Numer Algor (2017) 76:761–782
DOI 10.1007/s11075-017-0281-5

ORIGINAL PAPER

A feasible and effective technique in constructing ERKN methods for multi-frequency multidimensional oscillators in scientific computation

Hongli Yang[1,3] **· Xianyang Zeng**[2,3]

Received: 24 January 2016 / Accepted: 31 January 2017 / Published online: 17 February 2017

Abstract In last few years, many ERKN methods have been investigated for solving multi-frequency multidimensional second-order ordinary differential equations, and the numerical efficiency has been checked strongly in scientific computation. But in the constructions of (especially high-order) new ERKN methods, lots of time and effort are costed in presenting the practical order conditions firstly and then in adding some reasonable assumptions to get the coefficient functions finally. In this paper, a feasible and effective technique is given which makes the construction of ERKN methods finished in a few seconds or a few minutes, even for high-order integrators. Moreover, this technique does not need any more information and knowledge except the classical RKN method. And this paper also gives the theoretical explanation to guarantee that the ERKN method obtained from this technique has the same order and the same properties as the underlying RKN method.

The research was supported in part by the Science Foundations of the Nanjing Institute of Technology under Grant CKJA201410 and under Grant QKJA201404, by the Educational Reform Foundations of the Nanjing Institute of Technology under Grant JG201440, by the Natural Science Foundation of China under Grant 11671200.

✉ Hongli Yang
yanghongli1016@163.com

Xianyang Zeng
zxy@njit.edu.cn

1 Department of Mathematics and Physics, Nanjing Institute of Technology, Nanjing, People's Republic of China

2 Industrial Center, Nanjing Institute of Technology, Nanjing, People's Republic of China

3 Department of Mathematics, Nanjing University, Nanjing, People's Republic of China

Keywords ERKN methods · Symplectic conditions and symmetric conditions · Rooted tree theory · A feasible and effective technique · Scientific computation

Mathematics Subject Classification (2010) 65L05 · 65L06

1 Introduction

This paper focuses on numerical integrators solving multi-frequency and multidimensional perturbed oscillatory second-order ordinary differential equations (ODEs)

$$\begin{cases} \boldsymbol{q}''(t) + M\boldsymbol{q}(t) = \boldsymbol{f}\big(\boldsymbol{q}(t), \boldsymbol{q}'(t)\big), \qquad t \in [t_0, T], \\ \boldsymbol{q}(t_0) = \boldsymbol{q}_0, \quad \boldsymbol{q}'(t_0) = \boldsymbol{q}'_0, \end{cases} \tag{1}$$

where $M \in \mathbb{R}^{d\times d}$ is a constant matrix containing implicitly the frequencies of the problem. ODEs (1) arise in various fields of science and technology, such as applied mathematics, mechanics, physics, astronomy, molecular biology, and engineering [1–4]. In the case where the right-hand side of the systems does not depend on the derivative $\boldsymbol{q}'(t)$, the systems (1) are

$$\begin{cases} \boldsymbol{q}''(t) + M\boldsymbol{q}(t) = \boldsymbol{f}\big(\boldsymbol{q}(t)\big), \qquad t \in [t_0, T], \\ \boldsymbol{q}(t_0) = \boldsymbol{q}_0, \quad \boldsymbol{q}'(t_0) = \boldsymbol{q}'_0. \end{cases} \tag{2}$$

Furthermore, if M is a positive semi-definite symmetric matrix and $\boldsymbol{f}(\boldsymbol{q}) = -\nabla \boldsymbol{U}(\boldsymbol{q})$, then systems (2) become identical to multi-frequency and multidimensional oscillatory Hamiltonian systems

$$\begin{cases} \boldsymbol{p}' = -\nabla_{\boldsymbol{q}} H(\boldsymbol{p}, \boldsymbol{q}), \qquad \boldsymbol{p}(t_0) = \boldsymbol{p}_0, \\ \boldsymbol{q}' = \nabla_{\boldsymbol{p}} H(\boldsymbol{p}, \boldsymbol{q}), \qquad \boldsymbol{q}(t_0) = \boldsymbol{q}_0, \end{cases} \tag{3}$$

with the Hamiltonian

$$H(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{2}\boldsymbol{p}^{\intercal}\boldsymbol{p} + \frac{1}{2}\boldsymbol{q}^{\intercal}M\boldsymbol{q} + \boldsymbol{U}(\boldsymbol{q}), \tag{4}$$

where $\boldsymbol{U}(\boldsymbol{q})$ is a smooth potential function. For solving the multi-frequency and multidimensional perturbed oscillatory second-order ordinary differential equations, RK-type methods [2–21], exponential fitting and trigonometric fitting methods [2–6, 15, 20–28], multi-step methods [2–5, 8], energy-preserving methods [2–6, 17–19, 29–33], and collocation methods [2–4, 6, 18, 28, 29] have been proposed. These methods also have been deeply analyzed for Hamiltonian systems [5–7, 19–21, 32–36]. The ERKN methods [10, 14] are equivalent to the exponentially fitting RKN (EFRKN) methods [20, 21], but these methods correspond to different ideas and derivation. The ERKN integrators are proposed based on the variation of constants formula while the EFRKN methods are derived by applying the exponential fitting techniques to the multidimensional modified RKN methods. This paper prefers to the ERKN methods since the ERKN methods do not depend on the decomposition of M and then can be widely used in many fields [5, 8–15, 19, 20, 36–38].

In numerical applications, the efficiency and robustness of these integrators comparing with the classical RKN methods can be guaranteed since the ERKN methods make full use of the special structure of the ODEs (1). But by now, since the lack of some researches, in the construction of new ERKN method, people have to do the repetitive work which have been done similarly in constructing RKN method. In this paper, we will give a technique which makes the construction of ERKN method can be finished actually in a few seconds or a few minutes, even for high-order methods. It is greatly save the time and effort. This feasible and effective technique is on the basis of the special structure of a class of ERKN methods. The theoretical explanation would be presented in the order conditions, the symplectic conditions, and the symmetric conditions.

The rooted tree theory is most important in the RK-type methods. For the ERKN method solving the general systems (1), the rooted tree theory is on the basis of *the improved extended Nyström tree set (IEN-T set)* called as IEN-T theory [12, 16]. And for the ERKN method solving the special systems (2), the rooted tree theory is on the subset of IEN-T set, namely *the simplified special extended Nyström tree set (SSEN-T set)* and then the theory is called as SSEN-T theory [10, 11]. Since the coefficient functions of the interested class of ERKN methods mentioned in this paper are non-independent, the rooted tree theory for any kind of systems would bases on a subset of the underlying tree set. And we will conclude that the rooted tree theory for this special class of ERKN methods is actually on the basis of *the Nyström tree (N-T) set* for the general systems (1) and *the special Nyström tree (SN-T) set* for the special systems (2).

In this paper, we also present some theorems to guarantee that the special class of ERKN methods obtained from this technique share the same properties (such as order, symplectic property, symmetric property) with the underlying RKN methods. So, in this paper, we provide a feasible and efficient technique to construct some ERKN methods with special properties which are wanted in scientific computation.

The paper is organized as follows. Section 2 presents this technique and a special class of ERKN methods. Section 3 shows the feasibility and the effectiveness of the technique in constructing new ERKN methods. The theoretic explanation is studied in Sections 4 and 5. Section 4 presents the rooted tree theory for the special class of ERKN methods. In Section 5, theorems about the symplectic conditions and the symmetric conditions for the special class of ERKN methods are presented.

2 A special class of ERKN methods and a feasible and effective technique

In this section, we will first review the traditional RKN method and the ERKN method solving the general systems (1). And then basing on the traditional RKN method, we present a feasible and efficient technique to form a special class of ERKN methods which will make the construction of ERKN methods much easily. Moreover, in Sections 4 and 5, we will prove that this kind of ERKN method shares the same order, symplectic property and symmetric property with the underlying RKN method.

2.1 The RKN method and the ERKN method

The RKN method is firstly introduced by E.J. Nyström in German in 1925 to solve the second-order differential equations of the form $y'' = f(t, y, y')$. If the function in the right-hand side has the form $f(y, y') - My$, an s-stage traditional RKN method is defined by the following scheme

$$\begin{cases} Y_i = \boldsymbol{y}_n + c_i h \boldsymbol{y}'_n + h^2 \sum_{j=1}^{s} \bar{\alpha}_{ij} \Big(\boldsymbol{f}(Y_j, Y'_j) - MY_j \Big), \qquad i = 1, \ldots, s, \\ Y'_i = \boldsymbol{y}'_n + h \sum_{j=1}^{s} \alpha_{ij} \Big(\boldsymbol{f}(Y_j, Y'_j) - MY_j \Big), \qquad i = 1, \ldots, s, \\ \boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h \boldsymbol{y}'_n + h^2 \sum_{i=1}^{s} \bar{\beta}_i \Big(\boldsymbol{f}(Y_i, Y'_i) - MY_i \Big), \\ \boldsymbol{y}'_{n+1} = \boldsymbol{y}'_n + h \sum_{i=1}^{s} \beta_i \left(\boldsymbol{f}(Y_i, Y'_i) - MY_i \right), \end{cases} \tag{5}$$

with the Butcher tableau given in Table 1.

It is obviously that the RKN method (5) does not make full use of the special structure generated by the linear term $M\boldsymbol{y}$. If we make full use of the special structure and construct methods basing on the matrix-variation-of-constants formulas (6) and (7),

$$\begin{aligned} \boldsymbol{q}(t + \mu h) &= \phi_0(\mu^2 V)\boldsymbol{q}(t) + \mu h \phi_1(\mu^2 V)\boldsymbol{q}'(t) \\ &\quad + h^2 \int_0^{\mu} (\mu - z)\phi_1((\mu - z)^2 V)\boldsymbol{f}(\boldsymbol{q}(t + hz), \boldsymbol{q}'(t + hz))\mathrm{d}z, \end{aligned} \tag{6}$$

$$\begin{aligned} \boldsymbol{q}'(t + \mu h) &= \phi_0(\mu^2 V)\boldsymbol{q}'(t) - h\mu M \phi_1(\mu^2 V)\boldsymbol{q}(t) \\ &\quad + h \int_0^{\mu} \phi_0((\mu - z)^2 V)\boldsymbol{f}(\boldsymbol{q}(t + hz), \boldsymbol{q}'(t + hz))\mathrm{d}z, \end{aligned} \tag{7}$$

Table 1 The Butcher tableau of the RKN method (5)

c_1	$\bar{\alpha}_{11}$	$\bar{\alpha}_{12}$	$\cdots$	$\bar{\alpha}_{1s}$	α_{11}	α_{12}	$\cdots$	α_{1s}
c_2	$\bar{\alpha}_{21}$	$\bar{\alpha}_{22}$	$\cdots$	$\bar{\alpha}_{2s}$	α_{21}	α_{22}	$\cdots$	α_{2s}
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
c_s	$\bar{\alpha}_{s1}$	$\bar{\alpha}_{s2}$	$\cdots$	$\bar{\alpha}_{ss}$	α_{s1}	α_{s2}	$\cdots$	α_{ss}
	$\bar{\beta}_1$	$\bar{\beta}_2$	$\cdots$	$\bar{\beta}_s$	β_1	β_2	$\cdots$	β_s

where $\phi_i(V) = \sum_{p=0}^{+\infty} \frac{(-1)^p}{(2p+i)!} V^p$ with $i = 0, 1$, we can get the ERKN method. The ERKN method is specially defined for the systems (1). The one-dimensional ERKN method is defined in 2009 [10] firstly and then be generalized to the multidimensional ERKN method in 2010 [14].

Definition 1 An s-stage ERKN method solving the ODEs (1) is defined by the following scheme

$$\begin{cases} Q_i = \phi_0(c_i^2 V)\boldsymbol{q}_0 + c_i\phi_1(c_i^2 V)h\boldsymbol{q}_0' + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(V)\boldsymbol{f}(Q_j, Q_j'), \qquad i = 1, \ldots, s, \\ hQ_i' = -c_i V\phi_1(c_i^2 V)\boldsymbol{q}_0 + c_i\phi_0(c_i^2 V)h\boldsymbol{q}_0' + h^2 \sum_{j=1}^{s} a_{ij}(V)\boldsymbol{f}(Q_j, Q_j'), \qquad i = 1, \ldots, s, \\ \boldsymbol{q}_1 = \phi_0(V)\boldsymbol{q}_0 + \phi_1(V)h\boldsymbol{q}_0' + h^2 \sum_{i=1}^{s} \bar{b}_i(V)\boldsymbol{f}(Q_i, Q_i'), \\ h\boldsymbol{q}_1' = -V\phi_1(V)\boldsymbol{q}_0 + \phi_0(V)h\boldsymbol{q}_0' + h^2 \sum_{i=1}^{s} b_i(V)\boldsymbol{f}(Q_i, Q_i'), \end{cases} \tag{8}$$

where the coefficients c_i for $i = 1, \ldots, s$ are constant, the coefficients $\bar{a}_{ij}(V)$, $a_{ij}(V)$, $\bar{b}_i(V)$ and $b_i(V)$ for $i, j = 1, \ldots, s$ are functions of V and $V = h^2 M$.

The ERKN method (8) solving the systems (1) can be expressed in the Butcher's tableau as given in Table 2.

The excellent numerical behaviors of the ERKN method comparing to the RKN method are guaranteed since the special structure of the systems be preserved by the ERKN method. But by now, in order to construct ERKN method with special order or special properties, people have to do almost the same work with that occurs in the construction of the traditional RKN method.

Table 2 The Butcher tableaus of the ERKN method (8) for the general systems (1)

c_1	$\bar{a}_{11}(V)$	$\bar{a}_{12}(V)$	$\cdots$	$\bar{a}_{1s}(V)$	$a_{11}(V)$	$a_{12}(V)$	$\cdots$	$a_{1s}(V)$
c_2	$\bar{a}_{21}(V)$	$\bar{a}_{22}(V)$	$\cdots$	$\bar{a}_{2s}(V)$	$a_{21}(V)$	$a_{22}(V)$	$\cdots$	$a_{2s}(V)$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
c_s	$\bar{a}_{s1}(V)$	$\bar{a}_{s2}(V)$	$\cdots$	$\bar{a}_{ss}(V)$	$a_{s1}(V)$	$a_{s2}(V)$	$\cdots$	$a_{ss}(V)$
	$\bar{b}_1(V)$	$\bar{b}_2(V)$	$\cdots$	$\bar{b}_s(V)$	$b_1(V)$	$b_2(V)$	$\cdots$	$b_s(V)$

2.2 A technique and a special class of ERKN methods

In the construction of new ERKN methods, two steps can finish the construction in a few seconds or a few minutes. At first, we choose the coefficient functions $\big(c_i, \bar{a}_{ij}(V), a_{ij}(V), \bar{b}_i(V), b_i(V)\big)$ in the ERKN method (8) as

$$\begin{aligned} \bar{a}_{ij}(V) &= \bar{\gamma}_{ij}\phi_1((c_i-c_j)^2V),\ a_{ij}(V)=\gamma_{ij}\phi_0((c_i-c_j)^2V), \\ \bar{b}_i(V) &= \bar{\eta}_i\phi_1((1-c_i)^2V),\ b_i(V)=\eta_i\phi_0((1-c_i)^2V), \end{aligned} \tag{9}$$

namely, we approximate the integrals in (6) and (7) by the interpolation quadrature formulas. And then we can set these constant coefficients $\big(c_i, \bar{\gamma}_{ij}, \gamma_{ij}, \bar{\eta}_i, \eta_i\big)$ in (9) as $\big(c_i, \bar{\alpha}_{ij}, \alpha_{ij}, \bar{\beta}_i, \beta_i\big)$ for $i, j = 1, \ldots, s$ which are coefficients in the traditional RKN method (5). Thus, we obtain the ERKN method we are interested in.

Definition 2 An s-stage special class of ERKN methods solving the ODEs (1) is defined by the following scheme

$$\begin{cases} Q_i = \phi_0(c_i^2V)\boldsymbol{q}_0 + c_i\phi_1(c_i^2V)h\boldsymbol{q}_0' + h^2\sum\limits_{j=1}^{s}\bar{\alpha}_{ij}\phi_1((c_i-c_j)^2V)\boldsymbol{f}(Q_j, Q_j'), & i=1,\ldots,s, \\ hQ_i' = -c_iV\phi_1(c_i^2V)\boldsymbol{q}_0 + c_i\phi_0(c_i^2V)h\boldsymbol{q}_0' + h^2\sum\limits_{j=1}^{s}\alpha_{ij}\phi_0((c_i-c_j)^2V)\boldsymbol{f}(Q_j, Q_j'), & i=1,\ldots,s, \\ \boldsymbol{q}_1 = \phi_0(V)\boldsymbol{q}_0 + \phi_1(V)h\boldsymbol{q}_0' + h^2\sum\limits_{i=1}^{s}\bar{\beta}\phi_1((1-c_i)^2V)\boldsymbol{f}(Q_i, Q_i'), \\ h\boldsymbol{q}_1' = -V\phi_1(V)\boldsymbol{q}_0 + \phi_0(V)h\boldsymbol{q}_0' + h^2\sum\limits_{i=1}^{s}\beta_i\phi_0((1-c_i)^2V)\boldsymbol{f}(Q_i, Q_i'), \end{cases} \tag{10}$$

where $V = h^2M$ and the coefficients c_i, $\bar{\alpha}_{ij}$, α_{ij}, $\bar{\beta}_i$ and β_i for $i, j = 1, \ldots, s$ are constant.

It should be pointed out that the special class of ERKN methods (10) and the traditional RKN method (5) share the same coefficients. In the case of the special systems (2), the second equations in (10) and (5) are no longer needed, and then the Butcher tableaus of these two methods are given in Table 3.

Moreover, it will be proved that the ERKN method obtained from this approach has the same order, same symplectic property, and same symmetric property, as the underlying RKN method.

3 Construction of new ERKN methods

Tables 4, 5, 6, 7, 8 and 9 are examples of the constructing of the ERKN methods from the traditional RKN methods. It can be seen easily that it spends a few seconds or a few minutes to construct all these new ERKN methods. Actually these ERKN methods in this section have been studied in papers [5, 10, 16, 34]. While in these

Table 3 The Butcher tableaus of the RKN method (left) and the corresponding special class of ERKN methods (right) solving the systems (2)

c_1	$\bar{\alpha}_{11}$	$\bar{\alpha}_{12}$	$\cdots$	$\bar{\alpha}_{1s}$
c_2	$\bar{\alpha}_{21}$	$\bar{\alpha}_{22}$	$\cdots$	$\bar{\alpha}_{2s}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
c_s	$\bar{\alpha}_{s1}$	$\bar{\alpha}_{s2}$	$\cdots$	$\bar{\alpha}_{ss}$
	$\bar{\beta}_1$	$\bar{\beta}_2$	$\cdots$	$\bar{\beta}_s$
	β_1	β_2	$\cdots$	β_s

c_1	$\bar{\alpha}_{11}$	$\bar{\alpha}_{12}\phi_1((c_1-c_2)^2V)$	$\cdots$	$\bar{\alpha}_{1s}\phi_1((c_1-c_s)^2V)$
c_2	$\bar{\alpha}_{21}\phi_1((c_2-c_1)^2V)$	$\bar{\alpha}_{22}$	$\cdots$	$\bar{\alpha}_{2s}\phi_1((c_2-c_s)^2V)$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
c_s	$\bar{\alpha}_{s1}\phi_1((c_s-c_1)^2V)$	$\bar{\alpha}_{s2}\phi_1((c_s-c_2)^2V)$	$\cdots$	$\bar{\alpha}_{ss}$
	$\bar{\beta}_1\phi_1((1-c_1)^2V)$	$\bar{\beta}_2\phi_1((1-c_2)^2V)$	$\cdots$	$\bar{\beta}_s\phi_1((1-c_s)^2V)$
	$\beta_1\phi_0((1-c_1)^2V)$	$\beta_2\phi_0((1-c_2)^2V)$	$\cdots$	$\beta_s\phi_0((1-c_s)^2V)$

papers without exception the authors have to firstly give the practical order conditions and then consider some reasonable assumptions to get the coefficient functions finally, namely in these papers almost the same operation steps with that in the construction of the classical RKN methods [39, 40] have to do done.

These ERKN methods all show the better numerical behaviors in comparing with the traditional RKN methods and with some other famous methods. The last three ERKN methods follow from the famous three symplectic and symmetric RKN methods.

These ERKN methods are all explicit. Actually from the technique in this paper any ERKN method (explicit or implicit, low order or high order) can be obtained. For higher order RKN methods, we refer to Hairer & Wanner [41–43], to Albrecht [44], to Battin [45], to Beentjes & Gerritsen [46] and to Hairer [41, 47]. For symplecitc or symmetric RKN methods, we refer to Qin Meng-Zhao & Zhu Wen-jie [48], to Okunbor & Skeel [4, 49–51] and to Calvo & Sanz-Serna [4, 52, 53].

The rooted tree theory in the next section ensures the ERKN method (10) have the same order with the underlying RKN methods respectively. And the theorems in Section 5 ensure that if the underlying RKN method is symplectic (or/and symmetric), the ERKN method obtained from this technique is symplectic (or/and symmetric) too.

4 Rooted tree theory

In this section, we will give the rooted tree theory to guarantee the statement that the ERKN method (10) and the corresponding RKN method have the same order. At first, we will review the rooted tree theory for the ERKN integrators (8) [11, 16].

Table 4 A two-stage second-order RKN method (left) and the corresponding ERKN method (right) solving the systems (1)

0				
$\frac{2}{3}$	0		$\frac{2}{3}$	
	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$

0				
$\frac{2}{3}$	0		$\frac{2}{3}\phi_0(\frac{4}{9}V)$	
	$\frac{1}{4}\phi_1(V)$	$\frac{3}{4}\phi_1(\frac{1}{9}V)$	$\frac{1}{4}\phi_0(V)$	$\frac{1}{4}\phi_0(\frac{1}{9}V)$

Table 5 A three-stage third-order RKN method (left) and the corresponding ERKN method (right) solving the systems (1)

$$
\begin{array}{c|ccc|ccc}
0 & & & & & & \\
\frac{1}{2} & 0 & & & \frac{1}{2} & & \\
1 & 1 & 0 & & -1 & 2 & \\
\hline
 & \frac{1}{6} & \frac{2}{6} & 0 & \frac{1}{6} & \frac{4}{6} & \frac{1}{6}
\end{array}
\qquad
\begin{array}{c|ccc|ccc}
0 & & & & & & \\
\frac{1}{2} & 0 & & & \frac{1}{2}\phi_0(\frac{1}{4}V) & & \\
1 & \phi_1(V) & 0 & & -\phi_0(V) & 2\phi_0(\frac{1}{4}V) & \\
\hline
 & \frac{1}{6}\phi_1(V) & \frac{2}{6}\phi_1(\frac{1}{4}V) & 0 & \frac{1}{6}\phi_0(V) & \frac{4}{6}\phi_0(\frac{1}{4}V) & \frac{1}{6}I
\end{array}
$$

And then we present the simplified order conditions for the special class of ERKN methods (10). We will find that the rooted tree theory for the ERKN method (10) can actually be derived from the traditional bi-colored rooted tree sets which are originally presented for the RKN method.

Theorem 1 *([16]) An s-stage ERKN method (8) solving the systems (1) is of order r if and only if the following conditions are satisfied, for any* $\forall \tau \in$ *IEN-T*

$$\sum_{i=1}^{s} \bar{b}_i(V)\Phi_i(\tau) = \frac{\rho(\tau)!}{S(\tau)\gamma(\tau)}\phi_{\rho(\tau)+1}(V) + O(h^{r-\rho(\tau)}), \quad \rho(\tau) \leq r-1, \tag{11}$$

$$\sum_{i=1}^{s} b_i(V)\Phi_i(\tau) = \frac{\rho(\tau)!}{S(\tau)\gamma(\tau)}\phi_{\rho(\tau)}(V) + O(h^{r-\rho(\tau)+1}), \quad \rho(\tau) \leq r, \tag{12}$$

where the mappings $\rho(\tau)$*,* $\Phi_i(\tau)$*,* $S(\tau)$ *and* $\gamma(\tau)$ *are defined on the IEN-T set.*

If we consider the ERKN method (8) solving the special systems (2), we can obtain the order conditions theorem which is first introduced in paper [11]. In this special case the order conditions are based on the SSEN-T set.

Table 6 A three-stage third-order RKN method (above) and the corresponding ERKN method (below) solving the systems (1)

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8} & & & & \frac{1}{2} & & & \\
\frac{1}{2} & \frac{1}{8} & 0 & & & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & \frac{1}{2} & & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6}
\end{array}
$$

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8}\phi_1(\frac{1}{4}V) & & & & \frac{1}{2}\phi_0(\frac{1}{4}V) & & & \\
\frac{1}{2} & \frac{1}{8}\phi_1(\frac{1}{4}V) & 0 & & & 0 & \frac{1}{2}I & & \\
1 & 0 & 0 & \frac{1}{2}\phi_1(\frac{1}{4}V) & & 0 & 0 & \phi_0(\frac{1}{4}V) & \\
\hline
 & \frac{1}{6}\phi_1(V) & \frac{1}{6}\phi_1(\frac{1}{4}V) & \frac{1}{6}\phi_1(\frac{1}{4}V) & 0 & \frac{1}{6}\phi_0(V) & \frac{2}{6}\phi_0(\frac{1}{4}V) & \frac{2}{6}\phi_0(\frac{1}{4}V) & \frac{1}{6}I
\end{array}
$$

Table 7 A two-stage second-order symplectic and symmetric RKN method (left) and the corresponding ERKN method (right) solving the special systems (2)

$$\begin{array}{c|cc} 0 & & \\ 1 & \frac{1}{2} & \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|cc} 0 & & \\ 1 & \frac{1}{2}\phi_1(V) & \\ \hline & \frac{1}{2}\phi_1(V) & 0 \\ \hline & \frac{1}{2}\phi_0(V) & \frac{1}{2}I \end{array}$$

Theorem 2 *([11]) An s-stage ERKN method (8) solving the systems (2) is of order r if and only if the following conditions are satisfied, for any $\forall \tau \in$ SSEN-T*

$$\sum_{i=1}^{s} \bar{b}_i(V)\Phi_i(\tau) = \frac{\rho(\tau)!}{S(\tau)\gamma(\tau)}\phi_{\rho(\tau)+1}(V) + O(h^{r-\rho(\tau)}), \quad \rho(\tau) \le r-1, \tag{13}$$

$$\sum_{i=1}^{s} b_i(V)\Phi_i(\tau) = \frac{\rho(\tau)!}{S(\tau)\gamma(\tau)}\phi_{\rho(\tau)}(V) + O(h^{r-\rho(\tau)+1}), \quad \rho(\tau) \le r, \tag{14}$$

where the mappings $\rho(\tau)$, $\Phi_i(\tau)$, $S(\tau)$ and $\gamma(\tau)$ are defined on the SSEN-T set.

It should be pointed out that in the study of order conditions for the ERKN methods (8) [11, 16], if all coefficients are independent, one tree corresponds to one order condition and there is no redundant at all. But for the special class of ERKN methods (10), these theories are not satisfied enough since the coefficient functions are actually dependent and then there will be redundant order conditions. In the following we will present new order condition theories which make all redundant order conditions disappear. The following two Lemmas will be very important in bringing in these new order conditions.

Lemma 1 *For a given non-negative number m_1 and a given number k, assume that*

$$\sum_{i=1}^{s} A_i c_i^m = \frac{(B+m-1)!k!}{(B+m+k)!}, \quad \forall\, 0 < m \le m_1,$$

Table 8 Another two-stage second-order symplectic and symmetric RKN method (left) and the corresponding ERKN method (right) solving the special systems (2)

$$\begin{array}{c|cc} \frac{1}{4} & & \\ \frac{3}{4} & \frac{1}{4} & \\ \hline & \frac{3}{8} & \frac{1}{8} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|cc} \frac{1}{4} & & \\ \frac{3}{4} & \frac{1}{4}\phi_1(\frac{V}{4}) & \\ \hline & \frac{3}{8}\phi_1(\frac{9V}{16}) & \frac{1}{8}\phi_1(\frac{V}{16}) \\ \hline & \frac{1}{2}\phi_0(\frac{9V}{16}) & \frac{1}{2}\phi_0(\frac{V}{16}) \end{array}$$

Table 9 A three-stage fourth-order symplectic and symmetric RKN method [3, 51] where $c_1 = \frac{1}{6}(2 + \sqrt[3]{2} + \frac{1}{\sqrt[3]{2}})$ (above) and the corresponding ERKN method (below) solving the special systems (2)

c_1			
$\frac{1}{2}$	$\frac{1-2c_1}{12(1-2c_1)^2}$		
$1-c_1$	$\frac{1-2c_1}{6(1-2c_1)^2}$	$\frac{(1-2c_1)(1-6(1-c_1)c_1)}{3(1-2c_1)^2}$	
	$\frac{1-c_1}{6(1-2c_1)^2}$	$\frac{1-6(1-c_1)c_1}{3(1-2c_1)^2}$	$\frac{c_1}{6(1-2c_1)^2}$
	$\frac{1}{6(1-2c_1)^2}$	$\frac{2(1-6(1-c_1)c_1)}{3(1-2c_1)^2}$	$\frac{1}{6(1-2c_1)^2}$

c_1			
$\frac{1}{2}$	$\frac{1-2c_1}{12(1-2c_1)^2}\phi_1(\frac{(1-2c_1)^2V}{4})$		
$1-c_1$	$\frac{1-2c_1}{6(1-2c_1)^2}\phi_1((1-2c_1)^2V)$	$\frac{(1-2c_1)(1-6(1-c_1)c_1)}{3(1-2c_1)^2}\phi_1(\frac{(1-2c_1)^2V}{4})$	
	$\frac{1-c_1}{6(1-2c_1)^2}\phi_1((1-c_1)^2V)$	$\frac{1-6(1-c_1)c_1}{3(1-2c_1)^2}\phi_1(\frac{V}{4})$	$\frac{c_1}{6(1-2c_1)^2}\phi_1(c_1^2V)$
	$\frac{1}{6(1-2c_1)^2}\phi_0((1-c_1)^2V)$	$\frac{2(1-6(1-c_1)c_1)}{3(1-2c_1)^2}\phi_0(\frac{V}{4})$	$\frac{1}{6(1-2c_1)^2}\phi_0(c_1^2V)$

where B is a non-negative number. Then, we have

$$\sum_{i=1}^{s} A_i c_i^q (1-c_i)^{2p} = \frac{(B+q-1)!(2p+k)!}{(B+q+2p+k)!}, \quad \forall\, q \geq 0; \forall\, 2p+q \leq m_1.$$

Proof Using the mathematical induction, we can have that for any q, if $2p+q < m_1$

$$\begin{aligned}
\textstyle\sum_i A_i c_i^q (1-c_i)^{2p} &= \textstyle\sum_i A_i c_i^q (1-c_i)^{2p-2} - 2\sum_i A_i c_i^{q+1}(1-c_i)^{2p-2} + \sum_i A_i c_i^{q+2}(1-c_i)^{2p-2} \\
&= \frac{(B+q-1)!(2p-2+k)!}{(B+q+2p-2+k)!} - 2\frac{(B+q)!(2p-2+k)!}{(B+q+2p-1+k)!} + \frac{(B+q+1)!(2p-2+k)!}{(B+q+2p+k)!} \\
&= \frac{(B+q-1)!(2p+k)!}{(B+q+2p+k)!}.
\end{aligned}$$

The proof is finished. □

Lemma 2 *For any given $k > 0$,*

$$\sum_{q=0}^{2m} \frac{(-1)^q (k+q-1)!(k+2m+1)!}{q!(2m-q)!(k-1)!(k+q+1)!} = 2m+1. \tag{15}$$

Proof It can be completed by the mathematical induction for integral m (see the detail in Appendix). □

Theorem 3 *An s-stage special class of ERKN integrators* (10) *solving the systems* (2) *is of order r if and only if the following conditions are satisfied, for any* $\forall\tau \in$ *SN-T*

$$\sum_{i=1}^{s} \bar{\beta}_i \Phi_i(\tau) = \frac{1}{\rho(\tau)+1} \cdot \frac{1}{\gamma(\tau)}, \quad \rho(\tau) \le r-1, \tag{16}$$

$$\sum_{i=1}^{s} \beta_i \Phi_i(\tau) = \frac{1}{\gamma(\tau)}, \quad \rho(\tau) \le r, \tag{17}$$

where the mappings $\rho(\tau)$, $\Phi_i(\tau)$ *and* $\gamma(\tau)$ *are defined on the classical SN-T set* [3].

Proof The necessary part follows from Theorem 2, Definition of ϕ-functions and the special choice of coefficient functions $\bar{b}_i(V)$ and $b_i(V)$.

The sufficient part will be completed by two steps. At first, we will verify that if the following scheme

$$\sum_{i=1}^{s} \bar{\beta}_i \Phi_i(\tau) = \frac{1}{\rho(\tau)+1} \cdot \frac{1}{S(\tau)\gamma(\tau)}, \quad \rho(\tau) \le r-1, \tag{18}$$

$$\sum_{i=1}^{s} \beta_i \Phi_i(\tau) = \frac{1}{S(\tau)\gamma(\tau)}, \quad \rho(\tau) \le r, \tag{19}$$

is satisfied, an s-stage special class of ERKN integrators (10) is of order r. In fact, in this case, for any p, if $2p + \rho(\tau) \le r-1$, we have

$$\sum_{i=1}^{s} \bar{\beta}_i c_i^{2p} \Phi_i(\tau) = \sum_{i=1}^{s} \bar{\beta}_i \Phi_i(\hat{\tau}) = \frac{1}{\rho(\hat{\tau})+1} \cdot \frac{1}{S(\hat{\tau})\gamma(\hat{\tau})} = \frac{1}{(\rho(\tau)+2p+1)(\rho(\tau)+2p)} \cdot \frac{\rho(\tau)}{S(\tau)\gamma(\tau)}, \tag{20}$$

where $\hat{\tau}$ is an SSEN-T which are obtained from τ by attaching $2p$ new branches with a black vertex to the root of τ. And (20) follows from Definition 4.2 in [11], namely $\rho(\hat{\tau}) = \rho(\tau) + 2p$, $\Phi_i(\hat{\tau}) = c_i^{2p} \Phi_i(\tau)$, $\gamma(\hat{\tau}) = \dfrac{\rho(\tau)+2p}{\rho(\tau)} \gamma(\tau)$ and $S(\hat{\tau}) = S(\tau)$. Then from Lemma 1, for $k = 1$, we have

$$\sum_{i=1}^{s} \bar{\beta}_i (1-c_i)^{2p} \Phi_i(\tau) = \frac{(\rho(\tau)-1)!(2p+1)!}{(\rho(\tau)+2p+1)!} \cdot \frac{\rho(\tau)}{S(\tau)\gamma(\tau)}. \tag{21}$$

Inserting (21) into the Taylor series of the left side of order conditions (13) in Theorem 2

$$\sum_{i=1}^{s} \bar{b}_i(V)\Phi_i(\tau) = \sum_{2p \le r-\rho(\tau)-1} \frac{(-1)^p \sum_{i=1}^{s} \bar{\beta}_i (1-c_i)^{2p} \Phi_i(\tau)}{(2p+1)!} V^p + O(h^{r-\rho(\tau)}),$$

we have

$$\sum_{i=1}^{s} \bar{b}_i(V)\Phi_i(\tau) = \frac{\rho(\tau)!}{S(\tau)\gamma(\tau)} \phi_{\rho(\tau)+1}(V) + O(h^{r-\rho(\tau)}).$$

Similarly from (19), we can get (14). So, we complete the first step of the proof.

And in the next step, we will prove that for the special ERKN integrator (10), any tri-colored SSEN-T is redundant. With the disappear of meagre vertex, order conditions (18) and (19) are exactly order conditions (16) and (17) respectively.

Let u be a tri-colored SSEN-T as sketched in Fig. 1 and the rooted trees t (SSEN-Ts) are introduced with the encircled parts are assumed to be identical respectively. Here we will verify that order conditions (18) and (19) written from tree u can be implied by others written from some same order SSEN-Ts with less meagre vertices than u's. In fact, since Definition 4.2 in [11] gives $\Phi_i(u) = \frac{(-1)^m}{2m+1}\Phi_i(\tau_2)\bar{\alpha}_{jk}(c_j - c_k)^{2m}\Phi_k(\tau_1)$ and $\Phi_i(t) = \Phi_i(\tau_2)c_j^{2m-q}\bar{\alpha}_{jk}c_k^q\Phi_k(\tau_1)$, we have

$$\Phi_i(u) = \frac{(-1)^m}{2m+1}\sum_{q=0}^{2m}\frac{(-1)^q(2m)!}{q!(2m-q)!}\Phi_i(t).$$

If order conditions for trees t are true, then the left-hand side of the order condition (18) for tree u is

$$\sum \bar{\beta}_i\Phi_i(u) = \frac{(-1)^m}{2m+1}\sum_{q=0}^{2m}\frac{(-1)^q(2m)!}{q!(2m-q)!}\frac{1}{\rho(t)+1}\cdot\frac{1}{S(t)\gamma(t)}.$$

Definition 4.2 in [11] also gives that $\rho(u) = \rho(t)$, $S(u) = (-1)^m S(t)$ and $\frac{(2m)!}{\gamma(t)} = \frac{(\rho(\tau_1)+q-1)!}{(\rho(\tau_1)-1)!}\frac{(\rho(\tau_1)+2m+1)!}{(\rho(\tau_1)+q+1)!}\frac{1}{\gamma(u)}$. From Lemma 2, we have

$$\sum_{q=0}^{2m}\frac{(-1)^q(2m)!}{q!(2m-q)!}\frac{1}{\gamma(t)} = \sum_{q=0}^{2m}\frac{(-1)^q}{q!(2m-q)!}\frac{(\rho(\tau_1)+q-1)!}{(\rho(\tau_1)-1)!}\frac{(\rho(\tau_1)+2m+1)!}{(\rho(\tau_1)+q+1)!}\frac{1}{\gamma(u)} = (2m+1)\frac{1}{\gamma(u)},$$

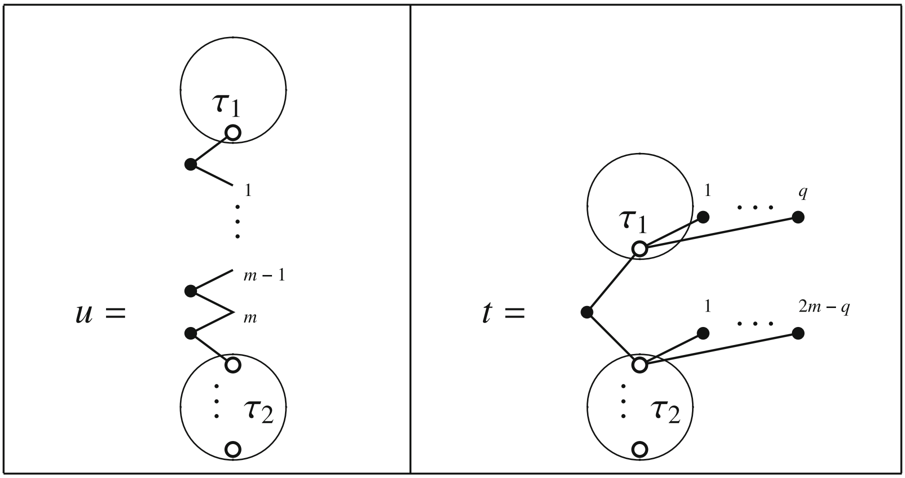

Fig. 1 Trees in Theorem 3

And then

$$\sum \bar{\beta}_i \Phi_i(u) = \frac{1}{\rho(u)+1} \frac{1}{S(u)\gamma(u)}.$$

Thus, by now, an SSEN-T with meagre vertices can be implied by some same order SSEN-Ts which all have less meagre vertices. Using the result repeatedly, the meagre vertices disappear, and any tri-colored rooted tree can by implied by bi-colored rooted trees. We then get the result. The proof is complete. □

If we consider the special class of ERKN integrators (10) solving the general systems (1), we can obtain the following theorem.

Theorem 4 *An s-stage special class of ERKN integrators* (10) *solving the general systems* (1) *is of order r if and only if the following conditions are satisfied, for any* $\forall \tau \in$ *N-T*

$$\sum_{i=1}^{s} \bar{\beta}_i \Phi_i(\tau) = \frac{1}{\rho(\tau)+1} \cdot \frac{1}{\gamma(\tau)}, \quad \rho(\tau) \le r-1, \tag{22}$$

$$\sum_{i=1}^{s} \beta_i \Phi_i(\tau) = \frac{1}{\gamma(\tau)}, \quad \rho(\tau) \le r, \tag{23}$$

where the mappings $\rho(\tau)$, $\Phi_i(\tau)$ *and* $\gamma(\tau)$ *are defined on the classical N-T set* [3].

Proof From Theorem 3, we just need to prove that any tri-colored IEN-T as sketched in Fig. 2, denoted by u, is redundant.

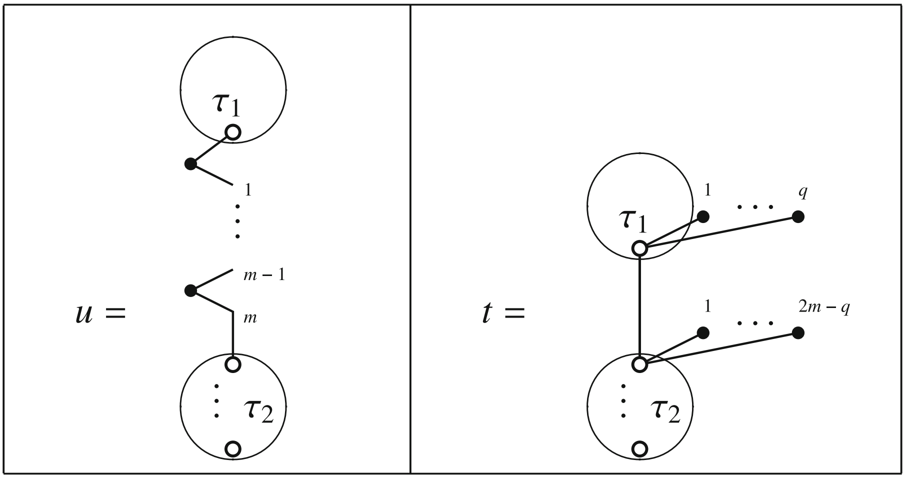

Fig. 2 Trees in Theorem 4

Let some rooted trees t sketched in Fig. 2 are introduced with the encircled parts are assumed to be identical respectively. And then we can complete the proof if the following result are verified

$$\Phi_i(u) = \frac{(-1)^m}{2m+1} \sum_{q=0}^{2m} \frac{(-1)^q (2m)!}{q!(2m-q)!} \Phi_i(t).$$

In fact, from Definition 4.2 in [16] $\Phi_i(u) = \frac{(-1)^m}{2m+1} \Phi_i(\tau_2)\alpha_{jk}(c_j - c_k)^{2m} \Phi_k(\tau_1)$ and $\Phi_i(t) = \Phi_i(\tau_2) c_j^{2m-q} \alpha_{jk} c_k^q \Phi_k(\tau_1)$, we can obtain the result. So the proof is complete. □

Theorems mentioned in this section tell us that the ERKN method (10) and the corresponding RKN method share the same order conditions which can be derived from the same rooted tree set solving the systems (1) (or (2)). And then these theorems ensure that the construction of the r-th order ERKN method (10) can be obtained much easily. Moreover, no more information and knowledge is needed except the classical ones.

5 Properties of the ERKN method

Symmetric methods and symplectic methods play a central role in the structuring-preserving integration of differential equations. In this section, we will show that the ERKN method (10) and the underlying RKN method have the same properties, such as symplectic and symmetric.

5.1 The symplectic conditions

In the study of the symplectic conditions for numerical integrators for Hamiltonian systems, the systems must be written as (2) with the matrix M is symmetric. The theory for symplectic methods can be traced back to 1988 and 1989. Pioneering work on symplectic integration is due to de Vogelaere (1956), Ruth (1983), and Feng Kang (1985). Books on the now well-developed subject are Sanz-Serna & Calvo (1994) and Leimkuhler & Reich (2004). Readers are referred to [32, 33, 35, 39, 52–57] et al.

Definition 3 A numerical one-step method $q_1 = \Phi_h(q_0)$ is called symplectic if the Jacobian matrix Φ'_h satisfies

$$\Phi_h'^T J \Phi_h' = J$$

with $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ where I is the identity matrix.

For standard ERKN method, X. Wu, B.Wang & J. Xia in paper [20] have presented the symplectic conditions as follows.

Theorem 5 *([20]) Consider the system (2) where M is a symmetric matrix. Then, the s-stage ERKN integrator (8) is symplectic if its coefficients satisfy*

$$b_i(V)\phi_0(V) + V\bar{b}_i(V)\phi_1(V) = d_i\phi_0(c_i^2 V), \quad i = 1, 2, \ldots, s, \tag{24}$$

$$b_i(V)\phi_1(V) - \bar{b}_i(V)\phi_0(V) = c_i d_i\phi_1(c_i^2 V), \quad i = 1, 2, \ldots, s, \tag{25}$$

$$\bar{b}_j(V)b_i(V) + d_j\bar{a}_{ji}(V) = \bar{b}_i(V)b_j(V) + d_i\bar{a}_{ij}(V), \quad i, j = 1, 2, \ldots, s, \tag{26}$$

where $d_i \in \mathbb{R}$.

If the ERKN method have special structure, these symplectic conditions can be simplified. Before this, we will give the following properties of the unconditionally convergent matrix-valued functions $\phi_i(V)$.

Lemma 3 *The matrix-valued functions $\phi_0(V)$ and $\phi_1(V)$ satisfy*

$$c_j\phi_1(c_j^2 V)\phi_0(c_i^2 V) - c_i\phi_0(c_j^2 V)\phi_1(c_i^2 V) = (c_j - c_i)\phi_1((c_j - c_i)^2 V), \tag{27}$$

$$\phi_0(c_j^2 V)\phi_0(c_i^2 V) + c_j c_i V\phi_1(c_j^2 V)\phi_1(c_i^2 V) = \phi_0((c_j - c_i)^2 V). \tag{28}$$

Proof By definitions of ϕ-functions, we have

$$c_j\phi_1(c_j^2 V)\phi_0(c_i^2 V) \;-\; c_i\phi_0(c_j^2 V)\phi_1(c_i^2 V) = \sum_{k=0}^{\infty}\frac{(-1)^k V^k c_j^{2k+1}}{(2k+1)!}\sum_{k=0}^{\infty}\frac{(-1)^k V^k c_i^{2k}}{(2k)!} - \sum_{k=0}^{\infty}\frac{(-1)^k V^k c_i^{2k+1}}{(2k+1)!}\sum_{k=0}^{\infty}\frac{(-1)^k V^k c_j^{2k}}{(2k)!}.$$

It follows from the Cauchy product $(\sum\limits_{n=0}^{\infty} a_n)(\sum\limits_{n=0}^{\infty} b_n) = \sum\limits_{n=0}^{\infty}\big(\sum\limits_{k=0}^{n} a_k b_{n-k}\big)$ that

$$\begin{aligned}
&c_j\phi_1(c_j^2 V)\phi_0(c_i^2 V) - c_i\phi_0(c_j^2 V)\phi_1(c_i^2 V)\\
&= \sum_{n=0}^{\infty}\Big(\sum_{k=0}^{n}\frac{(-1)^k V^k c_j^{2k+1}}{(2k+1)!}\frac{(-1)^{n-k} V^{n-k} c_i^{2n-2k}}{(2n-2k)!}\Big)\\
&- \sum_{n=0}^{\infty}\Big(\sum_{k=0}^{n}\frac{(-1)^{n-k} V^{n-k} c_i^{2n-2k+1}}{(2n-2k+1)!}\frac{(-1)^k V^k c_j^{2k}}{(2k)!}\Big)\\
&= \sum_{n=0}^{\infty}(-1)^n V^n\Big(\sum_{i=0}^{2n+1}\frac{c_j^i}{i!}\frac{(-c_i)^{2n+1-i}}{(2n+1-i)!}\Big).
\end{aligned}$$

Because of $\sum_{i=0}^{n} \frac{n!}{i!(n-i)!} a^i b^{n-i} = (a+b)^n$, we have the first identity. Similarly, we can obtain the second identity. This proof is complete. □

Theorem 6 *Consider the system* (2) *where M is a symmetric matrix. Then, the s-stage special class of ERKN integrator* (10) *is symplectic if its coefficients satisfy*

$$\bar{\beta}_i = \beta_i(1-c_i), \quad i = 1, 2, \ldots, s, \tag{29}$$

$$\beta_i(\bar{\beta}_j - \bar{\alpha}_{ij}) = \beta_j(\bar{\beta}_i - \bar{\alpha}_{ji}), \quad i, j = 1, 2, \ldots, s. \tag{30}$$

Proof Under the conditions (29), from the (28), we have

$$\begin{aligned} b_i(V)\phi_0(c_i^2 V) + V\bar{b}_i(V)\phi_1(V) &= \beta_i\Big(\phi_0((1-c_i)^2 V)\phi_0(V) + V(1-c_i)\phi_1((1-c_i)^2 V)\phi_1(V)\Big) \\ &= \beta_i\phi_0(c_i^2 V), \end{aligned}$$

and from the (27), we have

$$\begin{aligned} b_i(V)\phi_1(V) - \bar{b}_i(V)\phi_0(V) &= \beta_i\Big(\phi_0((1-c_i)^2 V)\phi_1(V) - (1-c_i)\phi_1((1-c_i)^2 V)\phi_0(V)\Big) \\ &= \beta_i c_i \phi_1(c_i^2 V). \end{aligned}$$

Under the conditions (29) and (30) , we have $\beta_i\beta_j(c_i - c_j) = \beta_i\bar{\alpha}_{ij} - \beta_j\bar{\alpha}_{ji}$, and then from the (27), we have

$$\begin{aligned} \bar{b}_j(V)b_i(V) - \bar{b}_i(V)b_j(V) &= \bar{\beta}_j\phi_1((1-c_j)^2 V)\beta_i\phi_0((1-c_i)^2 V) \\ &\quad -\bar{\beta}_i\phi_1((1-c_i)^2 V)\beta_j\phi_0((1-c_j)^2 V) \\ &= \beta_i\beta_j\Big((1-c_j)\phi_1((1-c_j)^2 V)\phi_0((1-c_i)^2 V) \\ &\quad -(1-c_i)\phi_1((1-c_i)^2 V)\phi_0((1-c_j)^2 V)\Big) \\ &= \beta_i\beta_j(c_i - c_j)\phi_1((c_i - c_j)^2 V) \\ &= \beta_i\bar{\alpha}_{ij}\phi_1((c_i - c_j)^2 V) - \beta_j\bar{\alpha}_{ji}\phi_1((c_i - c_j)^2 V) \\ &\quad = \beta_i\bar{a}_{ij}(V) - \beta_j\bar{a}_{ji}(V). \end{aligned}$$

So, from Theorem 5, we complete the proof. □

With the technique in this paper, symplectic ERKN methods (for example sixth-order symplectic ERKN method [38]) can be obtained easily.

5.2 The symmetric conditions

Numerical experiments indicate that symmetric methods applied to integrable and near-integrable reversible systems share similar properties to symplectic methods applied to (near-)integrable Hamiltonian systems: linear error growth, long-time near-conservation of first integrals, existence of invariant tori. The study of symmetric methods has its origin in the development of extrapolation methods (Gragg 1965, Stetter 1973), because the global error admits an asymptotic expansion in even powers of h. The notion of time-reversible methods is more common in the Computational Physics literature (Buneman 1967).

Definition 4 A numerical one-step method $q_1 = \Phi_h(q_0)$ is called *symmetric* or *time-reversible*, if it satisfies

$$\Phi_h \circ \Phi_{-h} = id \quad \text{or equivalently} \quad \Phi_h = \Phi_{-h}^{-1}.$$

Theorem 7 *An s-stage standard ERKN integrator* (8) *for the systems* (1) *is symmetric if its coefficients satisfy*

$$c_i = 1 - c_{s+1-i}, \quad i = 1, 2, \ldots, s, \tag{31}$$

$$b_i(V) = V\phi_1(V)\bar{b}_{s+1-i}(V) + \phi_0(V)b_{s+1-i}(V), \quad i = 1, 2, \ldots, s, \tag{32}$$

$$\begin{aligned}\bar{a}_{ij}(V) = {} & \phi_0(c_{s+1-i}^2 V)\bar{b}_j(V) - c_{s+1-i}\phi_1(c_{s+1-i}^2 V)b_j(V) \\ & + \bar{a}_{s+1-i,s+1-j}(V), \quad i, j = 1, 2, \ldots, s,\end{aligned} \tag{33}$$

$$\begin{aligned}a_{ij}(V) = {} & c_{s+1-i}V\phi_1(c_{s+1-i}^2 V)\bar{b}_j(V) + \phi_0(c_{s+1-i}^2 V)b_j(V) \\ & - a_{s+1-i,s+1-j}(V), \quad i, j = 1, 2, \ldots, s.\end{aligned} \tag{34}$$

Proof Exchanging $\left(\boldsymbol{q}_1, \boldsymbol{q}'_1\right) \leftrightarrow \left(\boldsymbol{q}_0, \boldsymbol{q}'_0\right)$ and $h \leftrightarrow -h$ in (8) gives

$$\begin{cases} Q_i^* = \phi_0(c_i^2 V)\boldsymbol{q}_1 - c_i\phi_1(c_i^2 V)h\boldsymbol{q}'_1 + h^2 \sum_{j=1}^{s} \bar{a}_{ij}(V)\boldsymbol{f}(Q_j^*, Q_j'^*), \\ Q_i'^* = c_i h M\phi_1(c_i^2 V)\boldsymbol{q}_1 + \phi_0(c_i^2 V)\boldsymbol{q}'_1 - h \sum_{j=1}^{s} a_{ij}(V)\boldsymbol{f}(Q_j^*, Q_j'^*), \\ \boldsymbol{q}_0 = \phi_0(V)\boldsymbol{q}_1 - \phi_1(V)h\boldsymbol{q}'_1 + h^2 \sum_{i=1}^{s} \bar{b}_i(V)\boldsymbol{f}(Q_i^*, Q_i'^*), \\ \boldsymbol{q}'_0 = hM\phi_1(V)\boldsymbol{q}_1 + \phi_0(V)\boldsymbol{q}'_1 - h \sum_{i=1}^{s} b_i(V)\boldsymbol{f}(Q_i^*, Q_i'^*). \end{cases} \tag{35}$$

From the last two equation in (35) and Lemma 3, we obtain

$$\begin{aligned} \boldsymbol{q}_1 &= \phi_0(V)\boldsymbol{q}_0 + \phi_1(V)h\boldsymbol{q}'_0 + h^2\sum_{i=1}^{s}\Big(\phi_1(V)b_i(V) - \phi_0(V)\bar{b}_i(V)\Big)\boldsymbol{f}(Q_i^*, Q_i'^*), \\ \boldsymbol{q}'_1 &= -hM\phi_1(V)\boldsymbol{q}_0 + \phi_0(V)\boldsymbol{q}'_0 + h\sum_{i=1}^{s}\Big(V\phi_1(V)\bar{b}_i(V) + \phi_0(V)b_i(V)\Big)\boldsymbol{f}(Q_i^*, Q_i'^*). \end{aligned} \tag{36}$$

Inserting (36) into the first two equations in (35), and from Lemma 3, we obtain

$$\begin{aligned} Q_i^* &= \phi_0((1-c_i)^2V)\boldsymbol{q}_0 + h(1-c_i)\phi_1((1-c_i)^2V)h\boldsymbol{q}'_0 \\ &+ h^2\sum_{j=1}^{s}\Big(\phi_0(c_i^2V)\big(\phi_1(V)b_j(V) - \phi_0(V)\bar{b}_j(V)\big) \\ &\qquad - c_i\phi_1(c_i^2V)\big(V\phi_1(V)\bar{b}_j(V) + \phi_0(V)b_j(V)\big) + \bar{a}_{ij}(V)\Big)\boldsymbol{f}(Q_j^*, Q_j'^*), \\ Q_i'^* &= -(1-c_i)hM\phi_1((1-c_i)^2V)\boldsymbol{q}_0 + \phi_0((1-c_i)^2V)\boldsymbol{q}'_0 \\ &+ h\sum_{j=1}^{s}\Big(c_iV\phi_1(c_i^2V)\big(\phi_1(V)b_j(V) - \phi_0(V)\bar{b}_j(V)\big) \\ &\qquad + \phi_0(c_i^2V)\big(V\phi_1(V)\bar{b}_j(V) + \phi_0(V)b_j(V)\big) - a_{ij}(V)\Big)\boldsymbol{f}(Q_j^*, Q_j'^*). \end{aligned} \tag{37}$$

Replacing all indices i and j in (36) and (37) by $s+1-i$ and $s+1-j$, respectively, we can see that the symmetric conditions for standard ERKN integrator (8) for the systems (1) are (31) – (34) and

$$\bar{b}_i(V) = \phi_1(V)b_{s+1-i}(V) - \phi_0(V)\bar{b}_{s+1-i}(V). \tag{38}$$

And since (38) is implied by (32), we complete the proof. □

Theorem 8 *([5]) An s-stage standard ERKN integrator* (8) *for the systems* (2) *is symmetric if its coefficients satisfy the conditions* (31) – (33).

For the special class of ERKN method (10) in this paper, we have following simplified symmetric conditions.

Theorem 9 *An s-stage special class of ERKN integrator* (10) *for the systems* (1) *is symmetric if its coefficients satisfy*

$$c_i = 1 - c_{s+1-i}, \quad i = 1, 2, \ldots, s, \tag{39}$$

$$\bar{\beta}_i = \beta_i(1-c_i), \quad i = 1, 2, \ldots, s, \tag{40}$$

$$\beta_i = \beta_{s+1-i}, \quad i = 1, 2, \ldots, s, \tag{41}$$

$$\bar{\alpha}_{ij} = \beta_j(c_i - c_j) + \bar{\alpha}_{s+1-i,s+1-j}, \quad i, j = 1, 2, \ldots, s, \tag{42}$$

$$\alpha_{ij} = \beta_j - \alpha_{s+1-i,s+1-j}, \quad i, j = 1, 2, \ldots, s \tag{43}$$

Proof Under the conditions (39) – (41), we have

$$\begin{aligned} V\phi_1(V)\bar{b}_{s+1-i}(V)+\phi_0(V)b_{s+1-i}(V) &= V\phi_1(V)\bar{\beta}_{s+1-i}\phi_1(c_i^2V)+\phi_0(V)\beta_{s+1-i}\phi_0(c_i^2V) \\ &= \beta_i\Big(c_iV\phi_1(V)\phi_1(c_i^2V)+\phi_0(V)\phi_0(c_i^2V)\Big), \end{aligned}$$

and then from the (28), we can obtain the conditions (32). Under the conditions (39) – (40) , we have

$$\begin{aligned} &\phi_0(c_{s+1-i}^2V)\bar{b}_j(V)-c_{s+1-i}\phi_1(c_{s+1-i}^2V)b_j(V)+\bar{a}_{s+1-i,s+1-j}(V) \\ &= \phi_0((1-c_i)^2V)\bar{\beta}_j\phi_1((1-c_j)^2V)-(1-c_i)\phi_1((1-c_i)^2V)\beta_j\phi_0((1-c_j)^2V) \\ &\quad +\bar{\alpha}_{s+1-i,s+1-j}\phi_1((c_j-c_i)^2V) \\ &= \Big((1-c_j)\phi_0((1-c_i)^2V)\phi_1((1-c_j)^2V) \\ &\quad -(1-c_i)\phi_1((1-c_i)^2V)\phi_0((1-c_j)^2V)\Big)\beta_j+\bar{\alpha}_{s+1-i,s+1-j}\phi_1((c_j-c_i)^2V), \end{aligned}$$

and then from the (27), we can get

$$\begin{aligned} \phi_0(c_{s+1-i}^2V)\bar{b}_j(V) \quad c_{s+1-i}\phi_1(c_{s+1-i}^2V)b_j(V)+\bar{a}_{s+1-i,s+1-j}(V) \\ = \Big(\beta_j(c_i-c_j)+\bar{\alpha}_{s+1-i,s+1-j}\Big)\phi_1((c_j-c_i)^2V), \end{aligned}$$

at last, we obtain the conditions (33) from the conditions (42). Similarly, from Lemma 3 and the conditions (43), we can obtain the conditions (34). The proof is complete. □

Theorem 10 *An s-stage special class of ERKN integrator* (10) *for the systems* (2) *is symmetric if its coefficients satisfy the conditions* (39) – (42).

These symplectic and symmetric conditions in the theorems have the same form with those for the classical RKN methods [3, 55].

6 Conclusion

In this paper, we give a feasible and effective technique to constructing ERKN methods. With this technique in numerical applications the the normal engineers can easily obtain the ERKN method (10) with the properties what they want in a few minutes or seconds. In fact, the ERKN method shares the same order, same symplectic property, and same symmetric property with the underlying RKN method.

The rooted tree thleory for the special kind of ERKN method (10) are also interesting. It is that for the special method the rooted tree theory is actually the classical bi-colored special Nyström rooted tree theory.

Acknowledgments The authors are grateful to the anonymous referees for their careful reading of the manuscript and for their invaluable comments and suggestions which improved this paper greatly.

Appendix: The proof of Lemma 2

At first, it is trivial for $m = 1$, and we prove this theorem using the mathematical induction. In fact,

$$\begin{aligned}
&\sum_{q=0}^{2(m+1)} \frac{(2m+2-q)(2m+1-q)(-1)^q (k+q-1)!(k+2(m+1)+1)!}{q!(2(m+1)-q)!(k-1)!(k+q+1)!} \\
&= (k+2m+3)(k+2m+2)\sum_{q=0}^{2m} \frac{(-1)^q (k+q-1)!(k+2m+1)!}{q!(2m-q)!(k-1)!(k+q+1)!},
\end{aligned} \tag{44}$$

$$\begin{aligned}
&\sum_{q=0}^{2(m+1)} \frac{q(2m+2-q)(-1)^q (k+q-1)!(k+2(m+1)+1)!}{q!(2(m+1)-q)!(k-1)!(k+q+1)!} \\
&= -(k+2m+3)k\sum_{q=1}^{2m+1} \frac{(-1)^{q-1}((k+1)+(q-1)-1)!((k+1)+2m+1)!}{(q-1)!(2m-(q-1))!((k+1)-1)!((k+1)+(q-1)+1)!},
\end{aligned} \tag{45}$$

$$\begin{aligned}
&\sum_{q=0}^{2(m+1)} \frac{q(q-1)(-1)^q (k+q-1)!(k+2(m+1)+1)!}{q!(2(m+1)-q)!(k-1)!(k+q+1)!} \\
&= (k+1)k\sum_{q=2}^{2m+2} \frac{(-1)^{q-1}((k+2)+(q-2)-1)!((k+2)+2m+1)!}{(q-2)!(2m-(q-2))!((k+2)-1)!((k+2)+(q-2)+1)!}.
\end{aligned} \tag{46}$$

Then, from following identity

$$(2m+2-q)(2m+1-q) + 2q(2m+2-q) + q(q-1) = (2m+2)(2m+1),$$

the sum of (44), (45) and (46) is given as

$$\begin{aligned}
&(2m+2)(2m+1)\sum_{q=0}^{2(m+1)} \frac{(-1)^q (k+q-1)!(k+2(m+1)+1)!}{q!(2(m+1)-q)!(k-1)!(k+q+1)!} \\
&= \Big((k+2m+3)(k+2m+2) - 2(k+2m+3)k + (k+1)k\Big)\cdot(2m+1) \\
&= (2m+3)(2m+2)(2m+1).
\end{aligned}$$

Then, we complete the proof.

References

1. Stiefel, E.L., Scheifele, G.: Linear and regular celestial mechanics. Springer-Verlag, New York (1971)
2. Butcher, J.C. Numerical methods for ordinary differential equations, 2nd edn. Wiley, Chichester (2008)
3. Hairer, E., Nørsett, S.P., Wanner, G.: Solving ordinary differential equations, vol. I. Nonstiff Problems, Springer-Verlag, Berlin (1993)
4. Hairer, E., Lubich, C., Wanner, G.: Geometric numerical integration: structure - preserving algorithms for ordinary differential equations, 2nd edn. Springer-Verlag, Berlin, Heidelberg (2006)

5. Wu, X., You, X., Wang, B.: Structure-Preserving algorithms for oscillatory differential equations. Springer-Verlag, Berlin Heidelberg (2013)
6. Wu, X., Liu, K., Shi, W.: Structure-Preserving algorithms for oscillatory differential equations, vol. II. Springer-Verlag Berlin Heidelberg and Science Press, Beijing, China (2015)
7. Wang, B., Wu, X.: A highly accurate explicit symplectic ERKN method for multi-frequency and multidimensional oscillatory Hamiltonian systems. Numer. Algor. **65**, 705–721 (2014)
8. Li, J., Wang, B., You, X., Wu, X.: Two-step extended RKN methods for oscillatory sysems. Comput. Phys. Commun. **182**, 2486–2507 (2011)
9. Wu, X., Wang, B., Liu, K., Zhao, H.: ERKN methods for long-term integration of multidimensional orbital problems. Appl. Math. Model. **37**, 2327–2336 (2013)
10. Yang, H., Wu, X., You, X., Fang, Y.: Extended RKN-type methods for numerical integration of perturbed oscillators. Comput. Phys. Comm **180**, 1777–1794 (2009)
11. Yang, H., Zeng, X., Wu, X., Ru, Z.: A simplified Nyström-tree theory for extended Runge-Kutta-Nyström integrators solving multi-frequency oscillatory systems. Comput. Phys. Comm **185**, 2841–2850 (2014)
12. You, X., Zhao, J., Yang, H., Fang, Y., Wu, X.: Order conditions for RKN methods solving general second-order oscillatory systems. Numer. Algor. **66**, 147–176 (2014)
13. Wu, X., Wang, B., Shi, W.: Effective integrators for nonlinear second-order oscillatory systems with a time-dependent frequency matrix. Appl. Math. Model. **37**, 6505–6518 (2013)
14. Wu, X., You, X., Shi, W., Wang, B.: ERKN integrators for systems of oscillatory second-order differential equations. Comput. Phys. Commun. **181**, 1873–1887 (2010)
15. Yang, H., Wu, X.: Trigonometrically-fitted ARKN methods for perturbed oscillators. Appl. Numer. Math. **58**, 1375–1395 (2008)
16. Zeng, X., Yang, H., Wu, X.: An improved tri-colored rooted-tree theory and order conditions for ERKN methods for general multi-frequency oscillatory systems, Numerical Algorithm, proceeding
17. Brugnano, L., Iavernaro, F., Trigiante, D.: A simple framework for the derivatiion and analysis of effective one-step methods for ODEs. Appl. Math. Comput. **218**, 8475–8485 (2012)
18. Hairer, E.: Energy-preserving variant of collocation methods. J. AIAM J. Numer. Anal. Ind. Appl. Math. **5**, 73–84 (2010)
19. Wu, X., Wang, B., Shi, W.: Efficient energy-perserving integrators for oscillatory Hamiltonian systems. J. Comput. Phys. **235**, 587–605 (2013)
20. Wu, X., Wang, B., Xia, J.: Explicit symplectic multidimensional exponential fitting modified Runge-Kutta-Nyström methods. BIT **52**, 773–795 (2012)
21. Blanes, S.: Explicit symplectic RKN methods for perturbed non-autonomous oscillators: Splitting, extended and exponentially fitting methods. Comput. Phys. Commun. **193**, 10C18 (2015)
22. Hochbruck, M., Ostermann, A.: Exponential integrators. Acta Numer. **19**, 209–286 (2010)
23. Hochbruck, M., Lubich, C.: A Gautschi - type method for oscillatory second - order differential equations. Numer. Math. **83**, 403–426 (1999)
24. Hochbruck, M., Lubich, C.: Exponential integrators for quantum-classical molecular dynamics. BIT **39**, 620–645 (1999)
25. Cox, S.M., Matthews, P.C.: Exponential time differencing for stiff systems. J. Comput. Phys. **176**(2), 430–455 (2002)
26. Franco, J.M.: Exponentially fitted explicit Runge-Kutta-Nyström methods. J. Comput. Appl. Math. **167**, 1–19 (2004)
27. Berland, H., Owren, B., Skaflestad, B.: B-series and order conditions for exponential integrators. SIAM J. Numer. Anal. **43**(4), 1715–1727 (2005)
28. Wang, B., Iserles, A., Wu, X.: Arbitrary-order trigonometric Fourier collocation methods for multi-frequency oscillatory systems. Found. Comput. Math. **16**, 151–181 (2016)
29. Brugnano, L., Iavernaro, F., Trigiante, D.: Energy and Quadratic Invariants Preserving integrators based upon Gauss collocation formulae. SIAM J. Numer. Anal. **50**, 2897–2916 (2012)
30. Cohen, D., Hairer, E., Lubich, C.: Numerical energy conservation for multi-frequency oscillatory differential equations. BIT **45**, 287–305 (2005)
31. Brugnano, L., Iavernaro, F.: Line integral methods which preserve all invariants of conservative problems. J. Comput. Appl. Math. **236**, 3905–3919 (2012)
32. Feng, K., Qin, M.Z.: Symplectic geometric algorithms for Hamiltionian systems, Zhejiang Publishing United Group, Zhejiang Science and Technology Publishing House. Hangzhou and Springer-Verlag, Berlin Heidelberg (2010)

33. Sanz-Serna, J.M., Calvo, M.P.: Numerical hamiltonian problems. Chapman & Hall, 2-6 Boundary Row, London SE1 8HN, UK (1994)
34. Wang, B., Yang, H.L., Meng, F.W.: Sixth-order symplectic and symmetric explicit ERKN schemes for solving multi-frequency oscillatory nonlinear Hamiltonian equations. Calcolo **53**, 1–14 (2016). doi:10.1007/s10092-016-0179-y
35. Chen, Z., You, X., Shi, W., Liu, Z.: Symmetric and symplectic ERNK methods for oscillatory Hamiltonian systems. Comput. Phys. Comm. **183**, 86–98 (2012)
36. Shi, W., Wu, X., Xia, J.: Explicit multi-symplectic extended leap-frog methods for Hamiltonian wave equations. J. Comput. Phys. **231**, 7671–7694 (2012)
37. Wang, B., Wu, X.: A Filon-type asymptotic approach to solving highly oscillatory second-order initial value problems. J. Comput. Phys. **243**, 210–223 (2013)
38. Wang, B., Wu, X., Zhao, H.: Novel improved multifimensional Strömer-Verlet formulas with applications to four aspects in scientific computation. Math. Comput. Model. **57**, 857–872 (2013)
39. Ruth, R.D.: A canonical integration technique. IEEE Trans. Nucl. Sci. **30**, 2669–2671 (1983)
40. Qin, M.Z., Zhu, W.J.: Construction of higher order symplectic schemes by somposition. Computing **47**, 309–321 (1992)
41. Hairer, E.: Méthodes de Nyström pour l'équation différentielle $y'' = f(x, y)$. Numer. Math. **27**, 283–300 (1977)
42. Hairer, E., Wanner, G.: On the Butcher group and general multi-value methods. Comuting **13**, 1–15 (1974)
43. Hairer, E., Wanner, G.: A theory for Nyström methods. Numer. Math. **25**, 383–400 (1976)
44. Albrecht, J.: Beiträge zum Runge-Kutta-Nerfahren. ZAMM **35**, 100–110 (1955)
45. Battin, R.H.: Resolution of Runge-Kutta-Nyström condition equations through eighth order. AIAA J. **14**, 1012–1021 (1976)
46. Beentjes, P.A., Gerritsen, W.J.: Higher order Runge-Kutta methods for the numerical solution of second order differential equations without first derivatives. Report NW 34/76, Mathematical Centrum, Amsterdam (1976)
47. Hairer, E.: A one-step method of order 10 for $y'' = f(x, y)$. IMA J. Num. Anal. **2**, 83–94 (1982)
48. Qin, M.Z., Zhu, W.J.: Canonical Runge-Kutta-Nystrom (RKN) methods for second order ordinary differential equations. Comput. Math. Applic. **22**, 85–95 (1991)
49. Okunbor, D., Skeel, R.D.: Explicit canonical methods for Hamiltonian systems. Math. Comput. **59**, 439–455 (1992)
50. Okunbor, D., Skeel, R.D.: Canoncal Runge-Kutta-Nyström methods of orders 5 and 6. J. Comput. Appl. Math. **51**, 375–382 (1994)
51. Okunbor, D., Skeel, R.D.: An explicit Runge-Kutta-Nyström method is canonical if and only if its adjoint is explicit. SIAM J. Numer. Anal. **29**, 521–527 (1992)
52. Calvo, M.P., Sanz-Serna, J.M.: High-order symplectic Runge-Kutta-Nyström methods. SIAM J. Sci. Comput. **14**, 1237–1252 (1993)
53. Calvo, M.P., Sanz-Serna, J.M.: Order conditions for canonical Runge-Kutta-Nyström methods. BIT **32**, 131–142 (1992)
54. Hong, J., Jiang, S., Li, C.: Explicit multi-symplectic methods for Klein-Gordon-Schrödinger equations. J. Comput. Phys. **228**, 250–273 (2009)
55. Suris, Y.B.: The canonicity of mappings generated by Runge-Kutta type methods when integrating the systems $\ddot{x} = -\partial U/\partial x$, Xh. Vychisl. Mat. I Mat. Fiz., **29**, 202-211 (in Russian); same as U.S.S.R. Comut. Maths. Phys., **29**, 138–144
56. Tocino, A., Vigo-Aguiar, J.: Symplectic conditions for exponential fitting Runge-Kutta-Nyström methods. Math. Comput. Modell. **42**, 873–876 (2005)
57. De Vogelaere, R.: Methods of integration which preserve the contact transformation property of the Hamiltonian equations Report, vol. 4. Department of Mathematics, University of Notre Dame, India (1956)