

Chapter 2

Continuous-Stage ERKN Integrators for Second-Order ODEs with Highly Oscillatory Solutions



In this chapter, continuous-stage extended Runge–Kutta–Nyström (CSERKN) integrators for solving highly oscillatory systems of second-order ODEs are derived and analysed. These integrators are incorporated into the special structure of highly oscillatory systems so that their internal stages and updates can integrate the associated highly oscillatory homogeneous systems exactly. When the underlying highly oscillatory systems are Hamiltonian systems, sufficient conditions for energy preservation are shown for CSERKN methods. The symmetry and stability of CSERKN integrators are also analysed in detail. Preliminary numerical results highlight the effectiveness of CSERKN methods.

2.1 Introduction

We consider the following system of second-order ordinary differential equations with oscillatory solutions

$$\begin{cases} q''(t) + Mq(t) = f(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, \quad q'(t_0) = q'_0, \end{cases} \quad (2.1)$$

where $M \in \mathbb{R}^{d \times d}$ is a symmetric positive semi-definite matrix that implicitly contains the dominant frequencies of the system, $q \in \mathbb{R}^d$ and $f(q) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a nonlinear function which is independent of q' . If $\|M\| \gg \max \left\{ 1, \left\| \frac{\partial f}{\partial q} \right\| \right\}$ then (2.1) is a highly oscillatory problem. This kind of problem frequently occurs in science and engineering fields such as quantum mechanics, astrophysics, quantum chemistry and electronics. It is particularly interesting when this highly oscillatory problem is obtained from a spatial semidiscretisation of a semilinear wave equation within the framework of the method of lines [1]. In practice, the system (2.1) can

be integrated with general purpose methods [2, 3] or other codes adapted to its special structure. However, it is worth noting that adaptive methods will be more efficient than general purpose methods since adaptive methods make good use of the information transmitted from the special structure of (2.1) introduced by the linear term $Mq(t)$.

For the particular case where $M = \omega^2 I_d$ with a single frequency $\omega > 0$ and the $d \times d$ identity matrix I_d , methods with frequency-dependent coefficients using techniques like trigonometrical/exponential fitting can be traced back to the 1960s (see, e.g. [4]). Here, we refer the reader to the reviews of the literature (see, [5, 6]) and the relevant papers (see, e.g. [7–18]). If M is a symmetric positive semi-definite matrix, exponential integrators (see, e.g. [19, 20]), adapted Runge–Kutta–Nyström (ARKN) methods (see [21, 22]) and other adaptive methods (see, e.g. [23–28]) have been developed. Wu et al. proposed and analysed extended Runge–Kutta–Nyström (ERKN) methods (see, e.g. [29–31]), whose internal stages and updates exactly integrate the following highly oscillatory homogeneous linear system

$$q''(t) + Mq(t) = 0 \quad (2.2)$$

associated with (2.1). This property plays an important role in oscillation-preserving integrators as stated in Chap. 1. The global error analysis of ERKN methods was presented and collocation techniques were also studied in [32–34].

If $f(q) = -\nabla U(q)$ for some smooth function $U(q)$, the system (2.1) is identical to a separable Hamiltonian system of the following form

$$\begin{cases} p'(t) = -\nabla_q H(p, q), \\ q'(t) = \nabla_p H(p, q), \end{cases} \quad (2.3)$$

with the initial values $q(t_0) = q_0$, $p(t_0) = p_0 = q_0'$, and the Hamiltonian

$$H(p, q) = \frac{1}{2}p^\top p + \frac{1}{2}q^\top Mq + U(q), \quad (2.4)$$

where $q : \mathbb{R} \rightarrow \mathbb{R}^d$ and $p : \mathbb{R} \rightarrow \mathbb{R}^d$ are known as generalised position and generalised momenta, respectively. It is clear that (2.3) is a highly oscillatory Hamiltonian system once $\|M\| \gg \max \left\{ 1, \left\| \frac{\partial f}{\partial q} \right\| \right\}$. As is known, for Hamiltonian system (2.3), the corresponding map is symplectic and the true solution preserves the energy $H(p, q)$ for all $t \in [t_0, T]$ (see, e.g. [35]). In the spirit of geometric numerical integration, an integrator that inherits such geometric properties as much as possible would be preferable. Unfortunately, however, it is often difficult to design numerical integrators which inherit both symplecticity and energy preservation. A numerical method which is energy preserving at each step and defined by a symplectic map has been discussed in [36, 37]. Since there is no symplectic B-series method that conserves arbitrary Hamiltonians [38, 39], methods satisfying one of

these properties have been developed in the past few decades [20]. Research work has shown that symplectic methods perform very well in approximately preserving the energy of Hamiltonian systems and we refer the reader to [20], for instance. However, it is worth noting that symplectic methods just approximately, rather than exactly, preserve the energy (2.4). In practical applications, apart from the accuracy of approximate solutions, high-precision energy-preserving integrators are also required. Moreover, in comparison with symplectic methods, energy-preserving integrators have better nonlinear stability characteristics, are easier to adapt the time step for, and are more suitable for the integration of chaotic systems (see, e.g. [40–43]). Therefore, energy-preserving algorithms are becoming more popular.

As is known, for first-order ordinary differential equations of the form

$$y'(t) = G(y(t)), \quad y(t_0) = y_0, \quad t \in [t_0, T], \quad (2.5)$$

continuous-stage Runge–Kutta (CSRK) methods were firstly researched in [44, 45]. Then, some relevant papers appeared (see, e.g. [46, 47]). Hairer proposed a family of CSRK methods and studied the corresponding energy conservation (see [48]). Miyatake and Butcher proved a sufficient and necessary energy-preserving condition of CSRK methods (see [49]). Recently, some developments in this field have been made (see, e.g. [50–52]). The exponentially and functionally-fitted version of the CSRK method appeared in [53, 54]. The conservation of energy has been approached by means of the definition of the discrete line integral [55–57].

More recently, for second-order ordinary differential equations of the form

$$q''(t) = F(q(t)), \quad q(t_0) = q_0, \quad q'(t_0) = q'_0, \quad t \in [t_0, T], \quad (2.6)$$

Tang et al. [58] discussed continuous-stage Runge–Kutta–Nyström (CSRKN) methods and studied symplecticity-preserving algorithms. Energy-preserving CSRKN methods were studied in [59]. The corresponding result in [58] has been extended to high-order symplectic CSRKN methods [60].

2.2 Extended Runge–Kutta–Nyström Methods

Suppose that M is a positive semi-definite matrix. We begin with the following matrix-valued ϕ -functions

$$\phi_j(M) = \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+j)!}, \quad j \geq 0, \quad M \in \mathbb{R}^{d \times d}. \quad (2.7)$$

which originally appeared in [22]. It can be observed from (2.7) that $j!\phi_j(M) \rightarrow I_d$ when $M \rightarrow \mathbf{0}$, where I_d is the $d \times d$ identity matrix. The following proposition

establishes the properties of matrix-valued ϕ -functions which will be used in Sect. 2.4 of this chapter.

Proposition 2.1 *The matrix-valued ϕ -functions defined by (2.7) satisfy:*

- (i) $M \in \mathbb{R}^{d \times d}$,

$$\begin{aligned}\phi_{j+2}(M) &= \int_0^1 \frac{(1-z)\phi_1(M(1-z)^2)z^j}{j!} dz, \quad j = 0, 1, \dots, \\ \phi_{j+1}(M) &= \int_0^1 \frac{\phi_0(M(1-z)^2)z^j}{j!} dz, \quad j = 0, 1, \dots; \end{aligned} \quad (2.8)$$

- (ii) *If M is invertible, then*

$$\phi_{j+2}(M) = M^{-1} \left(\frac{1}{j!} I_d - \phi_j(M) \right), \quad j = 0, 1, \dots; \quad (2.9)$$

- (iii) $\phi_0^2(M) + M\phi_1^2(M) = I_d$.

The proofs of Proposition 2.1 and further details about the matrix-valued ϕ -functions can be found in [22, 31]. As shown in Chap. 1 (see also [31]), an s -stage ERKN method for the numerical integration of the system (2.1) is defined as

$$\left\{ \begin{aligned} Q_i &= \phi_0(c_i^2 V)q_n + hc_i\phi_1(c_i^2 V)q'_n + h^2 \sum_{j=1}^s a_{ij}(V)f(Q_j), \quad i = 1, \dots, s, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q'_n + h^2 \sum_{i=1}^s \bar{b}_i(V)f(Q_i), \\ q'_{n+1} &= -hM\phi_1(V)q_n + \phi_0(V)q'_n + h \sum_{i=1}^s b_i(V)f(Q_i), \end{aligned} \right. \quad (2.10)$$

where c_i are real numbers, and $a_{ij}(V)$, $\bar{b}_i(V)$ and $b_i(V)$ for $i, j = 1, \dots, s$ are matrix-valued functions of $V = h^2 M$. The method (2.10) can be represented briefly in Butcher's notation by the following block tableau of coefficients:

$$\begin{array}{c|cc|c} c & \phi_0(c^2 V) & c\phi_1(c^2 V) & A(V) \\ \hline & \phi_0(V) & \phi_1(V) & \bar{b}^\top(V) \\ \hline & -hM\phi_1(V) & \phi_0(V) & b^\top(V) \end{array}$$

$$\begin{array}{c|c|c|c}
 c_1 & \phi_0(c_1^2 V) & c_1 \phi_1(c_1^2 V) & a_{11}(V) \cdots a_{1s}(V) \\
 \vdots & \vdots & \vdots & \vdots \quad \ddots \quad \vdots \\
 = c_s & \phi_0(c_s^2 V) & c_s \phi_1(c_s^2 V) & a_{s1}(V) \cdots a_{ss}(V) \\
 \hline
 & \phi_0(V) & \phi_1(V) & \bar{b}_1(V) \cdots \bar{b}_s(V) \\
 \hline
 & -hM\phi_1(V) & \phi_0(V) & b_1(V) \cdots b_s(V)
 \end{array} \tag{2.11}$$

The order conditions for an ERKN method (2.10) have been investigated in [31] by using the B-series theory associated with the set of extended special Nyström trees (see [61]). To learn more about this point the reader is referred to the relevant references for all the definitions and notations.

Let

$$a_{ij}(V) = \sum_{k=0}^{\infty} a_{ij}^{(2k)} V^k, \tag{2.12}$$

where the coefficients $a_{ij}^{(2k)}$ define the expansion of $a_{ij}(V)$. Then the local truncation errors of q_{n+1} and q'_{n+1} can be expanded in the form

$$\begin{aligned}
 e_{n+1} &= q_{n+1} - q(t_{n+1}) \\
 &= \sum_{\beta\tau \in \text{ESNT}} h^{\rho(\beta\tau)+1} \left(\frac{\gamma(\beta\tau)}{\rho(\beta\tau)!} \sum_{i=1}^s \bar{b}_i(V) \Phi_i(\beta\tau) - \phi_{\rho(\beta\tau)+1}(V) \right) \alpha(\beta\tau) F(\beta\tau)(q_n, q'_n), \\
 e'_{n+1} &= q'_{n+1} - q'(t_{n+1}) \\
 &= \sum_{\beta\tau \in \text{ESNT}} h^{\rho(\beta\tau)} \left(\frac{\gamma(\beta\tau)}{\rho(\beta\tau)!} \sum_{i=1}^s b_i(V) \Phi_i(\beta\tau) - \phi_{\rho(\beta\tau)}(V) \right) \alpha(\beta\tau) F(\beta\tau)(q_n, q'_n),
 \end{aligned}$$

where the set ESNT of extended special Nyström trees $\beta\tau$, functions $\rho(\beta\tau)$, $\alpha(\beta\tau)$ and elementary differential $F(\beta\tau)(q, q')$ are defined in [31, 61]. The following theorem states the order conditions for ERKN methods.

Theorem 2.1 *The ERKN method (2.10) is convergent of order p if and only if*

$$\begin{aligned}
 \sum_{i=1}^s \bar{b}_i(V) \Phi_i(\beta\tau) &= \frac{\rho(\beta\tau)!}{\gamma(\beta\tau)} \phi_{\rho(\beta\tau)+1}(V) + \mathcal{O}(h^{p-\rho(\beta\tau)}), \quad \rho(\beta\tau) \leq p-1, \\
 \sum_{i=1}^s b_i(V) \Phi_i(\beta\tau) &= \frac{\rho(\beta\tau)!}{\gamma(\beta\tau)} \phi_{\rho(\beta\tau)}(V) + \mathcal{O}(h^{p+1-\rho(\beta\tau)}), \quad \rho(\beta\tau) \leq p,
 \end{aligned} \tag{2.13}$$

where $\beta\tau \in \text{ESNT}$.

With regard to the follow-up work of ERKN methods, we refer the reader to [32], in which trigonometric Fourier collocation methods were studied. The symplectic conditions for ERKN methods were derived and analysed in [29, 30].

2.3 Continuous-Stage ERKN Methods and Order Conditions

Similarly to the CSRK method, Tang et al. considered the continuous-stage Runge–Kutta–Nyström (CSRKN) method for (2.6) as follows (see [58]).

Definition 2.1 Let $A_{\tau\sigma}$ be a function of variables $\tau, \sigma \in [0, 1]$ and \bar{B}_τ, B_τ and C_τ be functions of $\tau \in [0, 1]$. A continuous-stage Runge–Kutta–Nyström (CSRKN) method for solving (2.6) is defined by

$$\begin{cases} Q_\tau = q_n + hC_\tau q'_n + h^2 \int_0^1 A_{\tau\sigma} F(Q_\sigma) d\sigma, & \tau \in [0, 1], \\ q_{n+1} = q_n + hq'_n + h^2 \int_0^1 \bar{B}_\tau F(Q_\tau) d\tau, \\ q'_{n+1} = q'_n + h \int_0^1 B_\tau F(Q_\tau) d\tau. \end{cases} \quad (2.14)$$

The order conditions for CSRKN methods (2.14) have been given as those for classical RKN methods with $\sum, c_i, a_{ij}, \bar{b}_i$, and b_i , replaced by $\int_0^1, C_\tau, A_{\tau\sigma}, \bar{B}_\tau$, and B_τ , respectively. For a more detailed description of the order conditions of the CSRKN methods, we refer the reader to [58].

On the basis of the matrix-variation-of-constants formula of (2.1), applying the continuous-stage idea to the ERKN methods leads to continuous-stage extended Runge–Kutta–Nyström methods as follows.

Definition 2.2 An s -degree continuous-stage extended Runge–Kutta–Nyström (CSERKN) method for the numerical integration of the system (2.1) is defined by

$$\begin{cases} Q_\tau = C_\tau(V)q_n + hD_\tau(V)q'_n + h^2 \int_0^1 \bar{A}_{\tau\sigma}(V)f(Q_\sigma) d\sigma, & \tau \in [0, 1], \\ q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q'_n + h^2 \int_0^1 \bar{b}_\tau(V)f(Q_\tau) d\tau, \\ q'_{n+1} = -hM\phi_1(V)q_n + \phi_0(V)q'_n + h \int_0^1 b_\tau(V)f(Q_\tau) d\tau, \end{cases} \quad (2.15)$$

where Q_τ is a polynomial of degree s with respect to τ satisfying $Q_0 = q_n$ and $Q_1 = q_{n+1}$, $C_\tau(V)$, $D_\tau(V)$, $\bar{b}_\tau(V)$, and $b_\tau(V)$ are polynomials of degree s and depend on V , $\bar{A}_{\tau\sigma}(V)$ is a polynomial of degree s for τ , and $s - 1$ for σ and depend on V , where $\tau, \sigma \in [0, 1]$ and $V = h^2 M$. In addition, the relations $\bar{A}_{0\sigma}(V) = \mathbf{0}$ and $\bar{A}_{1\sigma}(V) = \bar{b}_\sigma(V)$ hold. The polynomials $C_\tau(V)$ and $D_\tau(V)$ satisfy

$$C_{c_i}(V) = \phi_0(c_i^2 V), \quad D_{c_i}(V) = c_i \phi_1(c_i^2 V), \quad (2.16)$$

where c_i for $i = 0, \dots, s$ are the fitting nodes, and one of them should be 1. We take $c_0 = 0$ and $c_s = 1$ in general. $C_\tau(V)$ and $D_\tau(V)$ can be expressed as

$$C_\tau(V) = \sum_{i=0}^s L_i(\tau) \phi_0(c_i^2 V), \quad D_\tau(V) = \sum_{i=0}^s L_i(\tau) c_i \phi_1(c_i^2 V), \quad (2.17)$$

where $L_i(\tau)$ for $i = 0, \dots, s$ are the following Lagrange interpolations functions

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

The CSERKN method can be expressed by the following block Butcher tableau

$$\begin{array}{c|ccc} C_\tau & C_\tau(V) & D_\tau(V) & \bar{A}_{\tau\sigma}(V) \\ \hline & \phi_0(V) & \phi_1(V) & \bar{b}_\tau(V) \\ \hline & -hM\phi_1(V) & \phi_0(V) & b_\tau(V) \end{array}. \quad (2.18)$$

A CSERKN method (2.15) is of order p , if for sufficiently smooth problem (2.1), the local truncation errors satisfy

$$e_{n+1} = q_{n+1} - q(t_{n+1}) = \mathcal{O}(h^{p+1}), \quad e'_{n+1} = q'_{n+1} - q'(t_{n+1}) = \mathcal{O}(h^{p+1}),$$

under the so-called local assumptions. In order to obtain the order conditions for CSERKN methods, it is assumed that

$$\bar{A}_{\tau\sigma}(V) = \sum_{k=0}^{\infty} \bar{A}_{\tau\sigma}^{(2k)} V^k, \quad (2.19)$$

where the coefficients $\bar{A}_{\tau\sigma}^{(2k)}$ define the expansion of $\bar{A}_{\tau\sigma}(V)$. Similarly to the analysis of the paper [31], we have

$$\begin{aligned} e_{n+1} &= q_{n+1} - q(t_{n+1}) \\ &= \sum_{\beta\tau \in \text{ESNT}} h^{\rho(\beta\tau)+1} \left(\frac{\gamma(\beta\tau)}{\rho(\beta\tau)!} \int_0^1 \bar{b}_\tau(V) \Phi_\tau(\beta\tau) d\tau - \phi_{\rho(\beta\tau)+1}(V) \right) \alpha(\beta\tau) F(\beta\tau)(q_n, q'_n), \\ e'_{n+1} &= q'_{n+1} - q'(t_{n+1}) \\ &= \sum_{\beta\tau \in \text{ESNT}} h^{\rho(\beta\tau)} \left(\frac{\gamma(\beta\tau)}{\rho(\beta\tau)!} \int_0^1 b_\tau(V) \Phi_\tau(\beta\tau) d\tau - \phi_{\rho(\beta\tau)}(V) \right) \alpha(\beta\tau) F(\beta\tau)(q_n, q'_n). \end{aligned}$$

The weights $\Phi_\tau(\beta\tau)$ can be given similarly to the ones for ERKN methods with \sum , c_i^k , $a_{ij}^{(2k)}$, $\bar{b}_i(V)$, and $b_i(V)$ replaced by \int_0^1 , $\sum_{i=1}^s L_i(\tau)c_i^k$, $\bar{A}_{\tau\sigma}^{(2k)}$, $\bar{b}_\tau(V)$, and $b_\tau(V)$, respectively. Therefore, we obtain the order conditions for a CSERKN method as follows.

Theorem 2.2 *The CSERKN method (2.15) is convergent of order p if and only if*

$$\begin{aligned} \int_0^1 \bar{b}_\tau(V) \Phi_\tau(\beta\tau) d\tau &= \frac{\rho(\beta\tau)!}{\gamma(\beta\tau)} \phi_{\rho(\beta\tau)+1}(V) + \mathcal{O}(h^{p-\rho(\beta\tau)}), \quad \rho(\beta\tau) \leq p-1, \\ \int_0^1 b_\tau(V) \Phi_\tau(\beta\tau) d\tau &= \frac{\rho(\beta\tau)!}{\gamma(\beta\tau)} \phi_{\rho(\beta\tau)}(V) + \mathcal{O}(h^{p+1-\rho(\beta\tau)}), \quad \rho(\beta\tau) \leq p, \end{aligned} \tag{2.20}$$

where $\beta\tau$ is the extended special Nyström-tree.

In what follows, we provide a list of the p -th order conditions (2.20) for the CSERKN method (2.15) up to the extended special Nyström trees with $\rho(\beta\tau) \leq 4$.

- For the tree $\beta\tau$ with $\rho(\beta\tau) = 1$, (2.20) gives

$$\int_0^1 \bar{b}_\tau(V) d\tau = \phi_2(V) + \mathcal{O}(h^{p-1}), \quad \int_0^1 b_\tau(V) d\tau = \phi_1(V) + \mathcal{O}(h^p).$$

- For the tree $\beta\tau$ with $\rho(\beta\tau) = 2$, it follows from (2.20) that

$$\begin{aligned} \int_0^1 \bar{b}_\tau(V) \sum_{i=0}^s L_i(\tau)c_i d\tau &= \phi_3(V) + \mathcal{O}(h^{p-2}), \\ \int_0^1 b_\tau(V) \sum_{i=0}^s L_i(\tau)c_i d\tau &= \phi_2(V) + \mathcal{O}(h^{p-1}). \end{aligned}$$

- For the trees $\beta\tau$ with $\rho(\beta\tau) = 3$, the order conditions are

$$\int_0^1 \bar{b}_\tau(V) \sum_{i=0}^s L_i(\tau) c_i^2 d\tau = 2\phi_4(V) + \mathcal{O}(h^{p-3}),$$

$$\int_0^1 \int_0^1 \bar{b}_\tau(V) \bar{A}_{\tau\sigma}^{(0)} d\tau d\sigma = \phi_4(V) + \mathcal{O}(h^{p-3}),$$

$$\int_0^1 b_\tau(V) \sum_{i=0}^s L_i(\tau) c_i^2 d\tau = 2\phi_3(V) + \mathcal{O}(h^{p-2}),$$

$$\int_0^1 \int_0^1 b_\tau(V) \bar{A}_{\tau\sigma}^{(0)} d\tau d\sigma = \phi_3(V) + \mathcal{O}(h^{p-2}).$$

- For the trees $\beta\tau$ with $\rho(\beta\tau) = 4$, we have

$$\int_0^1 \bar{b}_\tau(V) \sum_{i=0}^s L_i(\tau) c_i^3 d\tau = 6\phi_5(V) + \mathcal{O}(h^{p-4}),$$

$$\int_0^1 \int_0^1 \bar{b}_\tau(V) \sum_{i=0}^s L_i(\tau) c_i \bar{A}_{\tau\sigma}^{(0)} d\tau d\sigma = 3\phi_5(V) + \mathcal{O}(h^{p-4}),$$

$$\int_0^1 \int_0^1 \bar{b}_\tau(V) \bar{A}_{\tau\sigma}^{(0)} \sum_{i=0}^s L_i(\sigma) c_i d\tau d\sigma = \phi_5(V) + \mathcal{O}(h^{p-4}),$$

$$\int_0^1 b_\tau(V) \sum_{i=0}^s L_i(\tau) c_i^3 d\tau = 6\phi_4(V) + \mathcal{O}(h^{p-3}),$$

$$\int_0^1 \int_0^1 b_\tau(V) \sum_{i=0}^s L_i(\tau) c_i \bar{A}_{\tau\sigma}^{(0)} d\tau d\sigma = 3\phi_4(V) + \mathcal{O}(h^{p-3}),$$

$$\int_0^1 \int_0^1 b_\tau(V) \bar{A}_{\tau\sigma}^{(0)} \sum_{i=0}^s L_i(\sigma) c_i d\tau d\sigma = \phi_4(V) + \mathcal{O}(h^{p-3}).$$

Likewise, we can list more order conditions for trees with $\rho(\beta\tau) \geq 5$. It should be pointed out that, when $s \geq p$ and the abscissae c_1, c_2, \dots, c_s are distinct, we have $\sum_{i=0}^s L_i(\tau) c_i^p = \tau^p$.

2.4 Energy-Preserving Conditions and Symmetric Conditions

In what follows, we show sufficient conditions for energy preservation for a CSERKN method (2.15) when applied to the highly oscillatory Hamiltonian system (2.1).

Theorem 2.3 A CSERKN method (2.15) solving highly oscillatory Hamiltonian systems (2.1) is energy preserving if the coefficients satisfy

$$\begin{aligned} V\phi_0(V)\bar{b}_\tau(V) - V\phi_1(V)b_\tau(V) &= C'_\tau(V), \\ \phi_0(V)b_\tau(V) + V\phi_1(V)\bar{b}_\tau(V) &= D'_\tau(V), \\ b_\tau(V)b_\sigma(V) + V\bar{b}_\tau(V)\bar{b}_\sigma(V) &= \bar{A}'_{\tau\sigma}(V) + \bar{A}'_{\sigma\tau}(V), \end{aligned} \quad (2.21)$$

where $\bar{A}'_{\tau\sigma}(V) = \frac{\partial}{\partial \tau} \bar{A}_{\tau\sigma}(V)$, $C'_\tau(V) = \frac{d}{d\tau} C_\tau(V)$ and $D'_\tau(V) = \frac{d}{d\tau} D_\tau(V)$.

Proof For a CSERKN method (2.15) and Hamiltonian $H(p, q)$ determined by (2.4) with $p = q'$, we have

$$\begin{aligned} &H(p_{n+1}, q_{n+1}) - H(p_n, q_n) \\ &= \frac{1}{2} p_{n+1}^\top p_{n+1} + \frac{1}{2} q_{n+1}^\top M q_{n+1} + U(q_{n+1}) - \frac{1}{2} p_n^\top p_n - \frac{1}{2} q_n^\top M q_n - U(q_n) \\ &= \frac{1}{2} \left(-hM\phi_1(V)q_n + \phi_0(V)p_n + h \int_0^1 b_\tau(V) f(Q_\tau) d\tau \right)^\top \\ &\quad \cdot \left(-hM\phi_1(V)q_n + \phi_0(V)p_n + h \int_0^1 b_\tau(V) f(Q_\tau) d\tau \right) \\ &\quad + \frac{1}{2} \left(\phi_0(V)q_n + h\phi_1(V)p_n + h^2 \int_0^1 \bar{b}_\tau(V) f(Q_\tau) d\tau \right)^\top \\ &\quad \cdot M \left(\phi_0(V)q_n + h\phi_1(V)p_n + h^2 \int_0^1 \bar{b}_\tau(V) f(Q_\tau) d\tau \right) \\ &\quad + \int_0^1 [\nabla U(Q_\tau)]^\top dQ_\tau - \frac{1}{2} p_n^\top p_n - \frac{1}{2} q_n^\top M q_n. \end{aligned} \quad (2.22)$$

After some calculation, we obtain

$$\begin{aligned} &H(p_{n+1}, q_{n+1}) - H(p_n, q_n) \\ &= \frac{1}{2} p_n^\top \left(\phi_0^2(V) + V\phi_1^2(V) \right) p_n - \frac{1}{2} p_n^\top p_n + \frac{1}{2} q_n^\top M \left(\phi_0^2(V) + V\phi_1^2(V) \right) q_n - \frac{1}{2} q_n^\top M q_n \end{aligned}$$

$$\begin{aligned}
& + q_n^\top V \left(\phi_0(V) \int_0^1 \bar{b}_\tau(V) f(Q_\tau) d\tau - \phi_1(V) \int_0^1 b_\tau(V) f(Q_\tau) d\tau \right) \\
& + hp_n^\top \left(\phi_0(V) \int_0^1 b_\tau(V) f(Q_\tau) d\tau + V\phi_1(V) \int_0^1 \bar{b}_\tau(V) f(Q_\tau) d\tau \right) \\
& + \frac{h^2}{2} \left(\int_0^1 b_\tau(V) f(Q_\tau) d\tau \right)^\top \left(\int_0^1 b_\tau(V) f(Q_\tau) d\tau \right) \\
& + \frac{h^2}{2} \left(\int_0^1 \bar{b}_\tau(V) f(Q_\tau) d\tau \right)^\top V \left(\int_0^1 \bar{b}_\tau(V) f(Q_\tau) d\tau \right) \\
& + \int_0^1 [\nabla U(Q_\tau)]^\top d \left(C_\tau(V) q_n + hD_\tau(V) p_n + h^2 \int_0^1 \bar{A}_{\tau\sigma}(V) f(Q_\sigma) d\sigma \right).
\end{aligned} \tag{2.23}$$

It follows from Proposition 2.1 that

$$\begin{aligned}
& H(p_{n+1}, q_{n+1}) - H(p_n, q_n) \\
& = q_n^\top \int_0^1 \left(V\phi_0(V)\bar{b}_\tau(V) - V\phi_1(V)b_\tau(V) - C'_\tau(V) \right) f(Q_\tau) d\tau \\
& + hp_n^\top \int_0^1 \left(\phi_0(V)b_\tau(V) + V\phi_1(V)\bar{b}_\tau(V) - D'_\tau(V) \right) f(Q_\tau) d\tau \\
& + \frac{h^2}{2} \int_0^1 \int_0^1 f(Q_\tau)^\top b_\tau(V) b_\sigma(V) f(Q_\sigma) d\tau d\sigma \\
& + \frac{h^2}{2} \int_0^1 \int_0^1 f(Q_\tau)^\top V\bar{b}_\tau(V)\bar{b}_\sigma(V) f(Q_\sigma) d\tau d\sigma \\
& + h^2 \int_0^1 [\nabla U(Y_\tau)]^\top d \left(\int_0^1 \bar{A}_{\tau\sigma}(V) f(Q_\sigma) d\sigma \right).
\end{aligned}$$

Using the first two equations of (2.21) and $f(Q_\tau) = -\nabla U(Q_\tau)$, we obtain

$$\begin{aligned}
& H(p_{n+1}, q_{n+1}) - H(p_n, q_n) \\
& = \frac{h^2}{2} \int_0^1 \int_0^1 f(Q_\tau)^\top \left(b_\tau(V) b_\sigma(V) + V\bar{b}_\tau(V)\bar{b}_\sigma(V) - 2\bar{A}'_{\tau\sigma}(V) \right) f(Q_\sigma) d\tau d\sigma.
\end{aligned}$$

Letting $\tau \leftrightarrow \sigma$ and adding the resulting identities gives

$$H(p_{n+1}, q_{n+1}) - H(p_n, q_n) = \frac{h^2}{2} \int_0^1 \int_0^1 f(Q_\tau)^\top \left(b_\tau(V) b_\sigma(V) + V \bar{b}_\tau(V) \bar{b}_\sigma(V) \right. \\ \left. - \bar{A}'_{\tau\sigma}(V) - \bar{A}'_{\sigma\tau}(V) \right) f(Q_\sigma) d\tau d\sigma.$$

It then follows from the third equation of (2.21) that $H(p_{n+1}, q_{n+1}) - H(p_n, q_n) = 0$. The proof is complete. \square

Remark 2.4.1 When $V \rightarrow \mathbf{0}$ ($M \rightarrow \mathbf{0}$), the CSERKN method (2.15) reduces to CSRKN method. In this case, the energy-preserving conditions of (2.21) reduce to

$$b_\tau = D'_\tau, \\ b_\tau b_\sigma = \bar{A}'_{\tau\sigma} + \bar{A}'_{\sigma\tau}, \quad (2.24)$$

where $D'_\tau I$, $\bar{A}_{\tau\sigma} I_d$, $\bar{b}_\tau I_d$ and $b_\tau I_d$ are the limit values of $D'_\tau(V)$, $\bar{A}_{\tau\sigma}(V)$, $\bar{b}_\tau(V)$ and $b_\tau(V)$ as $V \rightarrow \mathbf{0}$. It follows from (2.17) that $D_\tau = \tau$ and $b_\tau = 1$. This result has been shown in [59].

A detailed investigation of the numerical integration of reversible systems has been made in [3], and it has been shown that symmetric integration methods often have excellent long-time behaviour for such systems. Therefore, we turn to the discussion about the symmetry of CSERKN methods.

Definition 2.3 (See [3]) The adjoint method Φ_h^* of a method Φ_h is defined as the inverse map of the original method with reversed time step $-h$, i.e., $\Phi_h^* = \Phi_{-h}^{-1}$. A method with $\Phi_h^* = \Phi_h$ is called symmetric.

The following theorem gives the symmetric conditions of CSERKN methods:

Theorem 2.4 A CSERKN methods (2.15) is symmetric if and only if the coefficients satisfy following conditions

$$\phi_1(V) b_\tau(V) - \phi_0(V) \bar{b}_\tau(V) = \bar{b}_{1-\tau}(V), \\ \phi_0(V) b_\tau(V) + V \phi_1(V) \bar{b}_\tau(V) = b_{1-\tau}(V), \\ C_\tau(V) \phi_0(V) + V D_\tau(V) \phi_1(V) = C_{1-\tau}(V), \\ C_\tau(V) \phi_1(V) - D_\tau(V) \phi_0(V) = D_{1-\tau}(V), \\ C_\tau(V) \left(\phi_1(V) b_\sigma(V) - \phi_0(V) \bar{b}_\sigma(V) \right) \\ - D_\tau(V) \left(\phi_0(V) b_\sigma(V) + V \phi_1(V) \bar{b}_\sigma(V) \right) + \bar{A}_{\tau\sigma}(V) = \bar{A}_{1-\tau, 1-\sigma}(V). \quad (2.25)$$

Proof Exchanging $q_{n+1} \leftrightarrow q_n$, $q'_{n+1} \leftrightarrow q'_n$, $t_{n+1} \leftrightarrow t_n$ and replacing h by $-h$ in scheme (2.15) leads to

$$\begin{aligned}\bar{Q}_\tau &= C_\tau(V)q_{n+1} - hD_\tau(V)q'_{n+1} + h^2 \int_0^1 \bar{A}_{\tau\sigma}(V)f(\bar{Q}_\sigma) d\sigma, \\ q_n &= \phi_0(V)q_{n+1} - h\phi_1(V)q'_{n+1} + h^2 \int_0^1 \bar{b}_\tau(V)f(\bar{Q}_\tau) d\tau, \\ q'_n &= hM\phi_1(V)q_{n+1} + \phi_0(V)q'_{n+1} - h \int_0^1 b_\tau(V)f(\bar{Q}_\tau) d\tau.\end{aligned}\tag{2.26}$$

Using (2.26) and Proposition 2.1, we obtain

$$\begin{aligned}q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q'_n \\ &\quad + h^2 \int_0^1 \left(\phi_1(V)b_\tau(V) - \phi_0(V)\bar{b}_\tau(V) \right) f(\bar{Q}_\tau) d\tau, \\ q'_{n+1} &= -hM\phi_1(V)q_n + \phi_0(V)q'_n \\ &\quad + h \int_0^1 \left(\phi_0(V)b_\tau(V) + V\phi_1(V)\bar{b}_\tau(V) \right) f(\bar{Q}_\tau) d\tau, \\ \bar{Q}_\tau &= \left(C_\tau(V)\phi_0(V) + VD_\tau(V)\phi_1(V) \right) q_n + \left(C_\tau(V)\phi_1(V) - D_\tau(V)\phi_0(V) \right) hq'_n \\ &\quad + h^2 \int_0^1 \left[C_\tau(V) \left(\phi_1(V)b_\sigma(V) - \phi_0(V)\bar{b}_\sigma(V) \right) \right. \\ &\quad \left. - D_\tau(V) \left(\phi_0(V)b_\sigma(V) + V\phi_1(V)\bar{b}_\sigma(V) \right) + \bar{A}_{\tau\sigma} \right] f(Q_\sigma) d\sigma.\end{aligned}\tag{2.27}$$

We replace all indices τ and σ by $1 - \tau$ and $1 - \sigma$, respectively, and denote $\bar{Q}_{1-\tau} = Q_\tau$. It is clear that the scheme defined by (2.27) coincides with the scheme (2.15) if and only if the coefficients satisfy the conditions (2.25). This proves the theorem. \square

Remark 2.4.2 When $V \rightarrow \mathbf{0}$ ($M \rightarrow \mathbf{0}$), the CSERKN method (2.15) reduces to a CSRKN method. In this case, the symmetric conditions reduce to

$$\begin{aligned}b_\tau - \bar{b}_\tau &= \bar{b}_{1-\tau}, \quad b_\tau = b_{1-\tau}, \\ b_\sigma - \bar{b}_\sigma - \tau b_\sigma + \bar{A}_{\tau\sigma} &= \bar{A}_{1-\tau, 1-\sigma}.\end{aligned}\tag{2.28}$$

where $\bar{A}_{\tau\sigma}I_d$, $\bar{b}_\tau I_d$ and $b_\tau I_d$ are the limit values of $\bar{A}_{\tau\sigma}(V)$, $\bar{b}_\tau(V)$ and $b_\tau(V)$ as $V \rightarrow \mathbf{0}$. This result has been given in [62].

2.5 Linear Stability Analysis

In order to analyse the stability of CSERKN methods, we consider the following linear scalar test equation

$$q''(t) + \omega^2 q(t) = -\varepsilon q(t), \quad (2.29)$$

where ω represents an estimate of the dominant frequency λ and $\varepsilon = \lambda^2 - \omega^2$ is the error of the estimate. Applying the CSERKN method (2.15) to (2.29) yields

$$\begin{aligned} Q_\tau &= C_\tau(V)q_n + hD_\tau(V)q'_n - z \int_0^1 \bar{A}_{\tau\sigma}(V)Q_\sigma d\sigma, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q'_n - z \int_0^1 \bar{b}_\tau(V)Q_\tau d\tau, \\ hq'_{n+1} &= -V\phi_1(V)q_n + h\phi_0(V)q'_n - z \int_0^1 b_\tau(V)Q_\tau d\tau, \end{aligned} \quad (2.30)$$

where $V = \omega^2 h^2$ and $z = \varepsilon h^2$. Considering Q_τ is a polynomial of degree s with respect to τ , we have

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

where $c_0 = 0$, $c_1 = 1$ and $Q_0 = q_n$, $Q_s = q_{n+1}$, and then obtain

$$\begin{aligned} Q_i &= C_i(V)q_n + hD_i(V)q'_n - z \int_0^1 \bar{A}_{i\sigma}(V) \left(\sum_{j=0}^s L_j(\sigma)Q_j \right) d\sigma, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q'_n - z \int_0^1 \bar{b}_\tau(V) \left(\sum_{i=0}^s L_i(\tau)Q_i \right) d\tau, \\ hq'_{n+1} &= -V\phi_1(V)q_n + h\phi_0(V)q'_n - z \int_0^1 b_\tau(V) \left(\sum_{i=0}^s L_i(\tau)Q_i \right) d\tau, \end{aligned} \quad (2.31)$$

where $C_i(V) = C_{c_i}(V)$, $D_i(V) = D_{c_i}(V)$ and $\bar{A}_{i\sigma}(V) = \bar{A}_{c_i\sigma}(V)$. We can express (2.31) in a vector form

$$\begin{aligned} Q &= C(V)q_n + hD(V)q'_n - z\bar{A}(V)Q, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q'_n - z\bar{B}(V)Q, \\ hq'_{n+1} &= -V\phi_1(V)q_n + h\phi_0(V)q'_n - zB(V)Q, \end{aligned} \quad (2.32)$$

where $Q = (Q_0, \dots, Q_s)^\top$ and

$$\begin{aligned}
 C(V) &= (C_0(V), \dots, C_s(V))^\top, \quad D(V) = (D_0(V), \dots, D_s(V))^\top, \\
 \bar{A}(V) &= \begin{pmatrix} \int_0^1 \bar{A}_{0\sigma}(V)L_0(\sigma)d\sigma & \dots & \int_0^1 \bar{A}_{0\sigma}(V)L_s(\sigma)d\sigma \\ \vdots & \ddots & \vdots \\ \int_0^1 \bar{A}_{s\sigma}(V)L_0(\sigma)d\sigma & \dots & \int_0^1 \bar{A}_{s\sigma}(V)L_s(\sigma)d\sigma \end{pmatrix}, \\
 \bar{B}(V) &= \left(\int_0^1 \bar{b}_\sigma(V)L_0(\sigma)d\sigma, \dots, \int_0^1 \bar{b}_\sigma(V)L_s(\sigma)d\sigma \right), \\
 B(V) &= \left(\int_0^1 b_\sigma(V)L_0(\sigma)d\sigma, \dots, \int_0^1 b_\sigma(V)L_s(\sigma)d\sigma \right).
 \end{aligned}$$

The elimination of the vector Q in (2.32) yields the recursion

$$\begin{pmatrix} q_{n+1} \\ hq'_{n+1} \end{pmatrix} = M(V, z) \begin{pmatrix} q_n \\ hq'_n \end{pmatrix}, \quad (2.33)$$

where

$$M = \begin{pmatrix} \phi_0(V) - z\bar{B}(V)N^{-1}C(V) & \phi_1(V) - z\bar{B}(V)N^{-1}D(V) \\ -V\phi_1(V) - zB(V)N^{-1}C(V) & \phi_0(V) - zB(V)N^{-1}D(V) \end{pmatrix}, \quad (2.34)$$

and $N = I + z\bar{A}(V)$. The matrix M is called the stability matrix. The behaviour of the numerical solution will depend on the spectral radius $\rho(M)$. Geometrically, the characterization of stability involves a two-dimensional region in (V, z) space for a CSERKN method.

Definition 2.4 For the CSERKN method (2.15) with the stability matrix $M(V, z)$, the region of the two-dimensional space

$$\Omega := \{(V, z) : V \geq 0, |\rho(M(V, z))| \leq 1\}$$

is called the region of stability. The closed surface defined by $\rho(M(V, z)) = 1$ and $V \geq 0$ is the stability boundary of the method.

Definition 2.5 Denoting $\zeta = \sqrt{V + z}$, the two quantities

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

are called the dispersion error and the dissipation error of the underlying CSERKN method, respectively. The method is said to be dispersive of order γ and dissipative

of order r , if $\phi(\zeta) = \mathcal{O}(\zeta^{\nu+1})$ and $d(\zeta) = \mathcal{O}(\zeta^{r+1})$, respectively. If $\phi(\zeta) = 0$ or $d(\zeta) = 0$, then the method is said to be zero dispersive or zero dissipative.

2.6 Construction of CSERKN Methods

In this section, we present second and fourth order symmetric and energy-preserving CSERKN schemes. The derivation process of higher-order methods is completely similar. In the construction of the method, we always choose $D_\tau = \tau$, as described in Remark 2.4.1.

In a CSERKN method, there is a restrictive relation between the internal and final stages for the consistency of the method, because q_{n+1} should coincide with Q_{c_s} while $c_s = 1$. Therefore, $\bar{b}_\sigma(V)$ should be expressed as $\bar{b}_\sigma(V) = \bar{A}_{1\sigma}(V)$.

2.6.1 The Case of Order Two

According to Definition 2.2, a one-degree CSERKN formulation has coefficients with the following form:

$$\bar{A}_{\tau\sigma}(V) = \bar{a}_{11}(V)\tau, \quad \bar{b}_\tau(V) = \bar{b}_1(V), \quad b_\tau(V) = b_1(V). \quad (2.35)$$

On the basis of the energy-preserving conditions (2.21), the coefficients satisfy

$$\begin{aligned} \bar{a}_{11}(V) &= \phi_2((c_1 - c_2)^2 V), \\ \bar{b}_1(V) &= \frac{(1 - c_2)^2 \phi_2((1 - c_2)^2 V) - (1 - c_1)^2 \phi_2((1 - c_1)^2 V)}{c_1 - c_2}, \\ b_1(V) &= \frac{(1 - c_2) \phi_1((1 - c_2)^2 V) - (1 - c_1) \phi_1((1 - c_1)^2 V)}{c_1 - c_2}. \end{aligned} \quad (2.36)$$

Under the assumption that the coefficients in (2.36) satisfy the symmetric conditions (2.25), we obtain

$$\begin{aligned} \bar{a}_{11}(V) &= \phi_2\left((2c_1 - 1)^2 V\right), \quad c_2 = 1 - c_1, \\ \bar{b}_1(V) &= \frac{c_1^2 \phi_2(c_1^2 V) - (1 - c_1)^2 \phi_2((1 - c_1)^2 V)}{2c_1 - 1}, \\ b_1(V) &= \frac{c_1 \phi_1(c_1^2 V) - (1 - c_1) \phi_1((1 - c_1)^2 V)}{2c_1 - 1}. \end{aligned} \quad (2.37)$$

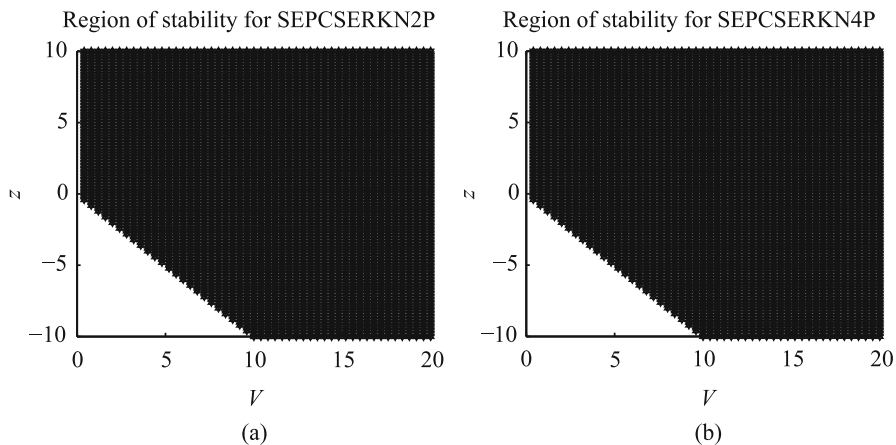


Fig. 2.1 The stability regions of the method SEPCSERKN2P (a) and the method SEPCSERKN4P (b)

Let $\bar{A}_{1\sigma}(V) = \bar{b}_\sigma(V)$ in (2.37), and this gives

$$\begin{aligned} c_1 &= 0, \quad c_2 = 1, \\ \bar{a}_{11}(V) &= \phi_2(V), \quad \bar{b}_1(V) = \phi_2(V), \quad b_1(V) = \phi_1(V). \end{aligned} \quad (2.38)$$

It then can be verified that the coefficients satisfy all the conditions of order two. We denote the CSERKN method determined by (2.38) as SEPCSERKN2P. With regard to the dispersion error and the dissipation error of the method SEPCSERKN2P, we have

$$\phi(\zeta) = \frac{\varepsilon^2 \zeta^3}{12(\varepsilon^2 + w^2)} + \mathcal{O}(\zeta^5), \quad d(\zeta) = 0.$$

This shows that the method is dispersive of order two and zero dissipative, respectively. The stability region of the method SEPCSERKN2P is depicted in Fig. 2.1a.

Remark 2.6.1 Actually, the method SEPCSERKN2P can be expressed as

$$\begin{cases} Q_\tau = (\tau\phi_0(V) + 1 - \tau)q_n + h\tau\phi_1(V)q'_n + h^2\tau \int_0^1 \phi_2(V)f(Q_\sigma) d\sigma, & \tau \in [0, 1], \\ q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q'_n + h^2 \int_0^1 \phi_2(V)f(Q_\tau) d\tau, \\ q'_{n+1} = -hM\phi_1(V)q_n + \phi_0(V)q'_n + h \int_0^1 \phi_1(V)f(Q_\tau) d\tau. \end{cases} \quad (2.39)$$

Using the first two expressions of (2.39), we write Q_τ as a linear combination of q_n and q_{n+1} .

$$Q_\tau = \tau q_{n+1} + (1 - \tau)q_n. \quad (2.40)$$

The method SEPCSERKN2P then can be expressed as

$$\begin{aligned} q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q'_n + h^2\phi_2(V) \int_0^1 f(\tau q_{n+1} + (1 - \tau)q_n) d\tau, \\ q'_{n+1} &= -hM\phi_1(V)q_n + \phi_0(V)q'_n + h\phi_1(V) \int_0^1 f(\tau q_{n+1} + (1 - \tau)q_n) d\tau. \end{aligned} \quad (2.41)$$

This formula (2.41) has been proposed in [63, 64] and is termed the adapted AVF (AAVF) formula in [64]. The authors in [65] studied the application of AAVF formula to Hamiltonian partial differential equations. Therefore, CSERKN methods can be thought of as an extension of the AAVF method (2.41).

2.6.2 The Case of Order Four

A two-degree CSERKN method has the coefficients of the form

$$\begin{aligned} \bar{A}_{\tau\sigma}(V) &= \bar{a}_{11}(V)\tau + \bar{a}_{12}(V)\tau\sigma + \bar{a}_{21}(V)\tau^2 + \bar{a}_{22}(V)\tau^2\sigma, \\ \bar{b}_\tau(V) &= \bar{b}_1(V) + \bar{b}_2(V)\tau, \quad b_\tau(V) = b_1(V) + b_2(V)\tau. \end{aligned} \quad (2.42)$$

It then follows from the first two energy-preserving conditions of (2.21) that

$$\begin{aligned} \bar{b}_1(V) &= \left((-c_2^2 + c_3^2)(1 - c_1)^2\phi_2((1 - c_1)^2V) + (c_1^2 - c_3^2)(1 - c_2)^2\phi_2((1 - c_2)^2V) \right. \\ &\quad \left. + (-c_1^2 + c_2^2)(1 - c_3)^2\phi_2((1 - c_3)^2V) \right) / \left((c_1 - c_2)(c_1 - c_3)(c_2 - c_3) \right), \\ \bar{b}_2(V) &= \left(2((c_2 - c_3)(1 - c_1)^2\phi_2((1 - c_1)^2V) + (-c_1 + c_3)(1 - c_2)^2\phi_2((1 - c_2)^2V) \right. \\ &\quad \left. + (c_1 - c_2)(1 - c_3)^2\phi_2((1 - c_3)^2V)) \right) / \left((c_1 - c_2)(c_1 - c_3)(c_2 - c_3) \right), \end{aligned}$$

$$\begin{aligned}
b_1(V) &= \left((c_2^2 - c_3^2)(1 - c_1)\phi_1((1 - c_1)^2V) + (-c_1^2 + c_3^2)(1 - c_2)\phi_1((1 - c_2)^2V) \right. \\
&\quad \left. + (c_1^2 - c_2^2)(1 - c_3)\phi_1((1 - c_3)^2V) \right) / \left((c_1 - c_2)(c_1 - c_3)(c_2 - c_3) \right), \\
b_2(V) &= 2 \left((-c_2 + c_3)(1 - c_1)\phi_1((1 - c_1)^2V) + (c_1 - c_3)(1 - c_2)\phi_1((1 - c_2)^2V) \right. \\
&\quad \left. + (-c_1 + c_2)(1 - c_3)\phi_1((1 - c_3)^2V) \right) / \left((c_1 - c_2)(c_1 - c_3)(c_2 - c_3) \right).
\end{aligned} \tag{2.43}$$

Using the last energy-preserving conditions of (2.21), we obtain

$$\begin{aligned}
\bar{a}_{11}(V) &= \frac{1}{2} \left(b_1^2(V) + \bar{b}_1^2(V)V \right), \\
\bar{a}_{21}(V) &= \frac{1}{2} \left(-a_{12}(V) + b_1(V)b_2(V) + \bar{b}_1(V)\bar{b}_2(V)V \right), \\
\bar{a}_{22}(V) &= \frac{1}{4} \left(b_2^2(V) + \bar{b}_2^2(V)V \right).
\end{aligned} \tag{2.44}$$

Letting the coefficients in (2.6.2) and (2.44) satisfy the symmetric conditions and $\bar{A}_{1\sigma}(V) = \bar{b}_\sigma(V)$, we obtain

$$\begin{aligned}
c_1 &= 0, \quad c_2 = \frac{1}{2}, \quad c_3 = 1, \quad \bar{a}_{11}(V) = 4\phi_2\left(\frac{1}{4}V\right) - 3\phi_2(V), \\
\bar{a}_{12}(V) &= -\phi_1^2\left(\frac{1}{16}V\right)\left(1 + \frac{V}{4}\phi_2\left(\frac{V}{4}\right)\right), \\
\bar{a}_{21}(V) &= \frac{1}{2}\phi_1^2\left(\frac{1}{16}V\right)\left(1 - \frac{3V}{4}\phi_2\left(\frac{V}{4}\right)\right), \quad \bar{a}_{22}(V) = \frac{V}{4}\phi_1^4\left(\frac{1}{16}V\right), \\
\bar{b}_1(V) &= 3\phi_2\left(V\right) - \phi_2\left(\frac{1}{4}V\right), \quad \bar{b}_2(V) = 2\phi_2\left(\frac{1}{4}V\right) - 4\phi_2(V), \\
b_1(V) &= -2\phi_1\left(\frac{1}{4}V\right) + 3\phi_1(V), \quad b_2(V) = 4\phi_1\left(\frac{1}{4}V\right) - 4\phi_1(V).
\end{aligned} \tag{2.45}$$

It can be verified that the coefficients satisfy all the conditions of order four. We denote the CSERKN method (2.15) determined by (2.45) as SEPCSERKN4P. Concerning the dispersion error and the dissipation error of the method SEPCSERKN4P, we have

$$\phi(\zeta) = \frac{\varepsilon^2(4\varepsilon^2 + 3w^2)\zeta^5}{2880(\varepsilon^2 + w^2)^2} + \mathcal{O}(\zeta^7), \quad d(\zeta) = 0,$$

which indicates that the method SEPCSERKN4P is dispersive of order four and zero dissipative, respectively. The stability region of the method SEPCSERKN4P is depicted in Fig. 2.1b.

2.7 Numerical Experiments

In this section, in order to demonstrate the superiority of the continuous-stage ERKN methods in comparison with the existing methods in the literature, we consider three model problems. Since these methods are implicit, iterative solutions are required. We use fixed point iteration with the tolerance 10^{-15} , and the maximum number of iterations is 100. The integrals appearing in the right-hand side of method (2.15) are integrated by using *quad* with the tolerance 10^{-12} . The integrators we select for comparison are

- EPCSRK2P: The energy-preserving CSRK method of order two derived in [48];
- EPCSRK4P: The energy-preserving CSRK method of order four derived in [48];
- SEPCSERKN2P: The symmetric and energy-preserving CSERKN method of order two presented in Sect. 2.6 of this chapter;
- SEPCSERKN4P: The symmetric and energy-preserving CSERKN method of order four presented in Sect. 2.6 of this chapter.

The numerical results are executed on the computer Lenovo M6600 (Inter(R) Pentium(R) CPU 3.00 GHz, 0.99 GB), and the programming language MATLAB is used.

Problem 2.1 We consider the Duffing equation

$$\begin{cases} q'' + \omega^2 q = 2k^2 q^3 - k^2 q, & t \in [0, t_{\text{end}}], \\ q(0) = 0, & q'(0) = \omega. \end{cases} \quad (2.46)$$

The Hamiltonian is given by

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

where $k = 0.03$. The exact solution of this initial-value problem is $q(t) = sn(\omega t; k/\omega)$, where sn is the so-called Jacobian elliptic function. We choose the frequency $\omega = 50$ in this experiment. Accordingly, this is a highly oscillatory Hamiltonian system.

We first solve this problem on the interval $[0, 100]$ with the stepsizes $h = 1/2^j$ for $j = 4, \dots, 7$ for each method. We then integrate the problem with a fixed stepsize $h = 1/100$ on the interval $[0, 100]$ to examine the preservation of the Hamiltonian for the four methods. The numerical results are presented in Fig. 2.2.

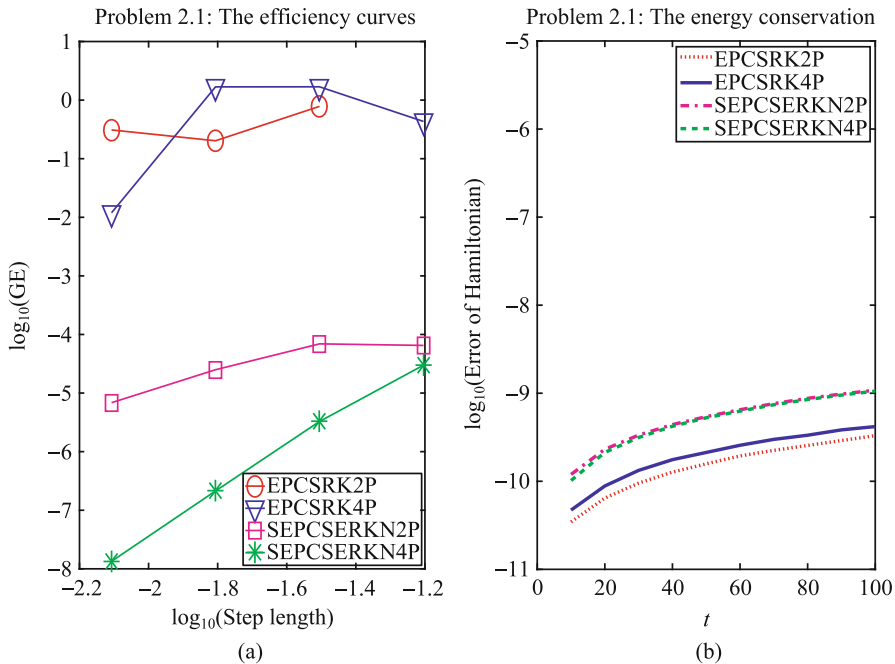


Fig. 2.2 Efficiency curves (a) and energy conservation (b) for Problem 2.1

Problem 2.2 We consider the two coupled oscillators with different frequencies [17]

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

The Hamiltonian of this system is given by

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

In this numerical experiment we choose $\varepsilon = 10^{-3}$. We first solve this problem on the interval $[0, 100]$ with the stepsizes $h = 1/2^j$ for $j = 2, \dots, 5$ for all the methods. We then integrate the problem with a fixed stepsize $h = 1/10$ on $[0, 100]$ and examine the preservation of the Hamiltonian. The numerical results are presented in Fig. 2.3.

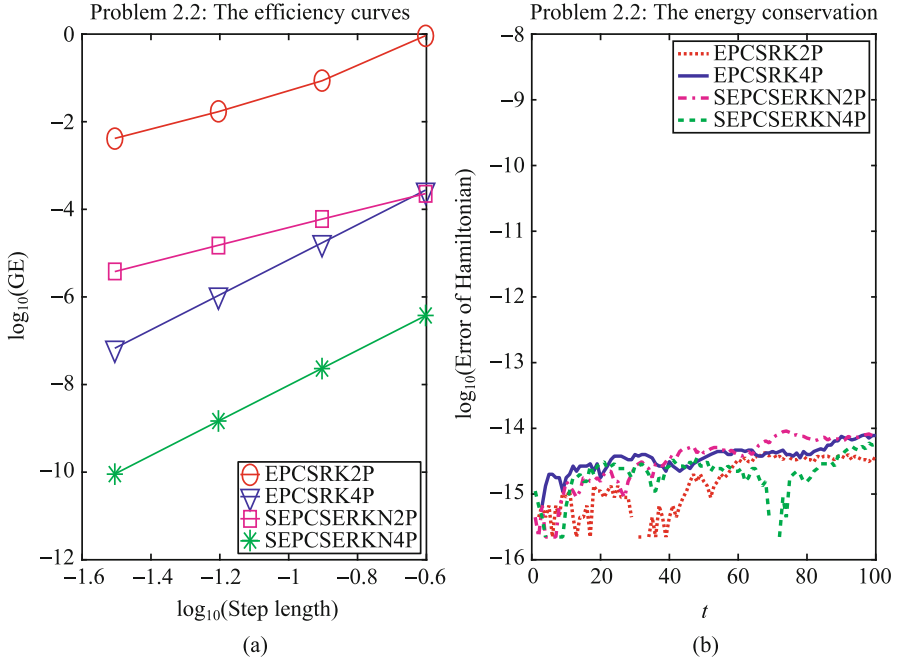


Fig. 2.3 Efficiency curves (a) and energy conservation (b) for Problem 2.2

Problem 2.3 Consider the semilinear wave equation

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = -\frac{1}{5}u^3, & 0 < x < 1, \quad t > 0, \\ u(0, t) = u(1, t) = 0, \quad u(x, 0) = \frac{\sin(\pi x)}{2}, \quad u_t(x, 0) = 0. \end{cases}$$

By using second-order symmetric differences, this problem is converted into a system of ODEs in time

$$\begin{cases} \frac{d^2 u_i}{dt^2} - \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = -\frac{1}{5}u_i^3, & 0 < t \leq t_{\text{end}}, \\ u_i(0) = \frac{\sin(\pi x_i)}{2}, \quad u'_i(0) = 0, \quad i = 1, \dots, N-1, \end{cases}$$

where $\Delta x = 1/N$ is the spatial mesh stepsize and $x_i = i\Delta x$. Then this semidiscrete oscillatory system has the form

$$\begin{cases} \frac{d^2 U}{dt^2} + MU = F(U), & 0 < t \leq t_{\text{end}}, \\ U(0) = \left(\frac{\sin(\pi x_1)}{2}, \dots, \frac{\sin(\pi x_{N-1})}{2} \right)^\top, \quad U'(0) = \mathbf{0}, \end{cases}$$

where $U(t) = (u_1(t), \dots, u_{N-1}(t))^T$ with $u_i(t) \approx u(x_i, t)$ for $i = 1, \dots, N-1$, and

$$M = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix}, \quad (2.47)$$

$$F(U) = \left(-\frac{1}{5}u_1^3, \dots, -\frac{1}{5}u_{N-1}^3 \right)^T.$$

The Hamiltonian of this system is given by

$$H(p, q) = \frac{1}{2}p^T p + \frac{1}{2}q^T M q + \frac{1}{20}e^T q^4,$$

where $e = (1, \dots, 1)^T$. In this numerical experiment we choose $N = 100$. We first solve this problem on the interval $[0, 100]$ with the stepsizes $h = 1/2^j$ for $j = 5, \dots, 8$. We then integrate the problem with a fixed stepsize $h = 1/128$ on $[0, 100]$ and examine the preservation of the Hamiltonian by each code. The numerical results are shown in Fig. 2.4.

It can be observed from Figs. 2.2, 2.3, and 2.4 of the three numerical experiments that the right-hand figures show all the integrators derived in this chapter preserve the Hamiltonian well. The results of the numerical experiments confirm that, for a given stepsize h , the SEPCSERKN integrators are more accurate than EPCSRK methods with the same convergence order.

Remark 2.7.1 In general, the computational cost per step of high order methods is larger than that of low order methods. In order to objectively evaluate these effects, we present in Fig. 2.5 the error versus CPU time for each problem, which indicates that SEPCSERKN4P is the best of these four methods. The related data are the same as those shown in Figs. 2.2a, 2.3a, and 2.4a.

2.8 Conclusions and Discussions

In this chapter, we derived and analysed continuous-stage extended Runge–Kutta–Nyström (CSERKN) methods for (2.1). This class of CSERKN methods is oscillation preserving since the internal stages and the updates exactly integrate the highly oscillatory homogeneous system (2.2) associated with (2.1). Symmetric and energy-preserving conditions for CSERKN methods were derived and analysed for highly oscillatory Hamiltonian systems. In terms of these conditions, two symmetric

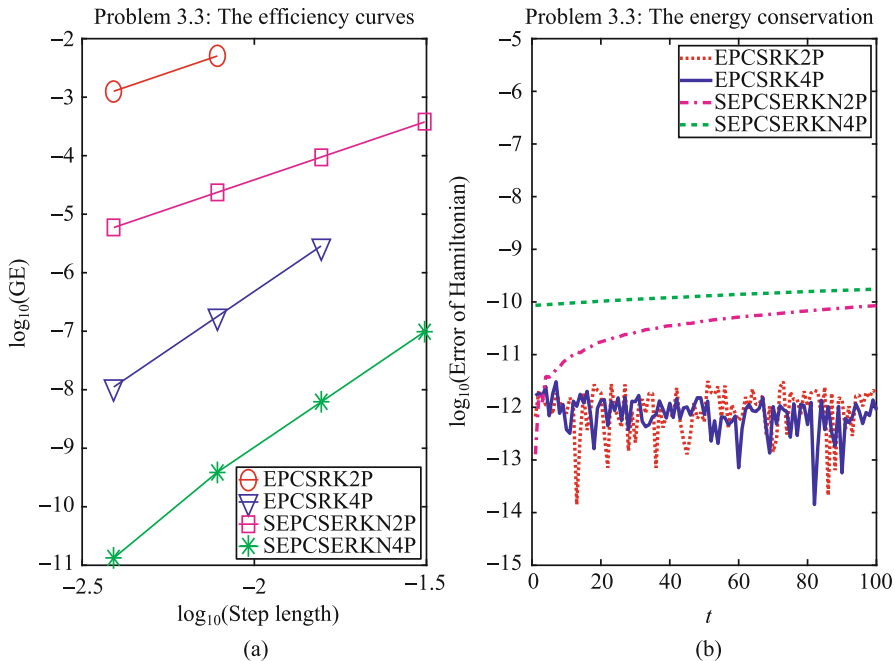


Fig. 2.4 Efficiency curves (a) and energy conservation (b) for Problem 3.3

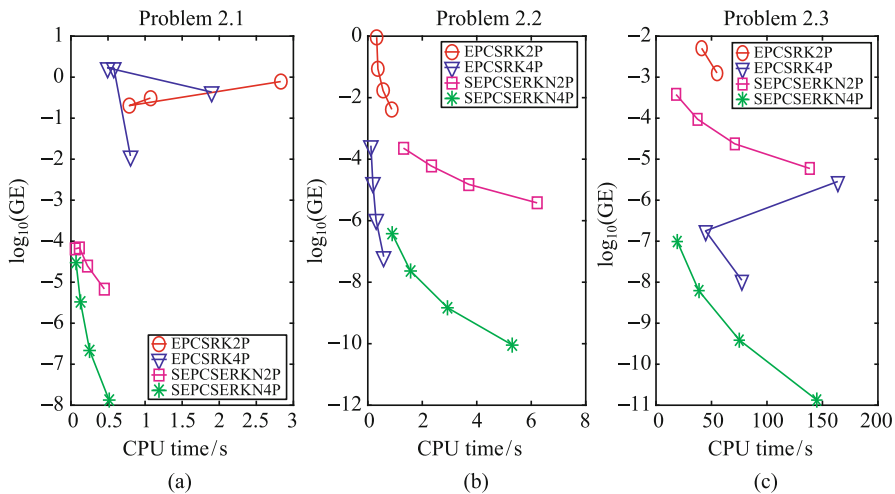


Fig. 2.5 The error versus CPU time for three problems

and energy-preserving CSERKN methods were constructed, of orders two and four respectively. The results of the numerical experiments show that the energy-preserving CSERKN methods preserve the energy well, and are more accurate than EPCSRK methods.

CSERKN methods for semilinear Hamiltonian wave equations could be investigated further. We expect that they may exactly preserve the energy of the underlying Hamiltonian wave equations, including the Klein–Gordon (KG) equation which has received a great deal of attention, both numerical and analytical. We refer the reader to [65] for this topic. A promising approach to the approximation is based on the so-called operator-variation-constants formula (the Duhamel Principle), and we refer the reader to some relevant papers [66–68]. In Chap. 11, symplectic approximations will be derived and analysed in detail for efficiently solving semilinear KG equations. Moreover, continuous-stage leap-frog schemes for semilinear Hamiltonian wave equations will be presented in Chap. 12.

The material in this chapter is based on the work by Li and Wu [69].

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