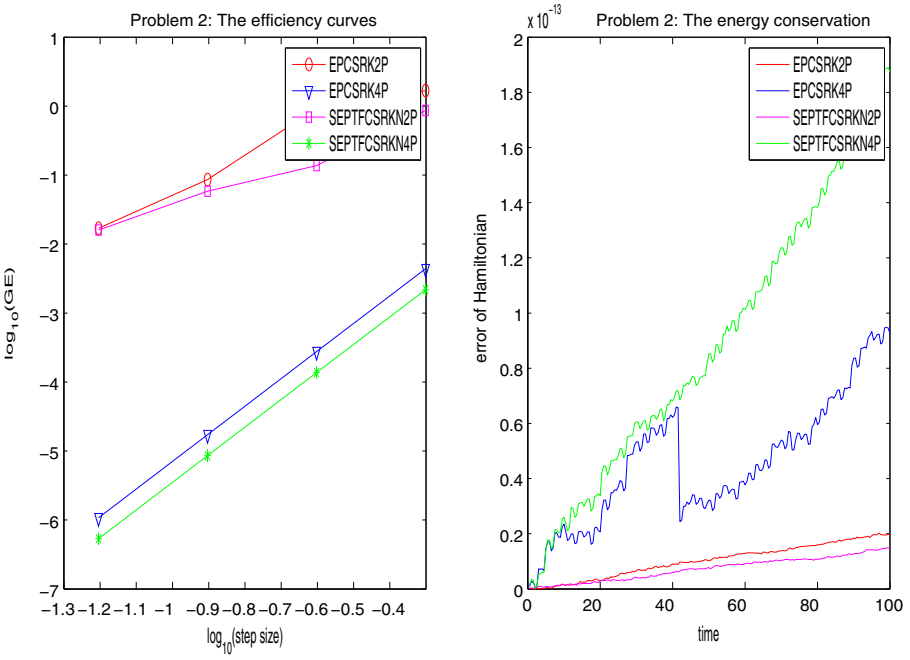

Fig. 3 Efficiency curves (left) and energy conservation (right) for problem 2

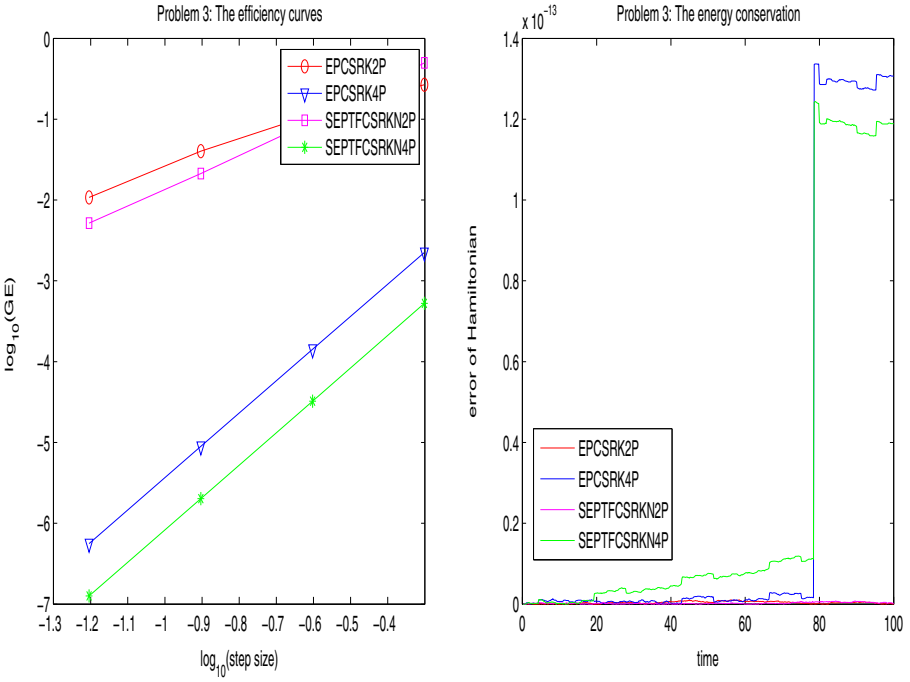

Fig. 4 Efficiency curves (left) and energy conservation (right) for problem 3

For the above three problems, the right figures show all schemes preserve the Hamiltonian well. The reason why the accuracy of the fourth-order schemes falls behind that of the second-order schemes might be due to the tolerance of *quad*. In the left figures, one can see that the errors are growing linearly with time for all four schemes. The results of the numerical experiments confirm that for a given step size h, our new methods are more accurate than CSRK methods with the same convergence order.

7 Conclusions and discussions

We present and study symmetric, energy-preserving, and trigonometrically fitted continuous-stage Runge-Kutta-Nyström (TFCSRKN) method in this paper. These methods integrate exactly second-order systems (1) whose solution can be expressed as linear combination of functions from the set of functions $\{\exp(\mathrm{i}wt), \exp(-\mathrm{i}wt)\}$ or equivalently the set $\{\cos(wt), \sin(wt)\}$ with w the approximation of the main frequency. The symmetric and energy-preserving conditions for TFCSRKN methods are derived. Based on these conditions, two new symmetric and energy-preserving methods of orders two and four, respectively, are constructed. The results of the numerical experiments confirm the theoretical expectations.

The determination of the main frequency w for a trigonometrically fitted method is a critical issue, because the coefficients of the trigonometrically fitted method depend on w. The knowledge of an estimation to the unknown frequency is needed in order to apply the numerical method efficiently. For the technique of frequency choice in trigonometrically fitted methods, the reader is referred to [35, 36].

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