

Chapter 6

The Construction of Arbitrary Order ERKN Integrators via Group Theory



This chapter presents the construction of arbitrary order extended Runge–Kutta–Nyström (ERKN) integrators. In general, ERKN methods are more effective than traditional Runge–Kutta–Nyström (RKN) methods in dealing with oscillatory Hamiltonian systems. However, the theoretical analysis for ERKN methods, such as the order conditions, the symplecticity conditions and the symmetric conditions, becomes much more complicated than that for RKN methods. Therefore, it is a bottleneck to construct high-order ERKN methods efficiently. This chapter first establishes the ERKN group Ω for ERKN methods and the RKN group G for RKN methods, respectively, and then shows that ERKN methods are a natural extension of RKN methods. That is, there exists an epimorphism η of the ERKN group Ω onto the RKN group G . This epimorphism gives a global insight into the structure of the ERKN group by the analysis of its kernel and the corresponding RKN group G . We also establish a particular mapping φ of G into Ω that each image element is an ideal representative element of the congruence class in Ω . Furthermore, an elementary theoretical analysis shows that this mapping φ can preserve many structure-preserving properties, such as the order, the symmetry and the symplecticity. From the epimorphism η together with its section φ , we may gain knowledge about the structure of the ERKN group Ω through the RKN group G .

6.1 Introduction

We are concerned in this chapter with initial value problems (IVP) of second-order oscillatory differential equations

$$\begin{cases} y''(t) + My(t) = f(y(t)), \\ y(t_0) = y_0, \quad y'(t_0) = y'_0, \end{cases} \quad (6.1)$$

with M a (symmetric) positive semi-definite matrix and $\|M\| \gg 1$, which frequently arise in many aspects of scientific and engineering computing, such as celestial mechanics, theoretical physics, chemistry and electronics. Effective numerical methods for solving this type of problems are of great importance (see, e.g. [4, 7–10, 13, 14]). Using the oscillatory structure introduced by the linear term My in (6.1), Yang et al. [34] proposed extended Runge–Kutta–Nyström (ERKN) methods. Much research effort on ERKN methods has been made and ERKN methods show notable efficiency and higher accuracy than the traditional Runge–Kutta–Nyström (RKN) methods in dealing with (6.1) (see, e.g. [28, 29, 31, 32, 35, 36]). It is clear that (6.1) becomes a Hamiltonian system once $f(y) = -\nabla U(y)$, where $U(y)$ is a smooth potential function. The symmetric conditions and symplectic conditions for ERKN methods have also been investigated [15, 16, 25, 27, 30]. However, it is very difficult to obtain a high-order ERKN method with some important structure properties, even though the order conditions, the symmetric conditions and the symplectic conditions have been well established.

On the one hand, we have known an important property of ERKN methods, that is, when $M \rightarrow \mathbf{0}$, each ERKN method reduces to a classical RKN method. This property implies that there exists an intrinsic relation between ERKN and RKN methods. On the other hand, the structural properties such as symmetry and symplecticity of RKN methods have been studied by many authors and very useful results have been achieved [1–3, 19–21, 23, 24, 26]. Taking account of these two points, in this chapter we attempt to clarify this intrinsic relation between ERKN and RKN methods by introducing an epimorphism η from the ERKN group Ω to the RKN group G . In particular, we establish a particular mapping η from G to Ω . Consequently, the properties of ERKN methods including the order, the symmetry, and the symplecticity, are inherited from the classical RKN methods via the mapping φ .

The plan of this chapter is as follows. In Sect. 6.2 we briefly review the classical RKN methods and then construct the RKN group G . In Sect. 6.3, the theories associated with the ERKN group Ω are established. Especially, we show that there exists an epimorphism η from Ω to G . In Sect. 6.4, we address the particular mapping φ from G to Ω in detail. It turns out that this mapping preserves the order, the symplecticity, and almost the symmetry. In Sect. 6.5 we carry out some numerical experiments for the high-order structure-preserving ERKN methods derived from the theoretical analysis in Sect. 6.4. The last section is concerned with conclusions and discussions.

6.2 Classical RKN Methods and the RKN Group

This section begins with an overview of the results on classical RKN methods for second-order initial value problems

$$\begin{cases} y''(t) = f(y(t)), \\ y(t_0) = y_0, \quad y'(t_0) = y'_0, \end{cases} \quad (6.2)$$

where the right-hand-side function f does not depend on the derivative y' and time t . As is well known, to approximate this autonomous system more efficiently than with traditional Runge–Kutta (RK) methods, the so-called Runge–Kutta–Nyström (RKN) methods were proposed [18]. An s -stage classical RKN method with a stepsize h for the problem (6.2) is defined as

$$\begin{cases} Y_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^s a_{ij} f(Y_j), & i = 1, \dots, s, \\ y_{n+1} = y_n + h y'_n + h^2 \sum_{i=1}^s \bar{b}_i f(Y_i), \\ y'_{n+1} = y'_n + h \sum_{i=1}^s b_i f(Y_i), \end{cases} \tag{6.3}$$

where a_{ij}, \bar{b}_i, b_i for $i, j = 1, \dots, s$ are real constants. Usually, the RKN method (6.3) can be briefly expressed in a Butcher Tableau

$$\begin{array}{c|cc} & c_1 & a_{11} \cdots a_{1s} \\ \hline c & A & \vdots \quad \vdots \\ \hline \bar{b}^\top & c_s & a_{s1} \cdots a_{ss} \\ \hline \bar{b}^\top & & \bar{b}_1 \cdots \bar{b}_s \\ \hline & & b_1 \cdots b_s \end{array} . \tag{6.4}$$

In order to establish an RKN group conveniently, we will specify an RKN method Φ with a stepsize h by Φ_h . Then $\Phi_{\gamma h}$ and $\Phi_{\beta h}$ are regarded as two different elements once $\gamma \neq \beta$, even though they share the same coefficients. To construct a group related to RKN methods, a binary composition is needed. Similarly to Hairer and Wanner [11] in 1974, we consider the composition of two RKN methods but matching allowance for their corresponding stepsizes.

We then introduce the following definition.

Definition 6.1 Suppose that Φ_h is an s -stage RKN method defined by (6.3) for the problem (6.2), Φ'_h is called an *essential 0-stepsize* form of Φ_h if the formula for Φ'_h reads

$$\begin{cases} Y_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^s a_{ij} f(Y_j), & i = 1, \dots, s, \\ y_{n+1} = y_n + h^2 \sum_{i=1}^s \bar{b}_i f(Y_i), \\ y'_{n+1} = y'_n + h \sum_{i=1}^s b_i f(Y_i). \end{cases} \tag{6.5}$$

Accordingly, Φ_h is called an h -stepsize form of Φ'_h .

Remark 6.1 From Definition 6.1, the only difference is in the second equation compared with (6.3). This is essential. That is, the equation

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^s \bar{b}_i f(Y_i),$$

for Φ_h has been changed into

$$y_{n+1} = y_n + h^2 \sum_{i=1}^s \bar{b}_i f(Y_i),$$

in (6.5) for Φ'_h . This means that the numerical solution $(y_{n+1}, y'_{n+1}) = \Phi_h(y_n, y'_n)$ approximates the exact solution at $t_n + h$, whereas $(y_{n+1}, y'_{n+1}) = \Phi'_h(y_n, y'_n)$ can only approximate to $(y(t_n), y'(t_n))$ at t_n . It is noted that if Ψ_h is a classical RKN method, then $\Psi_{0,h}$ is just the identity I . This implies that an RKN method $\Psi_{0,h}$ with the stepsize 0 is totally different from its *essential* 0-stepsize form Ψ'_h under our new definition.

Suppose that Φ_h^1 and Φ_h^2 are two RKN methods with s_1 stages and s_2 stages, respectively. Their coefficients are respectively denoted by $c = (c_1, \dots, c_{s_1})^\top$, $b = (b_1, \dots, b_{s_1})^\top$, $\bar{b} = (\bar{b}_1, \dots, \bar{b}_{s_1})^\top$, $A = (a_{ij})_{s_1 \times s_1}$ and $c^* = (c_1^*, \dots, c_{s_2}^*)^\top$, $b^* = (b_1^*, \dots, b_{s_2}^*)^\top$, $\bar{b}^* = (\bar{b}_1^*, \dots, \bar{b}_{s_2}^*)^\top$, $A^* = (a_{kj}^*)_{s_2 \times s_2}$. We next consider the composition of $\Phi_{\gamma h}^1$ and $\Phi_{\beta h}^2$. Taking (y_0, y'_0) as the starting value at t_0 and (y_1, y'_1) as the updated value after one step, we can express the composition law of $(y_1, y'_1) = (\Phi_{\beta h}^2 \circ \Phi_{\gamma h}^1)(y_0, y'_0)$ as

$$\left\{ \begin{array}{l} Y_i = y_0 + \gamma c_i h y'_0 + \gamma^2 h^2 \sum_{j=1}^{s_1} a_{ij} f(Y_j), \quad i = 1, \dots, s_1, \\ \tilde{y}_1 = y_0 + \gamma h y'_0 + \gamma^2 h^2 \sum_{i=1}^{s_1} \bar{b}_i f(Y_i), \\ \tilde{y}'_1 = y'_0 + \gamma h \sum_{i=1}^{s_1} b_i f(Y_i), \\ \tilde{Y}_k = \tilde{y}_1 + \beta c_k^* h \tilde{y}'_1 + \beta^2 h^2 \sum_{j=1}^{s_2} a_{kj}^* f(\tilde{Y}_j), \quad k = 1, \dots, s_2, \\ y_1 = \tilde{y}_1 + \beta h \tilde{y}'_1 + \beta^2 h^2 \sum_{i=1}^{s_2} \bar{b}_i^* f(\tilde{Y}_i), \\ y'_1 = \tilde{y}'_1 + \sum_{i=1}^{s_2} \beta h b_i^* f(\tilde{Y}_i). \end{array} \right. \quad (6.6)$$

Canceling \tilde{y}_1 and \tilde{y}'_1 from (6.6), we obtain the following simplified form

$$\left\{ \begin{array}{l} Y_i = y_0 + \gamma c_i h y'_0 + h^2 \sum_{j=1}^{s_1} \gamma^2 a_{ij} f(Y_j), \quad i = 1, \dots, s_1 \\ \tilde{Y}_k = y_0 + (\gamma + \beta c_k^*) h y'_0 + h^2 \left(\sum_{j=1}^{s_1} (\gamma^2 \tilde{b}_j + \gamma \beta c_k^* b_j) f(Y_j) + \sum_{j=1}^{s_2} \beta^2 a_{kj}^* f(\tilde{Y}_j) \right), \quad k = 1, \dots, s_2 \\ y_1 = y_0 + (\gamma + \beta) h y'_0 + h^2 \left(\sum_{i=1}^{s_1} (\gamma^2 \tilde{b}_i + \gamma \beta b_i) f(Y_i) + \sum_{i=1}^{s_2} \beta^2 \tilde{b}_i^* f(\tilde{Y}_i) \right), \\ y'_1 = y'_0 + h \left(\sum_{i=1}^{s_1} \gamma b_i f(Y_i) + \sum_{i=1}^{s_2} \beta b_i^* f(\tilde{Y}_i) \right). \end{array} \right. \quad (6.7)$$

Now let us have a further discussion on the formula (6.7). If $\gamma + \beta \neq 0$, we observe that (6.7) is just an RKN method $\Psi_{(\gamma+\beta)h}$ with the stepsize $(\gamma + \beta)h$. Meanwhile, by a careful calculation the Butcher tableau of RKN method Ψ_h reads

$$\begin{array}{c|cc} \gamma c/\delta & \gamma^2 A/\delta^2 & \\ (\gamma e + \beta c^*)/\delta & \tilde{A}/\delta^2 & \beta^2 A^*/\delta^2 \\ \hline & \tilde{b}^\top/\delta^2 & \beta^2 \tilde{b}^{*\top}/\delta^2 \\ \hline & \gamma b^\top/\delta & \beta b^{*\top}/\delta \end{array}, \quad (6.8)$$

where $\delta = \gamma + \beta$, $\tilde{A}_{ij} = \gamma^2 \tilde{b}_j + \gamma \beta c_i^* b_j$, $\tilde{b}_j = \gamma^2 \tilde{b}_j + \gamma \beta b_j$ for $i = 1, \dots, s_2$, $j = 1, \dots, s_1$, and $e = (1, \dots, 1)^\top$ is the $s_2 \times 1$ vector of units. It is clear that the updated value (y_1, y'_1) just approximates the exact value at $t_0 + (\gamma + \beta)h$.

However, for the case of $\gamma + \beta = 0$, the formula (6.7) is no longer of classical RKN type. In this case, $\Phi_{\beta h}^1 \circ \Phi_{\gamma h}^1$ is just an *essential 0-stepsize* RKN method, whose corresponding *h-stepsize* form can be expressed in the following Butcher tableau

$$\begin{array}{c|cc} \gamma c & \gamma^2 A & \\ \gamma e + \beta c^* & \tilde{A} & \beta^2 A^* \\ \hline & \tilde{b}^\top & \beta^2 \tilde{b}^{*\top} \\ \hline & \gamma b^\top & \beta b^{*\top} \end{array}, \quad (6.9)$$

where \tilde{A}_{ij} and \tilde{b}_j are the same as in formula (6.8). In this case, it should be noted that $\sum_i \gamma b_i + \sum_i \beta b_i^* = 0$ when $\gamma + \beta = 0$ and $\sum_i b_i = \sum_i b_i^* = 1$. Although this case is not significant in practice, it will be indispensable in the construction of an RKN group in the remainder of this chapter.

Define

$$G_1 := \{\Phi_{\alpha h} \mid \Phi_h \text{ is a classical RKN method for } \alpha \in \mathbb{R}\},$$

$G_0 := \{\Phi'_{\alpha h} \mid \Phi'_{\alpha h} \text{ is the essential 0-stepsize form of } \Phi_{\alpha h} \text{ and } \Phi_{\alpha h} \in G_1 \text{ with } \sum_i b_i = 0\}$, and $G = G_1 \cup G_0$.

We then have the following result.

Theorem 6.1 (G, \circ, I) is a group with respect to the composition \circ and the identity I .

Proof It is clear that the composition \circ is associative, and for each element $\Theta \in G$ we certainly have $\Theta \circ I = I \circ \Theta = \Theta$. Moreover, if Φ and Ψ are two arbitrary elements in G , from the formula (6.7) and the above analysis we know that $\Phi \circ \Psi \in G$. This shows the closure property of G under the product \circ . We next show that each element in G is invertible.

For an s -stage RKN method Λ_h defined by (6.3), the existing results [19] have revealed the existence of its adjoint method Λ_h^* . If the coefficients of the adjoint method are denoted by $c^* = (c_1^*, \dots, c_s^*)^\top$, $b^* = (b_1^*, \dots, b_s^*)^\top$, $\bar{b}^* = (\bar{b}_1^*, \dots, \bar{b}_s^*)^\top$, and $A^* = (a_{ij}^*)_{s \times s}$, then they satisfy

$$\begin{cases} c_i^* = 1 - c_{s+1-i}, \\ a_{ij}^* = (1 - c_{s+1-i})b_{s+1-j} - \bar{b}_{s+1-j} + a_{s+1-i, s+1-j}, \\ \bar{b}_j^* = b_{s+1-j} - \bar{b}_{s+1-j}, \\ b_j^* = b_{s+1-j}, \end{cases} \quad (6.10)$$

for $1 \leq i, j \leq s$. Certainly Λ_h^* belongs to G , and hence $\Lambda_{-h}^* \in G$. Furthermore, from the definition of adjoint methods, we have $\Lambda_h^{-1} = \Lambda_{-h}^*$ straightforwardly. Consequently, we have $\Lambda_h^{-1} \in G$, so does its essential 0-stepsize form $\Lambda_h'^{-1}$, namely, $\Lambda_h'^{-1} \in G$. This completes the proof. \square

Remark 6.2 Here, the above way of defining an RKN group has some nonessential differences from that of the RK group defined by Hairer and Wanner [11]. These differences actually rely on the following fact. If Φ_h and Ψ_h are two different RKN methods and they are not adjoint to each other, then the composition $\Phi_h \circ \Psi_{-h}^*$ does not belong to G_1 any more. Here Ψ_h^* denotes the adjoint method of Ψ_h . That is why we have additionally introduced Definition 6.1 and the set G_0 . Likewise, it is also needed to introduce another new definition (Definition 6.2) when constructing the ERKN group in the next section.

6.3 ERKN Group and Related Issues

6.3.1 Construction of ERKN Group

In this section, we are concerned with the group-structure analysis of the efficient integrator for the oscillatory second-order initial problem (6.1). It seems that classical

RKN methods could still be applied to these problems as numerical integrators, since one may move the term My from the left-hand side to the right-hand side of the differential equation and then the problem (6.1) can be also transformed to the type of (6.2). However, when $\|M\| \gg 1$, RKN methods may not be very effective methods for solving (6.1) and show bad numerical behavior. This is mainly caused by the highly oscillatory effect introduced by the linear term My . Taking account of this point, the extended Runge–Kutta–Nyström (ERKN) methods were proposed and designed especially for the oscillatory problem (6.1).

Based on the matrix-variation-of-constants formula [33], an s -stage ERKN method [34] for IVP (6.1) is defined by

$$\begin{cases} Y_i = \phi_0(c_i^2 V)y_n + c_i h \phi_1(c_i^2 V)y'_n + h^2 \sum_{j=1}^s a_{ij}(V)f(Y_j), & i = 1, \dots, s, \\ y_{n+1} = \phi_0(V)y_n + h \phi_1(V)y'_n + h^2 \sum_{i=1}^s \bar{b}_i(V)f(Y_i), \\ y'_{n+1} = -hM\phi_1(V)y_n + \phi_0(V)y'_n + h \sum_{i=1}^s b_i(V)f(Y_i). \end{cases} \quad (6.11)$$

Here, c_1, \dots, c_s are real constants, $b_i(V)$, $\bar{b}_i(V)$ and $a_{ij}(V)$ for $i, j = 1, \dots, s$ are matrix-valued functions of $V \equiv h^2 M$ which are usually expressed in formal series in terms of V

$$b_i(V) = \sum_{k=0}^{\infty} \frac{b_i^{(2k)}}{(2k)!} V^k, \quad \bar{b}_i(V) = \sum_{k=0}^{\infty} \frac{\bar{b}_i^{(2k)}}{(2k)!} V^k, \quad a_{ij}(V) = \sum_{k=0}^{\infty} \frac{a_{ij}^{(2k)}}{(2k)!} V^k, \quad (6.12)$$

and

$$\phi_j(V) := \sum_{k=0}^{\infty} \frac{(-1)^k V^k}{(2k+j)!}, \quad j = 0, 1, \dots \quad (6.13)$$

The properties related to $\phi_j(V)$ for $j = 0, 1, \dots$ can be found in [31] and the details are omitted here. We can also express the ERKN method (6.11) in a Butcher tableau

$$\begin{array}{c|ccc} & c_1 & \dots & a_{1s}(V) \\ \hline c & A(V) & \vdots & \vdots \\ \hline & \bar{b}(V)^{\top} & = c_s & a_{s1}(V) \dots a_{ss}(V) \\ \hline & \bar{b}(V)^{\top} & & \bar{b}_1(V) \dots \bar{b}_s(V) \\ \hline & & & b_1(V) \dots b_s(V) \end{array} \quad (6.14)$$

Proceeding in the same spirit as for RKN methods, we also introduce a new definition for ERKN methods as follows.

Definition 6.2 Suppose that Ψ_h is an s -stage ERKN method defined by (6.11) for the problem (6.1), Ψ'_h is called *essential 0-stepsiz*e form of Ψ_h if the formula for Ψ'_h reads

$$\left\{ \begin{array}{l} Y_i = \phi_0(c_i^2 V)y_n + c_i h \phi_1(c_i^2 V)y'_n + h^2 \sum_{j=1}^s a_{ij}(V)f(Y_j), \quad i = 1, \dots, s, \\ y_{n+1} = y_n + h^2 \sum_{i=1}^s \bar{b}_i(V)f(Y_i), \\ y'_{n+1} = y'_n + h \sum_{i=1}^s b_i(V)f(Y_i). \end{array} \right. \quad (6.15)$$

Then Ψ_h is called an h -stepsize form of Ψ'_h .

Suppose that Υ_h^1 and Υ_h^2 are two ERKN methods with s_1 stages and s_2 stages, respectively. The coefficients of Υ_h^1 are denoted as (c, b, \bar{b}, A) , and those of Υ_h^2 are additionally denoted with a star $(c^*, b^*, \bar{b}^*, A^*)$. We now consider the composition of $\Upsilon_{\gamma h}^1$ and $\Upsilon_{\beta h}^2$. After a careful calculation, we derive the scheme $\Upsilon_{\beta h}^2 \circ \Upsilon_{\gamma h}^1$ as follows

$$\left\{ \begin{array}{l} Y_i = \phi_0(\gamma^2 c_i^2 V)y_0 + \gamma c_i h \phi_1(\gamma^2 c_i^2 V)y'_0 + h^2 \sum_{j=1}^{s_1} \gamma^2 A_{ij}(\gamma^2 V)f(Y_j), \quad i = 1, \dots, s_1, \\ \tilde{Y}_k = \phi_0((\gamma + \beta c_k^*)^2 V)y_0 + (\gamma + \beta c_k^*)h \phi_1((\gamma + \beta c_k^*)^2 V)y'_0 \\ \quad + h^2 \left(\sum_{j=1}^{s_1} (\gamma^2 \bar{b}_j(\gamma^2 V)\phi_0(\beta^2 c_k^{*2} V) + \gamma \beta c_k^* b_j(\gamma^2 V)\phi_1(\beta^2 c_k^{*2} V))f(Y_j) \right. \\ \quad \left. + \sum_{j=1}^{s_2} \beta^2 A_{kj}^*(\beta^2 V)f(\tilde{Y}_j) \right), \quad k = 1, \dots, s_2, \\ y_1 = \phi_0((\gamma + \beta)^2 V)y_0 + (\gamma + \beta)h \phi_1((\gamma + \beta)^2 V)y'_0 \\ \quad + h^2 \left(\sum_{j=1}^{s_1} (\gamma^2 \bar{b}_j(\gamma^2 V)\phi_0(\beta^2 V) + \gamma \beta b_j(\gamma^2 V)\phi_1(\beta^2 V))f(Y_j) + \sum_{i=1}^{s_2} \beta^2 \bar{b}_i^*(\beta^2 V)f(\tilde{Y}_i) \right), \\ y'_1 = -(\gamma + \beta)h M \phi_1((\gamma + \beta)^2 V)y_0 + \phi_0((\gamma + \beta)^2 V)y'_0 \\ \quad + h \left(\sum_{j=1}^{s_1} (-\gamma^2 \beta V \bar{b}_j(\gamma^2 V)\phi_1(\beta^2 V) + \gamma \beta b_j(\gamma^2 V)\phi_0(\beta^2 V))f(Y_j) + \sum_{i=1}^{s_2} \beta b_i(\beta^2 V)f(\tilde{Y}_i) \right). \end{array} \right.$$

For the case $\gamma + \beta \neq 0$, gives that the composition $\Upsilon_{\beta h}^2 \circ \Upsilon_{\gamma h}^1$ indicates a new $\Upsilon_{\delta h}$, namely, an $(s_1 + s_2)$ -stage ERKN method with the stepsize $\delta h = (\gamma + \beta)h$, and Butcher tableau

$$\begin{array}{c|cc}
\gamma c/\delta & \gamma^2 A(\gamma^2/\delta^2 V)/\delta^2 & \\
(\gamma e + \beta c^*)/\delta & \bar{A}(V/\delta^2)/\delta^2 & \beta^2 A^*(\beta^2/\delta^2 V)/\delta^2 \\
\hline
& \bar{B}^\top(V/\delta^2)/\delta^2 & \beta^2 \bar{b}^{*\top}(\beta^2/\delta^2 V)/\delta^2 \\
& B^\top(V/\delta^2)/\delta & \beta b^{*\top}(\beta^2/\delta^2 V)/\delta
\end{array}, \quad (6.16)$$

where

$$\begin{cases}
\bar{A}_{ij}(V) = \gamma^2 \bar{b}_j(\gamma^2 V) \phi_0(\beta^2 c_i^{*2} V) + \gamma \beta c_i^* b_j(\gamma^2 V) \phi_1(\beta^2 c_i^{*2} V), \\
\bar{B}_j(V) = \gamma^2 \bar{b}_j(\gamma^2 V) \phi_0(\beta^2 V) + \gamma \beta b_j(\gamma^2 V) \phi_1(\beta^2 V), \\
B_j(V) = -\gamma^2 \beta V \bar{b}_j(\gamma^2 V) \phi_1(\beta^2 V) + \gamma b_j(\gamma^2 V) \phi_0(\beta^2 V),
\end{cases} \quad (6.17)$$

for $i = 1, \dots, s_2$, $j = 1, \dots, s_1$.

If $\gamma + \beta = 0$, the composition $\Upsilon' = \Upsilon_{\beta h}^2 \circ \Upsilon_{\gamma h}^1$ is also *essential 0-stepsize*, whose corresponding *h-stepsize* form can be expressed in the following Butcher tableau

$$\begin{array}{c|cc}
\gamma c & \gamma^2 A(\gamma^2 V) & \\
\gamma e + \beta c^* & \bar{A}(V) & \beta^2 A^*(\beta^2 V) \\
\hline
& \bar{B}^\top(V) & \beta^2 \bar{b}^{*\top}(\beta^2 V) \\
& B^\top(V) & \beta b^{*\top}(\beta^2 V)
\end{array}, \quad (6.18)$$

where $\bar{A}_{ij}(V)$, $\bar{B}_j(V)$, $B_j(V)$ have the same expression as (6.17) with $\sum_i \gamma b_i^{(0)} + \sum_i \beta b_i^{*(0)} = 0$.

Define

$$\Omega_1 := \{\Phi_{\alpha h} \mid \Phi_h \text{ is an ERKN method for } \alpha \in \mathbb{R}\},$$

$\Omega_0 := \{\Phi'_{\alpha h} \mid \Phi'_{\alpha h} \text{ is the essential 0-stepsize form of } \Phi_{\alpha h}, \Phi_{\alpha h} \in \Omega_1 \text{ with } \sum_i b_i^{(0)} = 0\}$, and $\Omega = \Omega_1 \cup \Omega_0$.

Then we have the following theorem.

Theorem 6.2 (Ω, \circ, I) is a group with respect to the composition \circ and the identity I .

The proof is similar to that of Theorem 6.1, except that the coefficients of the adjoint method of (6.11) can be expressed as

$$\begin{cases}
c_i^* = 1 - c_{s+1-i}, \\
a_{ij}^*(V) = \phi_0(c_{s+1-i}^2 V) \bar{b}_j(V) - c_{s+1-i} \phi_1(c_{s+1-i}^2 V) b_j(V) + a_{s+1-i, s+1-j}(V), \\
\bar{b}_j^*(V) = \phi_1(V) b_{s+1-j}(V) - \phi_0(V) \bar{b}_{s+1-j}(V), \\
b_j^*(V) = V \phi_1(V) \bar{b}_{s+1-j}(V) + \phi_0(V) b_{s+1-j}(V),
\end{cases} \quad (6.19)$$

for $1 \leq i, j \leq s$. Hence, we omit the details here.

6.3.2 The Relation Between the RKN Group G and the ERKN Group Ω

In the previous sections, we have established the RKN group (G, \circ, I) and the ERKN group (Ω, \circ, I) . A direct observation shows that when $M \rightarrow \mathbf{0}$, the oscillatory problem (6.1) becomes the traditional second-order initial value problem (6.2), and the ERKN method (6.11) hence reduces to the RKN method (6.3). This point indicates that there exists an inherent relationship between RKN methods and ERKN methods. Thus, ERKN methods are usually regarded as an extension of RKN methods. In the following, we will rigorously demonstrate this extension relationship.

In what follows, we will denote the coefficients of an RKN method in lower-case by (c, b, \bar{b}, a) and those of an ERKN method in upper-case by (C, B, \bar{B}, A) . As ERKN methods depend on the matrix M , for each element $\Psi \in \Omega$ we will denote it as $\Psi(M)$ to show this relevance if necessary. Then the word *reduces* can be defined as a map

$$\eta : \Omega \longrightarrow G, \quad \eta(\Psi) = \lim_{M \rightarrow \mathbf{0}} \Psi(M), \quad \forall \Psi \in \Omega.$$

As a continuation, we arrive at the following useful theorem.

Theorem 6.3 *The map η is an epimorphism of the group Ω onto the group G .*

Proof Suppose that Ψ^1 and Ψ^2 are two elements of Ω respectively with the stepsizes γh and βh , $\Phi^1 = \eta(\Psi^1)$, and $\Phi^2 = \eta(\Psi^2)$. From the composition laws (6.8) and (6.9) of RKN methods and those of ERKN methods (6.16) and (6.18), it can be easily verified that $\eta(\Psi^2 \circ \Psi^1) = \Phi^2 \circ \Phi^1 = \eta(\Psi^2) \circ \eta(\Psi^1)$. In addition, from the fact that $\eta(I) = I$, we conclude that η is a homomorphism of Ω into G .

We next show that η is surjective. For each element $\Phi \in G$, which is denoted by the coefficients (c, b, \bar{b}, a) , there exists $\Psi \in \Omega$, whose coefficients can be expressed as

$$C = c, \quad B(V) = b \otimes E_n, \quad \bar{B}(V) = \bar{b} \otimes E_n, \quad A(V) = a \otimes E_n, \quad (6.20)$$

where \otimes is the Kronecker product, E_n is an $n \times n$ identity matrix and n is the dimension of square matrix M . Obviously the coefficients (C, B, \bar{B}, A) define an element in Ω , and thus η is surjective. This completes the proof. \square

Corollary 6.1 *Let K be the kernel of η , i.e. $K = \eta^{-1}(I)$, then K is a normal subgroup of Ω . Moreover, the induced map $\bar{\eta}$ is an isomorphism of the quotient group $\bar{\Omega} = \Omega/K$ onto the group G .*

Theorem 6.3 actually gives a global view of ERKN methods by connecting them with classical RKN methods via the epimorphism map η . From Corollary 6.1, the map η defines a congruence relation \equiv by the normal subgroup K , where

$$\Phi \equiv \Psi \pmod{K} \quad \text{if} \quad \Phi^{-1} \circ \Psi \in K.$$

Then by finding a representative element Ψ for each congruence class $\bar{\Psi} \in \bar{\Omega}$, we can theoretically give all the elements in $\bar{\Psi}$, since for each $\Theta \in \bar{\Psi}$ there exists $\Gamma \in K$ such that $\Theta = \Psi \circ \Gamma$. This fact indicates that $\bar{\Psi}$ is the coset of Ψ relative to K , i.e. $\bar{\Psi} = \Psi \circ K$. Hence it only remains to describe the normal subgroup K in detail. This can be easily obtained from the following definition of K

$$K = \{ \Psi \in \Omega_0 | b_j^{(0)} = 0 \text{ and } \bar{b}_j^{(0)} = 0, \forall j \}.$$

6.4 A Particular Mapping of G into Ω

In Sect. 6.3, we have investigated the ERKN group as a whole. However, as mentioned in the previous section, we can just have a theoretical description for each congruence class $\bar{\Psi} \in \bar{\Omega}$, and this is not associated with the important properties of the method, such as the symplecticity, the symmetry and the order. Recalling Corollary 6.1 again, and taking account of the fact that $\bar{\Psi} = \Psi \circ K$, it is of great importance to select a representative element Ψ with favourable properties for the congruence class $\bar{\Psi}$, even though we cannot give a detailed analysis for each element in $\bar{\Psi}$.

Meanwhile, because $\eta(\bar{\Psi}) = \Phi \in G$, Φ inherits all the advantages of the ERKN elements in $\bar{\Psi}$. Hence all the ERKN elements in $\bar{\Psi}$ cannot have better structural properties than the reduced RKN element Φ . Taking account of this point, we may find this appropriate representative element Ψ with the help of the corresponding reduced RKN element Φ . In fact, what we are considering is to find a normal mapping φ from G into Ω , so that $\varphi(\Phi)$ can preserve as many properties as the original RKN method Φ does. A direct result about the potential mapping φ is that it should be the section of η . That is, the composition $\eta \circ \varphi = I$ is the identity on G . In this sense, the underlying mapping defined by (6.20) may be a straightforward candidate for φ . Unfortunately, most properties cannot be preserved in this easy way, and we have to reconsider a proper mapping φ .

From the variation-of-constants formula (see, e.g. [31, 32]) for the problem (6.2) and the problem (6.1), as well as the corresponding RKN method for (6.2) and ERKN integrator (6.11), we consider the following mapping:

$$\varphi : G \longrightarrow \Omega, \quad \begin{array}{c|c} c & a \\ \hline & \bar{b}^\top \\ \hline & b^\top \end{array} \longmapsto \begin{array}{c|c} C & A(V) \\ \hline & \bar{B}(V)^\top \\ \hline & B(V)^\top \end{array}, \quad (6.21)$$

where

$$\begin{cases} C_i = c_i, \\ A_{ij}(V) = a_{ij} \phi_1((c_i - c_j)^2 V), \\ \bar{B}_i(V) = \bar{b}_i \phi_1((1 - c_i)^2 V), \\ B_i(V) = b_i \phi_0((1 - c_i)^2 V), \end{cases}$$

for $1 \leq i, j \leq s$ and s is the stage of the RKN method. This mapping naturally maps a classical RKN method Φ to an ERRK method $\varphi(\Phi)$. Meanwhile, being a representative element for the congruence class $\overline{\varphi(\Phi)}$, we will show by the following several theorems that $\varphi(\Phi)$ almost preserves all the properties that the original RKN method Φ has.

Theorem 6.4 *If $\Phi \in G$ is symplectic, then $\varphi(\Phi) \in \Omega$ is symplectic.*

Proof From the definition of G , it is needed to verify that the result holds for all RKN methods. Hence we can suppose that Φ is an s -stage symplectic RKN method. The results from Suris [26] and Okunbor and Skeel [19] show that the coefficients of Φ should satisfy the following symplectic conditions:

$$\begin{cases} \bar{b}_i = (1 - c_i)b_i, & 1 \leq i \leq s, \\ \bar{b}_i b_j + b_i a_{ij} = \bar{b}_j b_i + b_j a_{ji}, & 1 \leq i, j \leq s. \end{cases} \quad (6.22)$$

We next show that the ERKN method $\varphi(\Phi)$, whose coefficients $C, A(V), \bar{B}(V), B(V)$ defined by (6.21), is symplectic. Although there is no sufficient and necessary conditions for the symplecticity of ERKN methods, we will prove that $\varphi(\Phi)$ satisfies the following conditions:

$$\begin{cases} \phi_0(V)B_i(V) + V\phi_1(V)\bar{B}_i(V) = d_i\phi_0(c_i^2V), & d_i \in \mathbb{R}, i = 1, 2, \dots, s, \\ \phi_1(V)B_i(V) - \phi_0(V)\bar{B}_i(V) = c_i d_i \phi_1(c_i^2V), & i = 1, 2, \dots, s, \\ \bar{B}_i B_j + d_i A_{ij} = \bar{B}_j B_i + d_j A_{ji}, & i, j = 1, 2, \dots, s, \end{cases} \quad (6.23)$$

which are sufficient conditions for symplectic ERKN methods originally proposed by Wu et al. [30].

The equations $\bar{B}_i(V) = \bar{b}_i \phi_1((1 - c_i)^2 V)$ and $B_i(V) = b_i \phi_0((1 - c_i)^2 V)$ exactly give the first two equations of (6.23), with $d_i = b_i$. Then, inserting the expression of $A(V), \bar{B}(V), B(V)$ into the the third equation of (6.23), we obtain

$$\begin{aligned} & \bar{B}_i B_j + d_i A_{ij} - (\bar{B}_j B_i + d_j A_{ji}) \\ &= (1 - c_i)b_i b_j \phi_1((1 - c_i)^2 V)\phi_0((1 - c_j)^2 V) + b_i a_{ij} \phi_1((c_i - c_j)^2 V) \\ & \quad - ((1 - c_j)b_j b_i \phi_1((1 - c_j)^2 V)\phi_0((1 - c_i)^2 V) + b_j a_{ji} \phi_1((c_i - c_j)^2 V)) \\ &= (b_i b_j (c_j - c_i) + b_i a_{ij} - b_j a_{ji}) \phi_1((c_i - c_j)^2 V) \\ &= 0. \end{aligned}$$

The last equation directly follows from (6.22). This completes the proof. \square

Theorem 6.5 *If $\Phi \in G$ is symmetric and the coefficients satisfy the simplifying assumption $\bar{b}_i = b_i(1 - c_i)$, then $\varphi(\Phi) \in \Omega$ is symmetric.*

Proof Similarly to Theorem 6.4, we only need to verify the case that Φ is an s -stage RKN method. Hence, we need to derive the symmetric conditions of ERKN methods [16, 27]

$$\begin{cases} c_i = 1 - c_{s+1-i}, \\ A_{ij}(V) = \phi_0(c_{s+1-i}^2 V) \bar{B}_j(V) - c_{s+1-i} \phi_1(c_{s+1-i}^2 V) B_j(V) + A_{s+1-i, s+1-j}(V), \\ \bar{B}_j(V) = \phi_1(V) B_{s+1-j}(V) - \phi_0(V) \bar{B}_{s+1-j}(V), \\ B_j(V) = V \phi_1(V) \bar{B}_{s+1-j}(V) + \phi_0(V) B_{s+1-j}(V), \end{cases} \quad (6.24)$$

from the symmetric conditions of RKN methods [12],

$$\begin{cases} c_i = 1 - c_{s+1-i}, \\ a_{ij} = (1 - c_{s+1-i}) b_{s+1-j} - \bar{b}_{s+1-j} + a_{s+1-i, s+1-j}, \\ \bar{b}_j = b_{s+1-j} - \bar{b}_{s+1-j}, \\ b_j = b_{s+1-j}. \end{cases} \quad (6.25)$$

The first equation of (6.24) naturally holds. On noting that $b_j = b_{s+1-j}$ and $\bar{b}_j = b_j(1 - c_j)$, we have

$$\begin{aligned} & \phi_1(V) B_{s+1-j} - \phi_0(V) \bar{B}_{s+1-j} \\ &= b_{s+1-j} \phi_1(V) \phi_0((1 - c_{s+1-j})^2 V) - b_{s+1-j} (1 - c_{s+1-j}) \phi_0(V) \phi_1((1 - c_{s+1-j})^2 V) \\ &= b_j \phi_1(V) \phi_0(c_j^2 V) - b_j c_j \phi_1(V) \phi_0(c_j^2 V) \\ &= b_j (1 - c_j) \phi_1((1 - c_j)^2 V) \\ &= \bar{B}_j(V), \end{aligned}$$

and

$$\begin{aligned} & V \phi_1(V) \bar{B}_{s+1-j} + \phi_0(V) B_{s+1-j} \\ &= b_{s+1-j} (1 - c_{s+1-j}) V \phi_1(V) \phi_1((1 - c_{s+1-j})^2 V) + b_{s+1-j} \phi_0(V) \phi_0((1 - c_{s+1-j})^2 V) \\ &= b_j (c_j V \phi_1(V) \phi_1(c_j^2 V) + \phi_0(V) \phi_0(c_j^2 V)) \\ &= b_j \phi_0((1 - c_j)^2 V) \\ &= B_j(V). \end{aligned}$$

These give the third and fourth equations of (6.24). Furthermore, it follows from (6.25) and the simplifying assumption $a_{ij} = b_j(c_i - c_j) + a_{s+1-i, s+1-j}$. We thus have

$$\begin{aligned} & \phi_0(c_{s+1-i}^2 V) \bar{B}_j(V) - c_{s+1-i} \phi_1(c_{s+1-i}^2 V) B_j(V) + A_{s+1-i, s+1-j}(V) \\ &= b_j (1 - c_j) \phi_0((1 - c_i)^2 V) \phi_1((1 - c_j)^2 V) - b_j (1 - c_i) \phi_1((1 - c_i)^2 V) \phi_0((1 - c_j)^2 V) \\ & \quad + a_{s+1-i, s+1-j} \phi_1((c_i - c_j)^2 V) \\ &= (b_j(c_i - c_j) + a_{s+1-i, s+1-j}) \phi_1((c_i - c_j)^2 V), \\ &= a_{ij} \phi_1((c_i - c_j)^2 V) \\ &= A_{ij}(V), \end{aligned}$$

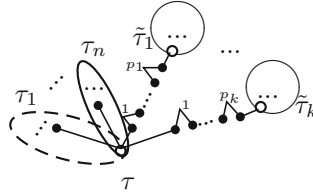


Fig. 6.1 Figure of tree $\tau = \tau_1 \times \tau_2 \times \dots \times \tau_n \times (W_+ b_+ (b_+ B_+)^{p_1} (\tilde{\tau}_1)) \times \dots \times (W_+ b_+ (b_+ B_+)^{p_k} (\tilde{\tau}_k))$

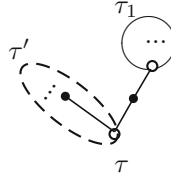


Fig. 6.2 Figure of tree $\tau = (W_+ b_+ (b_+ B_+)^0 (\tau_1)) \times \tau'$

and consequently the second equation of (6.24) is satisfied. This completes the proof. \square

Remark 6.3 Although the condition $\bar{b}_i = b_i(1 - c_i)$ required by Theorem 6.5, looks like an additional simplifying condition, in fact this assumption is already contained in the symplectic conditions for RKN methods in Theorem 6.4.

The following theorem is related to the order of a numerical method and the corresponding order conditions. Hence it seems plausible to gain some knowledge of special Nyström tree (SNT) and simplified special extended Nyström tree (SSENT), which is respectively designed to deal with order conditions of RKN and ERKN methods. Further details concerning SNT and SSENT can be found in [12, 35]. For the convenience of the proof, we introduce the following two definitions and a basic lemma, which will be used in the proof of the theorem later.

Definition 6.3 The degree of merge node $d(\tau)$ on SSENT are recursively defined as follows.

1. $d(\tau) = 0$, if $\tau \in SNT$;
2. $d(\tau) = k + \sum_{j=1}^n d(\tau_j) + \sum_{i=1}^k d(\tilde{\tau}_i)$, if $\tau = \tau_1 \times \tau_2 \times \dots \times \tau_n \times (W_+ b_+ (b_+ B_+)^{p_1} (\tilde{\tau}_1)) \times \dots \times (W_+ b_+ (b_+ B_+)^{p_k} (\tilde{\tau}_k))$ and $\tau_i, \tilde{\tau}_j \in SSENT, p_i \in \mathbb{N}_+$ (see Fig. 6.1).

Definition 6.4 If $\tau = (W_+ b_+ (b_+ B_+)^0 (\tau_1)) \times \tau'$ (see Fig. 6.2), then we define τ_1 to be the first generation of τ . We recursively define that τ_n is the n th ($n \geq 2$) generation of τ , if there exists $\tau_0 \in SSENT$ that τ_n is the first generation of τ_0 and τ_0 is the $(n - 1)$ th generation of τ .

Lemma 6.1 *If $\tau = \tau_1 \times \tau_2$, $\tau_1, \tau_2 \in SSENT$, then the order $\rho(\tau)$, the sign $s(\tau)$, the density $\gamma(\tau)$, and the weight $\Phi_i(\tau)$ satisfy*

$$\begin{aligned} \rho(\tau) &= \rho(\tau_1) + \rho(\tau_2) - 1, & s(\tau) &= s(\tau_1) \cdot s(\tau_2), \\ \gamma(\tau) &= \rho(\tau) \cdot \frac{\gamma(\tau_1)}{\rho(\tau_1)} \cdot \frac{\gamma(\tau_2)}{\rho(\tau_2)}, & \Phi_i(\tau) &= \Phi_i(\tau_1) \cdot \Phi_i(\tau_2). \end{aligned} \quad (6.26)$$

This lemma can be directly obtained from the definition of order, density and sign of an SSENT tree. Hence, we omit the remaining details of the proof here.

Theorem 6.6 *If $\Psi \in G$ is of order p ($p \geq 1$), then $\varphi(\Psi) \in \Omega$ is also of order p .*

Proof Suppose that Ψ is an s -stage RKN method. The theorem can be stated as follows.

If the order conditions [12]

$$\begin{cases} \sum_{i=1}^s \bar{b}_i \Phi_i(\tau) = \frac{1}{(\rho(\tau) + 1)\gamma(\tau)}, & \forall \tau \in SNT_m, \quad m \leq p - 1, \\ \sum_{i=1}^s b_i \Phi_i(\tau) = \frac{1}{\gamma(\tau)}, & \forall \tau \in SNT_m, \quad m \leq p, \end{cases} \quad (6.27)$$

hold for Ψ , then the order conditions [35]

$$\begin{cases} \sum_{i=1}^s \bar{B}_i \Phi_i(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)s(\tau)} \phi_{\rho(\tau)+1} + \mathcal{O}(h^{p-\rho(\tau)}), & \forall \tau \in SSENT_m, \quad m \leq p - 1, \\ \sum_{i=1}^s B_i \Phi_i(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)s(\tau)} \phi_{\rho(\tau)} + \mathcal{O}(h^{p-\rho(\tau)+1}), & \forall \tau \in SSENT_m, \quad m \leq p, \end{cases} \quad (6.28)$$

also hold for $\varphi(\Psi)$ under the mapping (6.21).

We will prove this theorem by induction. To this end, the degree of merge node $d(\tau)$ is used as an indicator. To show this in detail, we split the proof in two parts with $d(\tau) = 0$ and $d(\tau) > 0$ for all $\tau \in SSENT$. As stated in [35], we should first note that SNT is in fact a subset of SSENT. In the first part of the proof we will show that for each $\tau \in SNT$, i.e. $d(\tau) = 0$, the statement of (6.28) holds.

Noting that $s(\tau) = 1$ holds for all $\tau \in SNT$, we can rewrite (6.28) as an equivalent form

$$\begin{cases} \sum_{i=1}^s \bar{B}_i^{(2l)} \Phi_i(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)} \frac{(-1)^l (2l)!}{(\rho(\tau) + 1 + 2l)!}, & \forall \tau \in SNT_m, \quad 2l \leq p - m - 2, \\ \sum_{i=1}^s B_i^{(2l)} \Phi_i(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)} \frac{(-1)^l (2l)!}{(\rho(\tau) + 2l)!}, & \forall \tau \in SNT_m, \quad 2l \leq p - m - 1, \end{cases} \quad (6.29)$$

with the definitions of matrix-valued functions (6.12–6.13). Furthermore, taking account of the mapping (6.21) and (6.12–6.13), we obtain the following equations


$$\begin{cases} A_{ij}^{(2k)} = a_{ij}(c_i - c_j)^k \frac{(-1)^k}{2k + 1}, \\ \bar{B}_j^{(2k)} = \bar{b}_j(1 - c_j)^k \frac{(-1)^k}{2k + 1}, \\ B_j^{(2k)} = b_j(1 - c_j)^k (-1)^k, \end{cases} \quad (6.30)$$

for the constants $A_{ij}^{(2k)}$, $B_j^{(2k)}$, $\bar{B}_j^{(2k)}$ by comparing the corresponding coefficients of each term V^k . Inserting the new expressions of (6.30) into (6.29) gives

$$\begin{cases} \sum_{i=1}^s \bar{b}_i(1 - c_i)^{2l} \Phi_i(\tau) = \frac{1}{\gamma(\tau)} \frac{\rho(\tau)!(2l + 1)!}{(\rho(\tau) + 1 + 2l)!}, \quad \forall \tau \in SNT_m, \quad m + 2l + 1 \leq p - 1, \\ \sum_{i=1}^s b_i(1 - c_i)^{2l} \Phi_i(\tau) = \frac{1}{\gamma(\tau)} \frac{\rho(\tau)!(2l)!}{(\rho(\tau) + 2l)!}, \quad \forall \tau \in SNT_m, \quad m + 2l + 1 \leq p. \end{cases} \quad (6.31)$$

This means that we only need show the correctness of (6.31) instead of (6.28).

Noting that $\Phi_i(\tau)$ is the weight of SNT tree τ , then $c_i^k \Phi_i(\tau)$ will be the weight of

a new SNT tree $\tau' = \tau_0 \times \tau$, where $\tau_0 =$  .

Considering Lemma 6.1, and noting that $\gamma(\tau_0) = \rho(\tau_0) = k + 1$, we then have

$$\rho(\tau') = \rho(\tau) + k, \quad \gamma(\tau') = \rho(\tau) \cdot \frac{\gamma(\tau)}{\rho(\tau_0)} \cdot \frac{\gamma(\tau)}{\rho(\tau_0)} = \gamma(\tau) \frac{\rho(\tau) + k}{\rho(\tau)}, \quad \Phi_i(\tau') = c_i^k \Phi_i(\tau). \quad (6.32)$$

For any $k \leq 2l$, it can be deduced that $k + \rho(\tau) \leq p$, i.e. $\rho(\tau') \leq p$. Thus, together with the order conditions (6.27) for the special SNT tree τ' and (6.32), the following equations

$$\begin{cases} \sum_{i=1}^s \bar{b}_i(c_i^k \Phi_i(\tau)) = \frac{\rho(\tau)}{\gamma(\tau)(\rho(\tau) + k)(\rho(\tau) + k + 1)}, \quad \forall \tau \in SNT_m, \quad m + k + 1 \leq p - 1, \\ \sum_{i=1}^s b_i(c_i^k \Phi_i(\tau)) = \frac{\rho(\tau)}{\gamma(\tau)(\rho(\tau) + k)}, \quad \forall \tau \in SNT_m, \quad m + k + 1 \leq p. \end{cases} \quad (6.33)$$

are satisfied. Multiplying by $(-1)^k C_{2l}^k$ the two sides of (6.33) and summing over k from 0 to $2l$, we obtain

$$\left\{ \begin{aligned} \sum_{k=0}^{2l} (-1)^k C_{2l}^k \sum_{i=1}^s \bar{b}_i (c_i^k \Phi_i(\tau)) &= \sum_{i=1}^s \bar{b}_i (1 - c_i)^{2l} \Phi_i(\tau) \\ &= \sum_{k=0}^{2l} (-1)^k C_{2l}^k \frac{\rho(\tau)}{\gamma(\tau)(\rho(\tau) + k)(\rho(\tau) + k + 1)}, \\ \sum_{k=0}^{2l} (-1)^k C_{2l}^k \sum_{i=1}^s b_i (c_i^k \Phi_i(\tau)) &= \sum_{i=1}^s b_i (1 - c_i)^{2l} \Phi_i(\tau) \\ &= \sum_{k=0}^{2l} (-1)^k C_{2l}^k \frac{\rho(\tau)}{\gamma(\tau)(\rho(\tau) + k)}. \end{aligned} \right. \quad (6.34)$$

Comparing (6.31) with (6.34), it can be concluded that if the two conditions,

$$\left\{ \begin{aligned} \sum_{k=0}^{2l} (-1)^k C_{2l}^k \frac{\rho(\tau)}{(\rho(\tau) + k)(\rho(\tau) + k + 1)} &= \frac{\rho(\tau)!(2l + 1)!}{(\rho(\tau) + 1 + 2l)!} \\ \sum_{k=0}^{2l} (-1)^k C_{2l}^k \frac{\rho(\tau)}{(\rho(\tau) + k)} &= \frac{\rho(\tau)!(2l)!}{(\rho(\tau) + 2l)!}, \end{aligned} \right. \quad (6.35)$$

hold for any $\rho(\tau) \leq p$, the Eq. (6.31) will be satisfied. Here C_{2l}^k denotes the binomial coefficient $\frac{(2l)!}{k!(2l-k)!}$. It is clear that (6.35) is just a special case of the two identical equations

$$\left\{ \begin{aligned} \sum_{k=0}^{2l} (-1)^k C_{2l}^k \frac{n}{(n+k)(n+k+1)} &= \frac{n!(2l+1)!}{(n+1+2l)!}, \quad \forall n \in \mathbb{N}_+, \\ \sum_{k=0}^{2l} (-1)^k C_{2l}^k \frac{n}{(n+k)} &= \frac{n!(2l)!}{(n+2l)!}, \quad \forall n \in \mathbb{N}_+. \end{aligned} \right. \quad (6.36)$$

Hence, the proof of this part is complete.

For the second part of the proof, we suppose that the order conditions for $\varphi(\Psi)$ hold for any $d(\tau) = K$ ($\rho(\tau) \leq p$). This means that the equations

$$\left\{ \begin{aligned} \sum_{i=1}^s \bar{B}_i \Phi_i(\tau) &= \frac{\rho(\tau)!}{\gamma(\tau)s(\tau)} \phi_{\rho(\tau)+1} + \mathcal{O}(h^{p-\rho(\tau)}), \\ \sum_{i=1}^s B_i \Phi_i(\tau) &= \frac{\rho(\tau)!}{\gamma(\tau)s(\tau)} \phi_{\rho(\tau)} + \mathcal{O}(h^{p-\rho(\tau)+1}), \end{aligned} \right. \quad (6.37)$$

are satisfied for $\tau \in SSENT$, $d(\tau) = K$ ($\rho(\tau) \leq p$). We turn to showing that (6.37) also holds for any $\tau \in SSENT$ with $d(\tau) = K + 1$ ($\rho(\tau) \leq p$).

Suppose that $\tau \in SSENT$, $\rho(\tau) \leq p$ and $d(\tau) = K + 1$. It follows from Definitions 6.3 and 6.4 that there must exist two integers $l \geq 1$, $n \geq 0$ and a corresponding *SSENT* tree τ_n in τ , where τ_n with the particular form $\tau_n = (W_+ b_+ (b_+ B_+)^l(\tau_0))$ is the n th generation of τ . Here, it is convenient to suppose that τ_{k+1} is the first generation of τ_k for $1 \leq k \leq n - 1$ and τ_1 is the the first generation of τ , that is

$$\tau = (W_+ b_+ (b_+ B_+)^0(\tau_1)) \times \tau'_1, \quad \tau_k = (W_+ b_+ (b_+ B_+)^0(\tau_k + 1)) \times \tau'_{k+1},$$

where τ'_k may be some *SSENT* tree depending on τ . Using Lemma 6.1, we have the following formula

$$\begin{cases} s(\tau_k) = s(\tau_{k+1}) \cdot s(\tau'_{k+1}), \\ \rho(\tau_k) = \rho(\tau_{k+1}) + \rho(\tau'_{k+1}) + 1, \\ \gamma(\tau_k) = \rho(\tau_k)(\rho(\tau_{k+1}) + 1)\gamma(\tau_{k+1}) \frac{\gamma(\tau'_{k+1})}{\rho(\tau'_{k+1})}. \end{cases} \quad (6.38)$$

Recursively iterating (6.38) implies that

$$\begin{cases} s(\tau) = s(\tau_n) \cdot \prod_{k=1}^n s(\tau'_{k+1}), \\ \rho(\tau) = \rho(\tau_{k+1}) + n + \sum_{k=1}^n \rho(\tau'_{k+1}), \\ \gamma(\tau) = \rho(\tau)(\rho(\tau_n) + 1)\gamma(\tau_n) \cdot \prod_{k=1}^{n-1} \rho(\tau_k)(\rho(\tau_k) + 1) \cdot \prod_{k=1}^n \frac{\gamma(\tau'_{k+1})}{\rho(\tau'_{k+1})}. \end{cases} \quad (6.39)$$

Modifying the *SSENT* tree τ by merely replacing τ_n with $\tilde{\tau}_n$, we obtain a new tree $\tilde{\tau}$ (certainly τ_k will become a new one $\tilde{\tau}_k$ and τ'_k remains the same). Let $\delta = \rho(\tau_n) - \rho(\tilde{\tau}_n)$. Then it follows from (6.39) that

$$\begin{cases} s(\tilde{\tau}) = s(\tau) \cdot \frac{s(\tilde{\tau}_n)}{s(\tau_n)}, \\ \rho(\tau) - \rho(\tilde{\tau}) = \rho(\tau_1) - \rho(\tilde{\tau}_1) = \dots = \rho(\tau_n) - \rho(\tilde{\tau}_n) = \delta, \\ \gamma(\tilde{\tau}) = \gamma(\tau) \frac{\gamma(\tilde{\tau}_n)}{\gamma(\tau_n)} \left(1 - \frac{\delta}{\rho(\tau)}\right) \left(1 - \frac{\delta}{\rho(\tau_n) + 1}\right) \cdot \prod_{k=1}^{n-1} \left(1 - \frac{\delta}{\rho(\tau_k)}\right) \left(1 - \frac{\delta}{\rho(\tau_k) + 1}\right). \end{cases} \quad (6.40)$$

For $\tau_n = (W_+ b_+ (b_+ B_+)^l(\tau_0))$ (see Fig. 6.3), we can derive

$$\begin{cases} s(\tau_n) = (-1)^l s(\tau_0), \\ \rho(\tau_n) = \rho(\tau_0) + 2l + 2, \\ \gamma(\tau_n) = \gamma(\tau_0) \frac{(\rho(\tau_0) + 2l + 2)!}{\rho(\tau_0)!(2l)!}. \end{cases} \quad (6.41)$$

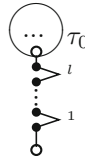


Fig. 6.3 Figure of tree $\tau_n = (W_+ b_+(b_+ B_+)^l)(\tau_0)$

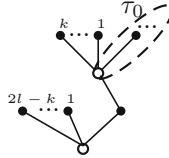


Fig. 6.4 Figure of tree $\tilde{\tau}_n$

We now consider $\tilde{\tau}_n$ (see Fig. 6.4) with the particular form

$$\tilde{\tau}_n = \overbrace{\circ \times \circ \times \dots \times \circ}^{2l-k \text{ folds}} \times (W_+ b_+(b_+ B_+)^0(\tau_0 \times \overbrace{\circ \times \dots \times \circ}^{k \text{ folds}})), \quad 0 \leq k \leq 2l.$$

We then have

$$\begin{cases} s(\tilde{\tau}_n) = s(\tau_0), \\ \rho(\tilde{\tau}_n) = \rho(\tau_0) + 2l + 2, \\ \gamma(\tilde{\tau}_n) = (\rho(\tau_0) + k)(\rho(\tau_0) + k + 1)(\rho(\tau_0) + 2l + 2) \frac{\gamma(\tau_0)}{\rho(\tau_0)}. \end{cases} \tag{6.42}$$

Combining (6.40) with (6.41–6.42), we derive the following equations

$$\begin{cases} s(\tilde{\tau}) = s(\tau) \cdot (-1)^l, \\ \rho(\tilde{\tau}) = \rho(\tau), \text{ i.e. } \delta = 0, \\ \gamma(\tilde{\tau}) = \gamma(\tau) \frac{(\rho(\tau_0) + k)(\rho(\tau_0) + k + 1)(\rho(\tau_0) - 1)!(2l)!}{(\rho(\tau_0) + 2l + 1)!}. \end{cases} \tag{6.43}$$

Keep in mind that the weights of τ and $\tilde{\tau}(k)$ (here we concretely denote the new tree $\tilde{\tau}$ as $\tilde{\tau}(k)$ since it really depends on k) can be respectively expressed as

$$\left\{ \begin{array}{l} \Phi_i(\tau) = \sum_{\mu=1}^s \sum_{\nu=1}^s \Delta_{\mu} A_{\mu\nu}^{(2l)} \Xi_{\nu} = \sum_{\mu=1}^s \sum_{\nu=1}^s \Delta_{\mu} a_{\mu\nu} (c_{\mu} - c_{\nu})^{2l} \frac{(-1)^l}{2l+1} \Xi_{\nu}, \\ \Phi_i(\tilde{\tau}(k)) = \sum_{\mu=1}^s \sum_{\nu=1}^s c_{\mu}^{2l-k} \Delta_{\mu} a_{\mu\nu} c_{\nu}^k \Xi_{\nu}, \end{array} \right. \quad (6.44)$$

where Δ_{μ} , Ξ_{ν} are some summation depending on other branches of τ . It follows from (6.44) that

$$\Phi_i(\tau) = \sum_{k=0}^{2l} \frac{(-1)^{l+k} C_{2l}^k}{2l+1} \Phi_i(\tilde{\tau}(k)). \quad (6.45)$$

Moreover, from Definition 6.3, the equation $d(\tilde{\tau}(k)) = d(\tau) - 1 = K$ holds for any $0 \leq k \leq 2l$. By the assumption in this part we know that the order conditions (6.37) are satisfied for such $\tilde{\tau}(k)$ ($0 \leq k \leq 2l$). Combining the Eq. (6.45) with the order conditions for $\tilde{\tau}(k)$, we have

$$\left\{ \begin{array}{l} \sum_{i=1}^s \bar{B}_i \Phi_i(\tau) = \sum_{k=0}^{2l} \frac{(-1)^{l+k} C_{2l}^k}{2l+1} \sum_{i=1}^s \bar{B}_i \Phi_i(\tilde{\tau}(k)) \\ \quad = \sum_{k=0}^{2l} \frac{(-1)^{l+k} C_{2l}^k}{2l+1} \frac{\rho(\tilde{\tau}(k))!}{\gamma(\tilde{\tau}(k))s(\tilde{\tau}(k))} \phi_{\rho(\tilde{\tau}(k))+1} + \mathcal{O}(h^{p-\rho(\tilde{\tau}(k))}), \\ \sum_{i=1}^s B_i \Phi_i(\tau) = \sum_{k=0}^{2l} \frac{(-1)^{l+k} C_{2l}^k}{2l+1} \sum_{i=1}^s B_i \Phi_i(\tilde{\tau}(k)) \\ \quad = \sum_{k=0}^{2l} \frac{(-1)^{l+k} C_{2l}^k}{2l+1} \frac{\rho(\tilde{\tau}(k))!}{\gamma(\tilde{\tau}(k))s(\tilde{\tau}(k))} \phi_{\rho(\tilde{\tau}(k))} + \mathcal{O}(h^{p-\rho(\tilde{\tau}(k))+1}). \end{array} \right. \quad (6.46)$$

Taking account of the formula (6.43), which is related to τ and the new *SENT* tree $\tilde{\tau}(k)$, the equations in (6.46) imply that

$$\left\{ \begin{array}{l} \sum_{i=1}^s \bar{B}_i \Phi_i(\tau) = \sum_{k=0}^{2l} \frac{(-1)^k C_{2l}^k (\rho(\tau_0) + 2l + 1)!}{(\rho(\tau_0) + k)(\rho(\tau_0) + k + 1)(\rho(\tau_0) - 1)!(2l + 1)!} \cdot \frac{\rho(\tau)!}{\gamma(\tau)s(\tau)} \phi_{\rho(\tau)+1} \\ \quad + \mathcal{O}(h^{p-\rho(\tau)}), \\ \sum_{i=1}^s B_i \Phi_i(\tau) = \sum_{k=0}^{2l} \frac{(-1)^k C_{2l}^k (\rho(\tau_0) + 2l + 1)!}{(\rho(\tau_0) + k)(\rho(\tau_0) + k + 1)(\rho(\tau_0) - 1)!(2l + 1)!} \cdot \frac{\rho(\tau)!}{\gamma(\tau)s(\tau)} \phi_{\rho(\tau)} \\ \quad + \mathcal{O}(h^{p-\rho(\tau)+1}), \end{array} \right. \quad (6.47)$$

by replacing $s(\tilde{\tau}(k))$, $\gamma(\tilde{\tau}(k))$, $\rho(\tilde{\tau}(k))$ with $s(\tau)$, $\gamma(\tau)$, $\rho(\tau)$. Comparing (6.47) with (6.37), we observe that whether the order conditions are satisfied for τ depends on the following equation

$$\sum_{k=0}^{2l} \frac{(-1)^k C_{2l}^k (\rho(\tau_0) + 2l + 1)!}{(\rho(\tau_0) + k)(\rho(\tau_0) + k + 1)(\rho(\tau_0) - 1)!(2l + 1)!} = 1. \quad (6.48)$$

It has also been known that (6.48) is just a special case of the identity

$$\sum_{k=0}^{2l} \frac{(-1)^k C_{2l}^k (n+2l+1)!}{(n+k)(n+k+1)(n-1)!(2l+1)!} = 1, \quad n, l \in \mathbb{N}_+.$$

Hence, (6.37) also holds for any $\tau \in SSENT$ that $d(\tau) = K + 1$ ($\rho(\tau) \leq p$).

Since both the base case and the inductive step have been demonstrated by the above two processes, we have completed the proof of this theorem. \square

The theorems established in this section essentially reveal the relation between classical RKN methods and ERKN methods. An original and natural way to construct certain high-order ERKN methods is based on the order conditions (6.28), by which only general fifth/sixth order ERKN methods have now been found and it is quite difficult to find an arbitrarily high order ERKN method due to the high complexity. However, the theoretical results stated above can provide us with another simple way to construct high-order ERKN methods. In this way, we only need to find its corresponding reduced RKN method and these have been well studied in the literature. Furthermore, ERKN methods with particular properties, such as symmetry and symplecticity, can also be obtained via the mapping (6.21) and their reduced RKN methods. Finally, we are able to obtain knowledge of ERKN methods by studying RKN methods instead of ERKN methods themselves, especially in the construction of high-order ERKN methods.

6.5 Numerical Experiments

In order to show applications of the results presented in the previous section, we conduct some numerical experiments. First, we select some classical RKN methods as follows:

- RKN3s4: the three-stage symmetric symplectic Runge–Kutta–Nyström method of order four proposed by Forest and Ruth [6];
- RKN7s6: the seven-stage symmetric symplectic Runge–Kutta–Nyström method of order six given by Okunbor and Skeel [21];
- RKN6s6: the six-stage Runge–Kutta–Nyström method of order six given by Papakostas and Tsitourasy [22];
- RKN16s10: the sixteen-stage Runge–Kutta–Nyström method of order ten presented by Dormand, El-Mikkawy and Prince [5].

Then from the mapping (6.21), their corresponding ERKN methods are also obtained with the individual properties maintained. We denote their corresponding ERKN methods as ERKN3s4, ERKN7s6, ERKN6s6, and ERKN16s10, respectively.

During the numerical experiments, we will display the efficiency curves and the conservation of energy for each Hamiltonian system. It should be noted that, the numerical solution obtained by RKN16s10 with a small stepsize is used as the standard reference solution, if the analytical solution cannot be explicitly given.

Problem 6.1 We first consider an orbital problem with perturbation [29]

$$\begin{cases} q_1'' = -q_1 - \frac{2\varepsilon + \varepsilon^2}{r^5}q_1, & q_1(0) = 1, & q_1'(0) = 0, \\ q_2'' = -q_2 - \frac{2\varepsilon + \varepsilon^2}{r^5}q_2, & q_2(0) = 0, & q_2'(0) = 1 + \varepsilon, \end{cases}$$

where $r = \sqrt{q_1^2 + q_2^2}$, and the analytical solution is given by

$$q_1(t) = \cos(t + \varepsilon t), \quad q_2(t) = \sin(t + \varepsilon t),$$

with the Hamiltonian

$$H = \frac{p_1^2 + p_2^2}{2} + \frac{q_1^2 + q_2^2}{2} - \frac{2\varepsilon + \varepsilon^2}{3(q_1^2 + q_2^2)^{\frac{3}{2}}}.$$

We numerically integrate the problem on the interval $[0, 1000]$ with $\varepsilon = 10^{-3}$. It is clear from the efficiency curves in Fig. 6.5a that ERKN methods are usually superior to their corresponding reduced RKN methods with respect to the global error (GE), and a high-order RKN/ERKN method also shows better performance than a low-order RKN/ERKN method in dealing with an oscillatory problem. Figure 6.5b demonstrates that symplectic methods (RKN3s4, RKN7s6, ERKN3s4, ERKN7s6) show their good energy-conservation property for the Hamiltonian, while the other methods without symplecticity lead to a linear energy dissipation on a long-term scale. The detailed results on the energy conservation for ERKN3s4 and ERKN7s6 are shown in Fig. 6.6. All these results from Figs. 6.5 and 6.6 are consistent with those of classical numerical methods, and show that ERKN methods obtained by the map φ with the reduced RKN methods are remarkably efficient and effective.

Problem 6.2 We consider the Hénon–Heilse system

$$\begin{cases} q_1'' + q_1 = -2q_1q_2, \\ q_2'' + q_2 = -q_1^2 + q_2^2, \end{cases} \quad (6.49)$$

with the initial conditions $q_1(0) = \sqrt{\frac{5}{48}}$, $p_2(0) = \frac{1}{4}$, $q_2(0) = p_1(0) = 0$. The Hamiltonian of the system is given by

$$H(p, q) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2q_2 - \frac{1}{3}q_2^3.$$

We first integrate this problem on the interval $[0, 1000]$ with different stepsizes. The efficiency curves for each method are shown in Fig. 6.7a, which indicate the comparable efficiency for ERKN methods to their corresponding reduced RKN ones, since $\|M\|$ now nearly has the same magnitude as $\|\frac{\partial f}{\partial q}\|$. This phenomenon also

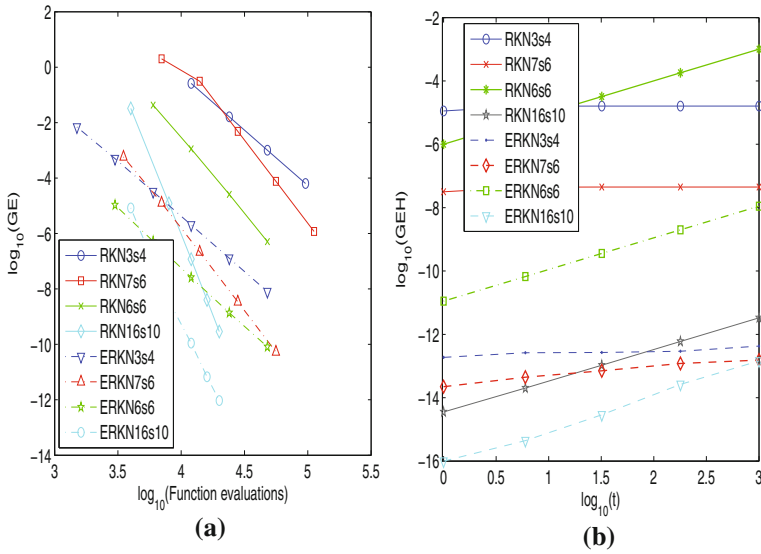


Fig. 6.5 Results for Problem 6.1: **a** The log-log plot of maximum global error GE against number of function evaluations; **b** the logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t)$ with the stepsize $h = 1$

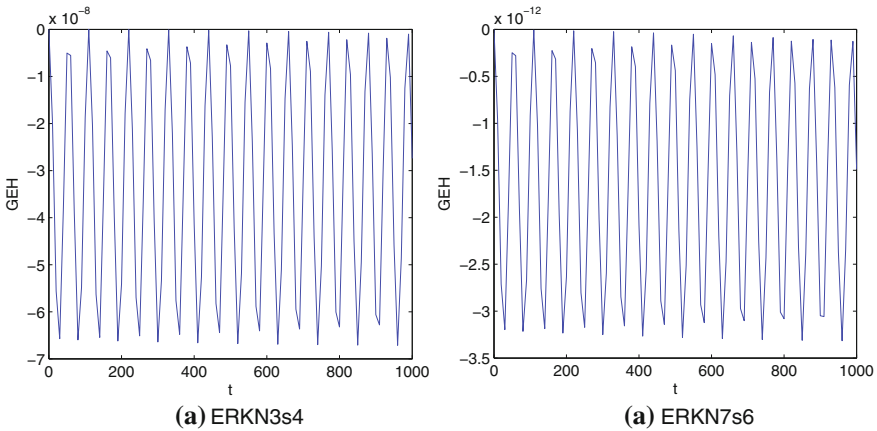


Fig. 6.6 Results for Problem 6.1: the global error for Hamiltonian of symplectic methods ERKN3s4 and ERKN7s6 with the stepsize $h = 2$

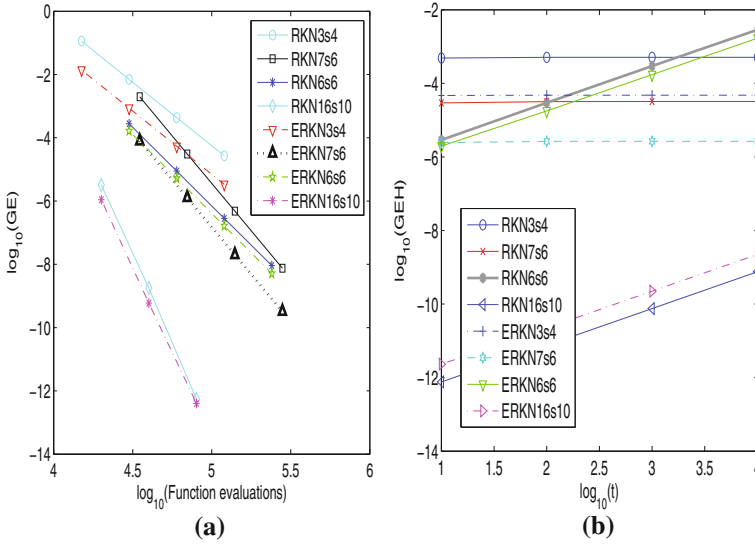


Fig. 6.7 Results for Problem 6.2: **a** The log-log plot of maximum global error GE against the number of function evaluations; **b** the logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t)$ with the stepsize $h = 0.5$

occurs in Fig. 6.7b, where the energy-conservation curve for each method is plotted. Besides, we can also observe from Fig. 6.7 that the difference between symplectic methods is a little more remarkable than that between non-symplectic ones. The good energy-conservation property of symplectic ERKN methods (ERKN3s4 and ERKN7s6) is clearly shown in Fig. 6.8, which demonstrates that the symplecticity is maintained by the mapping φ very well.

Problem 6.3 We consider the sine-Gordon equation [13] with the periodic boundary conditions

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \sin u, & -5 \leq x \leq 5, t \geq 0, \\ u(-5, t) = u(5, t). \end{cases} \quad (6.50)$$

A semi-discretization on the spatial variable with the second-order symmetric differences gives the following differential equations in time

$$\frac{d^2 U}{dt^2} + MU = F(U), \quad (6.51)$$

where $U(t) = (u_1(t), \dots, u_N(t))^T$ with $u_i(t) \approx u(x_i, t)$, $x_i = -5 + i\Delta x$ for $i = 1, \dots, N$, $\Delta x = 10/N$, and

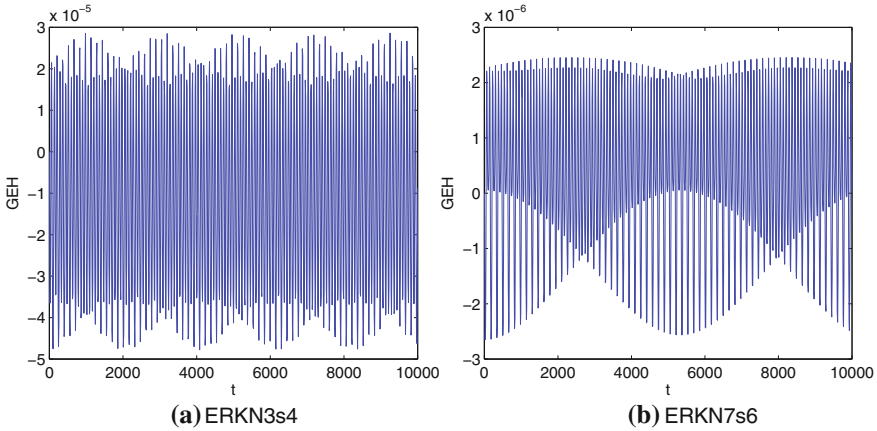


Fig. 6.8 Results for Problem 6.2: the global error for Hamiltonian of symplectic methods ERKN3s4 and ERKN7s6 with the stepsize $h = 0.5$

$$M = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}$$

$$F(U) = -\sin(U) = -(\sin u_1, \dots, \sin u_N)^\top.$$

The corresponding Hamiltonian is given by

$$H(U', U) = \frac{1}{2}U'^\top U' + \frac{1}{2}U^\top M U - (\cos u_1 + \dots + \cos u_N).$$

For this problem, we take the initial conditions as

$$U(0) = (\pi)_{i=1}^N, \quad U_i(0) = \sqrt{N} \left(0.01 + \sin\left(\frac{2\pi i}{N}\right) \right)_{i=1}^N,$$

with $N = 64$. For the efficiency curves in Fig. 6.9a, we integrate the problem for $t_{end} = 10$ with the different stepsizes. Figure 6.9a shows the good efficiency and accuracy of all the ERKN methods. In Fig. 6.9b, all methods give rise to energy dissipation even if the method is symplectic. This phenomenon is mainly caused by the chaotic behavior of the problem, in which a sufficiently small perturbation may lead to a significant error after a long time, and this increase is always exponential. It can be observed from Fig. 6.10 that the numerical reference solution obtained by RKN16s10 obviously shows notable difference between the initial interval $[0, 100]$ and the terminal interval $[900, 1000]$. Figure 6.11 gives a further demonstration that the global errors of RKN7s6 and ERKN7s6 increase nearly in an exponential fashion

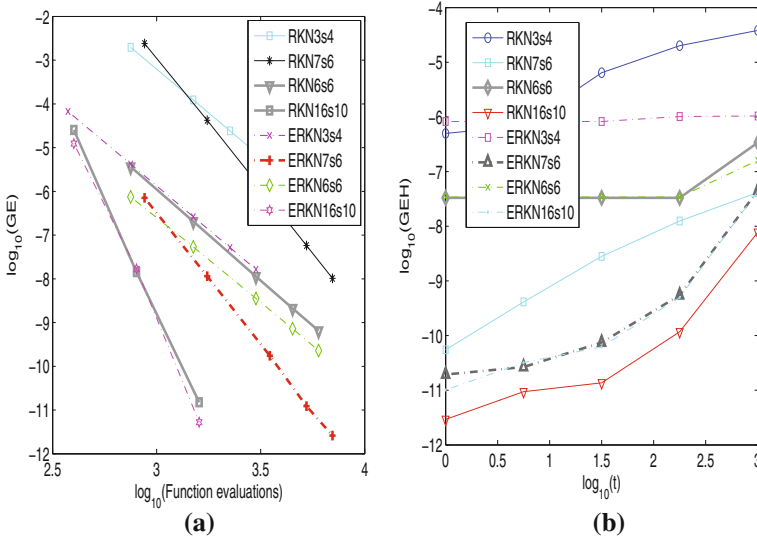


Fig. 6.9 Results for Problem 6.3: **a** The log-log plot of maximum global error GE against number of function evaluations; **b** the logarithm of the maximum global error of Hamiltonian $GEH = \max|H_n - H_0|$ against $\log_{10}(t)$ with the stepsize $h = 0.01$

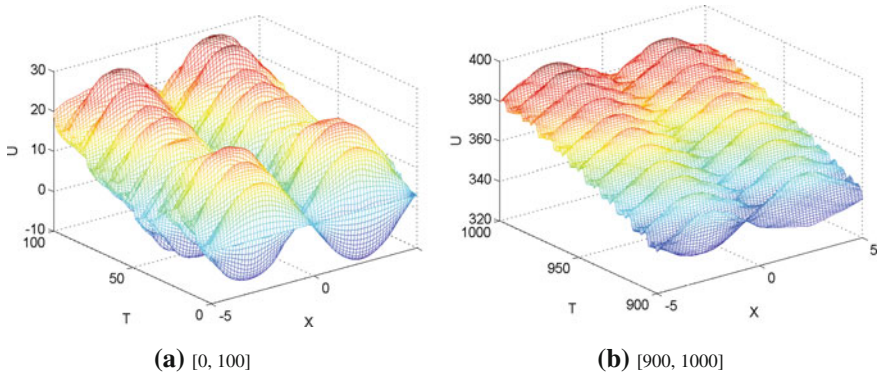


Fig. 6.10 Results for Problem 6.3: The numerical reference solution in different interval obtained by RKN16s10 with the stepsize $h = 0.001$

with time t . This may lead to non-conservation for symplectic methods in practical numerical computations.

Problem 6.4 We consider the Fermi-Pasta-Ulam problem (see, e.g. [10]), which can be expressed by a Hamiltonian system with the Hamiltonian

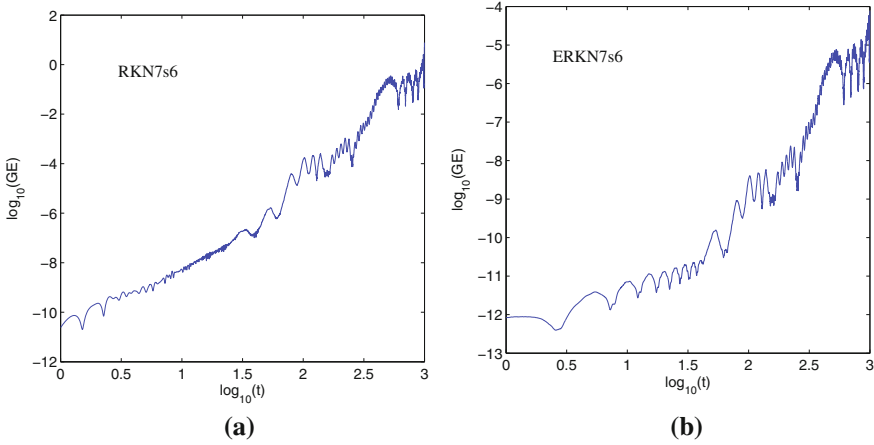


Fig. 6.11 Results for Problem 6.3: the global error for RKN7s6 and ERKN7s6 with the stepsize $h = 0.01$, respectively

$$\begin{aligned}
 H(y, x) = & \frac{1}{2} \sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2} \sum_{i=1}^m x_{m+i}^2 + \frac{1}{4} \left((x_1 - x_{m+1})^4 \right. \\
 & \left. + \sum_{i=1}^{m-1} (x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4 \right),
 \end{aligned} \tag{6.52}$$

where x_i represents a scaled displacement of the i th stiff spring, x_{m+i} is a scaled expansion (or compression) of the i th stiff spring, and y_i, y_{m+i} are their velocities (or momenta).

The corresponding Hamiltonian system is given by

$$\begin{cases} x' = H_y(y, x), \\ y' = -H_x(y, x), \end{cases} \tag{6.53}$$

which can be also written in the equivalent form of the oscillatory second-order differential equations

$$x''(t) + Mx(t) = -\nabla_x U(x), \tag{6.54}$$

where

$$y = x', \quad M = \begin{pmatrix} \mathbf{0}_{m \times m} & \mathbf{0}_{m \times m} \\ \mathbf{0}_{m \times m} & \omega^2 I_{m \times m} \end{pmatrix},$$

$$U(x) = \frac{1}{4} \left((x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1} (x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4 \right).$$

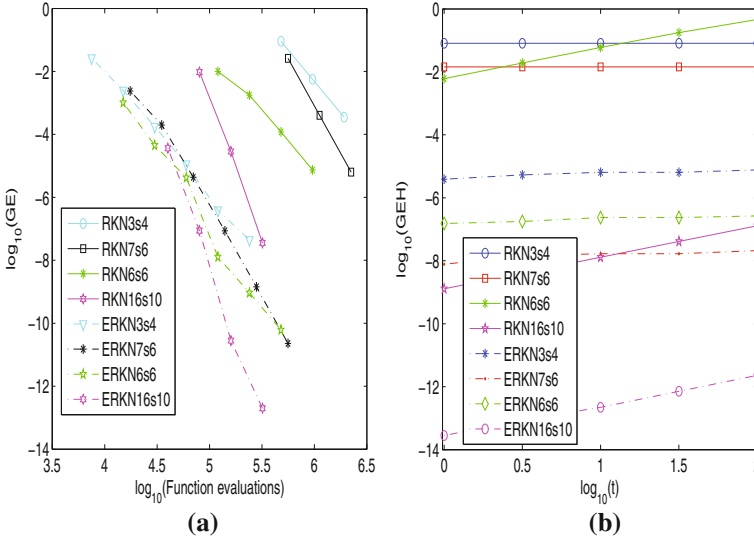


Fig. 6.12 Results for Problem 6.4: **a** The log-log plot of maximum global error GE against the number of function evaluations; **b** the logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t)$ with the stepsize $h = 0.005$

In the experiment, we choose

$$m = 3, \quad x_1(0) = 1, \quad y_1(0) = 1, \quad x_4(0) = \frac{1}{\omega}, \quad y_1(0) = 1, \quad \omega = 200,$$

and choose zero for the remaining initial values. The numerical results are shown in Fig. 6.12. Similarly to Problem 6.3, we also integrate the equation over a short interval with $t_{end} = 20$ to decrease the influence of chaotic behavior. Both figures show good efficiency in the global error and energy error for the ERKN methods. In particular, symplecticity is also maintained by the map φ , such as ERKN3s4 and ERKN7s6 in Fig. 6.13 display a stable energy conservation in the sense of numerical computation.

6.6 Conclusions and Discussions

In this chapter, we studied in greater depth the ERKN methods for solving (6.1) based on the group structure of numerical methods. After the construction of the RKN group and the ERKN group, we first presented the inherent relationship between ERKN and RKN methods, that is, there exists an epimorphism η of the ERKN group onto the RKN group. This epimorphism gives a clear and exact meaning for the word *extension* from RKN methods to ERKN methods and describes the ERKN group in

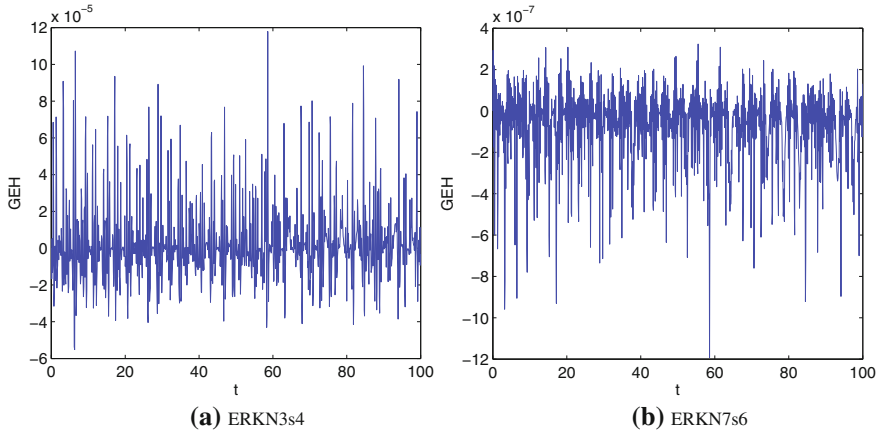


Fig. 6.13 Results for Problem 6.4: the global error for Hamiltonian of symplectic methods ERKN3s4 and ERKN7s6 with the stepsize $h = 0.01$

terms of the RKN group in the sense of structure preservation. Moreover, we established the particular mapping φ defined by (6.21), which maps an RKN method to an ERKN method. A series of theorems about the mapping show that the image element can be regarded as an ideal representative element for each congruence class of the ERKN group. That is, the image ERKN element almost preserves as many properties as the RKN element does. This mapping φ also provides us with an effective approach to constructing arbitrarily high order (symmetric or symplectic) ERKN methods, whereas the original way based directly on order conditions (symmetric or symplectic conditions) is more complicated. Furthermore, the numerical simulations in Sect. 6.5 strongly support our theoretical analysis in Sect. 6.4, and the numerical results are really promising. The high-order structure-preserving ERKN methods obtained in such a simple and effective way show better efficiency and accuracy than their corresponding reduced methods (letting $V = 0$), namely, the RKN methods.

Remember that the exponential Fourier collocation methods for first-order differential equations were derived and analysed in Sect. 6.3. Accordingly, the next chapter will present trigonometric collocation methods for multi-frequency and multidimensional second-order oscillatory systems.

The material of this chapter is based on the recent work by Mei and Wu [17].

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