

Chapter 5

Exponential Collocation Methods for Conservative or Dissipative Systems



The main purpose of this chapter is to present exponential collocation methods (ECMs) for solving conservative or dissipative systems. ECMs can be of arbitrarily high order and preserve exactly or approximately first integrals or Lyapunov functions. In particular, the application of ECMs to stiff gradient systems is discussed in detail, and it turns out that ECMs are unconditionally energy-diminishing and strongly damped even for very stiff gradient systems. As a consequence of this discussion, arbitrary-order trigonometric/RKN collocation methods are also presented and analysed for second-order highly oscillatory/general systems. The chapter is accompanied by numerical results that demonstrate the potential value of this research.

5.1 Introduction

In this chapter, we consider systems of ordinary differential equations (ODEs) of the form

$$y'(t) = Q\nabla H(y(t)), \quad y(0) = y_0 \in \mathbb{R}^d, \quad t \in [0, T], \quad (5.1)$$

where Q is an invertible and $d \times d$ real matrix, and $H : \mathbb{R}^d \rightarrow \mathbb{R}$ is defined by

$$H(y) = \frac{1}{2}y^\top My + V(y). \quad (5.2)$$

Here M is a $d \times d$ symmetric real matrix, and $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is a differentiable function.

It is important to note that the system (5.1) exhibits remarkable geometrical/physical structures, which should be preserved by a numerical method in the spirit of geometric numerical integration. In fact, if the matrix Q is skew symmetric, then (5.1) is a conservative system with the first integral H : i.e.,

$$H(y(t)) \equiv H(y_0) \quad \text{for any } t \geq 0.$$

If the matrix Q is negative semi-definite, then (5.1) is a dissipative system with the Lyapunov function H : i.e.,

$$H(y(t_2)) \leq H(y(t_1)) \quad \text{if } t_2 \geq t_1.$$

Throughout this chapter, we call H energy for both cases in a broad sense. The objective of this chapter is to design and analyse a class of arbitrary-order exponential energy-preserving collocation methods which can preserve first integrals or Lyapunov functions of the underlying conservative/dissipative system (5.1).

It is convenient to express

$$A = QM, \quad g(y(t)) = Q\nabla V(y(t)).$$

We then rewrite the system (5.1) as

$$y'(t) = Ay(t) + g(y(t)), \quad y(0) = y_0 \in \mathbb{R}^d. \quad (5.3)$$

As is known, the exact solution of (5.1) or (5.3) can be represented by the variation-of-constants formula (the Duhamel Principle)

$$y(t) = e^{tA}y_0 + t \int_0^1 e^{(1-\tau)tA} g(y(\tau)) d\tau. \quad (5.4)$$

The system (5.1) or (5.3) plays a prominent role in a wide range of applications in physics and engineering, including mechanics, astronomy, molecular dynamics, and in problems of wave propagation in classical and quantum physics (see, e.g. [1–4]). Some highly oscillatory problems and semidiscrete PDEs such as semilinear Schrödinger equations fit this pattern. Among typical examples are the multi-frequency highly oscillatory Hamiltonian systems with the Hamiltonian

$$H(p, q) = \frac{1}{2}p^\top \bar{M}^{-1}p + \frac{1}{2}q^\top \bar{K}q + U(q), \quad (5.5)$$

where \bar{K} is a symmetric positive semi-definite stiffness matrix, \bar{M} is a symmetric positive definite mass matrix, and $U(q)$ is a smooth potential with moderately bounded derivatives.

As an interesting class of numerical methods for (5.3), exponential integrators have been widely investigated and developed in recent decades, and we refer the reader to [5–17] for example. Exponential integrators make good use of the variation-of-constants formula (5.4), and their performance has been evaluated on a range of test problems. A systematic survey of exponential integrators is presented in [2]. However, apart from symplectic exponential integrators (see, e.g. [18]), most existing publications dealing with exponential integrators focus on the construction and analysis of the schemes and pay little attention to energy-preserving exponential integrators which can preserve the first integrals/Lyapunov functions. Energy-preserving exponential integrators, especially higher-order schemes have not been well researched yet in the literature.

On the other hand, various effective energy-preserving methods have been proposed and researched for (5.3) in the special case of $A = 0$, such as the average vector field (AVF) method [19–21], discrete gradient (DG) methods [22–24], Hamiltonian Boundary Value Methods (HBVMs) [25–28], the Runge–Kutta-type energy-preserving collocation (RKEPC) methods [29, 30], time finite elements (TFE) methods [31–35], and energy-preserving exponentially-fitted (EPEF) methods [36, 37]. Some numerical methods preserving Lyapunov functions have also been studied for (5.3) with $A = 0$ (see, e.g. [38–40]). It is noted that all these methods are constructed and studied for the special case $A = 0$ and thus they do not take advantage of the structure brought by the linear term Ay in the system (5.3). These methods could be applied to (5.3) with $A \neq 0$ if the right-hand side of (5.3) is considered as a whole (function), i.e., $y' = f(y) \equiv Ay + g(y)$.

Recently, in order to take advantage of the structure of the underlying system and preserve its energy simultaneously, a novel energy-preserving method has been studied in [41, 42] for second-order ODEs and a new energy-preserving exponential scheme for the conservative or dissipative system has been researched in [43]. However, those two kinds of methods are both based on the AVF methods and thence they are only of order two, in general. This may not be sufficient to deal with some practical problems for high-precision numerical simulations in sciences and engineering.

On noting the above observation, we are concerned in this chapter with deriving and analysing structure-preserving exponential collocation methods. To this end we make good use of the variation-of-constants formula and the structure introduced by the underlying system. These exponential integrators can in such a way exactly or approximately preserve the first integral or the Lyapunov function of (5.1). Very recently, there have been some publications on the numerical solution of Hamiltonian PDEs, and the analysis is related to the approach of this chapter (see, e.g. [44–48]).

5.2 Formulation of Methods

Following [34], we begin by defining the finite-dimensional function spaces Y_h as follows:

$$Y_h = \text{span} \{ \tilde{\varphi}_0(\tau), \dots, \tilde{\varphi}_{r-1}(\tau) \} \\ = \left\{ \tilde{w} : \tilde{w}(\tau) = \sum_{i=0}^{r-1} \tilde{\varphi}_i(\tau) W_i, \tau \in [0, 1], W_i \in \mathbb{R}^d \right\}, \quad (5.6)$$

where $\{\tilde{\varphi}_i\}_{i=0}^{r-1}$ are supposed to be linearly independent on $I = [0, T]$ and sufficiently smooth. We use $\tilde{\varphi}_i(\tau)$ to denote $\varphi_i(\tau h)$ for all the functions φ_i throughout this chapter and $h > 0$ is the stepsize. With this definition, we consider another finite-dimensional function space X_h such that $\tilde{w}' \in Y_h$ for any $\tilde{w} \in X_h$.

We introduce the idea of the formulation of methods. Find $\tilde{u}(\tau)$ with $\tilde{u}(0) = y_0$, satisfying

$$\tilde{u}'(\tau) = A\tilde{u}(\tau) + \mathcal{P}_h g(\tilde{u}(\tau)), \quad (5.7)$$

where the projection operation \mathcal{P}_h is given by (see [34])

$$\langle \tilde{v}(\tau), \mathcal{P}_h \tilde{w}(\tau) \rangle = \langle \tilde{v}(\tau), \tilde{w}(\tau) \rangle \quad \text{for any } \tilde{v}(\tau) \in Y_h \quad (5.8)$$

and the inner product $\langle \cdot, \cdot \rangle$ is defined by (see [34])

$$\langle w_1, w_2 \rangle = \langle w_1(\tau), w_2(\tau) \rangle_\tau = \int_0^1 w_1(\tau) \cdot w_2(\tau) d\tau.$$

With regard to the projection operation \mathcal{P}_h , we have the following property (see [34]) which is needed in this chapter.

Lemma 5.1 *The projection $\mathcal{P}_h \tilde{w}$ can be explicitly expressed as*

$$\mathcal{P}_h \tilde{w}(\tau) = \langle P_{\tau, \sigma}, \tilde{w}(\sigma) \rangle_\sigma,$$

where

$$P_{\tau, \sigma} = (\tilde{\varphi}_0(\tau), \dots, \tilde{\varphi}_{r-1}(\tau)) \Theta^{-1} (\tilde{\varphi}_0(\sigma), \dots, \tilde{\varphi}_{r-1}(\sigma))^\top, \\ \Theta = ((\tilde{\varphi}_i(\tau), \tilde{\varphi}_j(\tau)))_{0 \leq i, j \leq r-1}. \quad (5.9)$$

When h tends to 0, the limit of $P_{\tau, \sigma}$ exists. If $P_{\tau, \sigma}$ is computed by a standard orthonormal basis $\{\tilde{\psi}_0, \dots, \tilde{\psi}_{r-1}\}$ of Y_h under the inner product $\langle \cdot, \cdot \rangle$, then Θ

is an identity matrix and $P_{\tau,\sigma}$ has a simpler expression:

$$P_{\tau,\sigma} = \sum_{i=0}^{r-1} \tilde{\psi}_i(\tau) \tilde{\psi}_i(\sigma). \quad (5.10)$$

As $\tilde{u}(\tau) = u(\tau h)$, (5.7) can be expressed in

$$u'(\tau h) = Au(\tau h) + \langle P_{\tau,\sigma}, g(u(\sigma h)) \rangle_{\sigma}.$$

Applying the variation-of-constants formula (5.4) to (5.7), we obtain

$$\begin{aligned} \tilde{u}(\tau) = u(\tau h) &= e^{\tau h A} y_0 + \tau h \int_0^1 e^{(1-\xi)\tau h A} \langle P_{\xi\tau,\sigma}, g(u(\sigma h)) \rangle_{\sigma} d\xi \\ &= e^{\tau h A} y_0 + \tau h \int_0^1 e^{(1-\xi)\tau h A} \langle P_{\xi\tau,\sigma}, g(\tilde{u}(\sigma)) \rangle_{\sigma} d\xi \end{aligned} \quad (5.11)$$

Inserting (5.10) into (5.11) yields

$$\begin{aligned} \tilde{u}(\tau) &= e^{\tau h A} y_0 + \tau h \int_0^1 e^{(1-\xi)\tau h A} \int_0^1 \sum_{i=0}^{r-1} \tilde{\psi}_i(\xi\tau) \tilde{\psi}_i(\sigma) g(\tilde{u}(\sigma)) d\sigma d\xi \\ &= e^{\tau h A} y_0 + \tau h \int_0^1 \sum_{i=0}^{r-1} \int_0^1 e^{(1-\xi)\tau h A} \tilde{\psi}_i(\xi\tau) d\xi \tilde{\psi}_i(\sigma) g(\tilde{u}(\sigma)) d\sigma. \end{aligned}$$

We are now in a position to define exponential collocation methods.

Definition 5.1 An exponential collocation method for solving the system (5.1) or (5.3) is defined as follows:

$$\tilde{u}(\tau) = e^{\tau h A} y_0 + \tau h \int_0^1 \bar{A}_{\tau,\sigma}(A) g(\tilde{u}(\sigma)) d\sigma, \quad y_1 = \tilde{u}(1), \quad (5.12)$$

where h is a stepsize,

$$\bar{A}_{\tau,\sigma}(A) = \int_0^1 e^{(1-\xi)\tau h A} P_{\xi\tau,\sigma} d\xi = \sum_{i=0}^{r-1} \int_0^1 e^{(1-\xi)\tau h A} \tilde{\psi}_i(\xi\tau) d\xi \tilde{\psi}_i(\sigma), \quad (5.13)$$

and $\{\tilde{\psi}_0, \dots, \tilde{\psi}_{r-1}\}$ is a standard orthonormal basis of Y_h . We denote the method as ECr.

Remark 5.1 Once the stepsize h is chosen, the method (5.12) approximates the solution of (5.1) in the time interval I_0 . Obviously, the obtained result can be considered as the initial condition for a new initial value problem and it can be approximated in the next time interval I_1 . In general, the method can be extended to the approximation of the solution in the interval $[0, T]$.

Remark 5.2 It can be observed that the ECr method (5.12) exactly integrates the homogeneous linear system $y' = Ay$. The scheme (5.12) can be classified into the category of exponential integrators (which can be thought of as continuous-stage exponential integrators). This is an interesting and important class of numerical methods for first-order ODEs (see, e.g. [2, 13, 14, 49, 50]). In [43], the authors researched a new energy-preserving exponential scheme for the conservative or dissipative system. Here we note that its order is only two since this scheme combines the ideas of DG and AVF methods. We have proposed a kind of arbitrary-order exponential Fourier collocation methods in [16]. However, those methods cannot preserve energy exactly. Fortunately, we will show that the ECr method (5.12) can be of arbitrarily high order and can preserve energy exactly or approximately, and which is different from the existing exponential integrators in the literature. This feature is significant and makes the methods more efficient and robust.

Remark 5.3 In the case of $M = 0$ and $Q = \begin{pmatrix} O_{d_1 \times d_1} & -I_{d_1 \times d_1} \\ I_{d_1 \times d_1} & O_{d_1 \times d_1} \end{pmatrix}$, (5.1) is a Hamiltonian system. In this special case, if we choose X_h and Y_h as

$$Y_h = \text{span} \{ \tilde{\varphi}_0(\tau), \dots, \tilde{\varphi}_{r-1}(\tau) \},$$

$$X_h = \text{span} \left\{ 1, \int_0^\tau \tilde{\varphi}_0(s) ds, \dots, \int_0^\tau \tilde{\varphi}_{r-1}(s) ds \right\},$$

then the ECr method (5.12) becomes the following energy-preserving Runge–Kutta type collocation methods

$$\tilde{u}(\tau) = y_0 + \tau h \int_0^1 \int_0^1 P_{\xi\tau,\sigma} d\xi g(\tilde{u}(\sigma)) d\sigma, \quad y_1 = \tilde{u}(1),$$

which yields the functionally-fitted TFE method derived in [34]. Moreover, under the above choices of M and Q , if Y_h is particularly generated by the shifted Legendre polynomials on $[0, 1]$, then the ECr method (5.12) reduces to the RKEPC method of order $2r$ given in [30] or HBVM(∞, r) presented in [26]. Consequently, the ECr method (5.12) can be regarded as a generalisation of these existing methods in the literature.

5.3 Methods for Second-Order ODEs with Highly Oscillatory Solutions

We first consider the following systems of second-order ODEs with highly oscillatory solutions

$$q''(t) - Nq'(t) + \Upsilon q(t) = -\nabla U(q(t)), \quad q(0) = q_0, \quad q'(0) = q'_0, \quad t \in [0, T], \quad (5.14)$$

where N is a symmetric negative semi-definite matrix, Υ is a symmetric positive semi-definite matrix, and $U : \mathbb{R}^d \rightarrow \mathbb{R}$ is a differentiable function. By introducing $p = q'$, (5.14) can be transformed into

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} 0 & I \\ -I & N \end{pmatrix} \nabla H(p, q) \quad (5.15)$$

with

$$H(p, q) = \frac{1}{2} p^\top p + \frac{1}{2} q^\top \Upsilon q + U(q). \quad (5.16)$$

This is exactly the same as the problem (5.1). Since N is symmetric negative semi-definite, (5.15) is a dissipative system with the Lyapunov function (5.16). In the particular case $N = 0$, (5.15) becomes a conservative Hamiltonian system with the first integral (5.16). This is an important highly oscillatory system which has been investigated by many researchers (see, e.g. [4, 51–58]).

Applying the ECr method (5.12) to (5.15) yields the trigonometric collocation method for second-order highly oscillatory systems. In particular, for Hamiltonian systems

$$q''(t) + \Upsilon q(t) = -\nabla U(q(t)), \quad (5.17)$$

the case where $N = 0$ in (5.14), the ECr method (5.12) leads to the following form.

Definition 5.2 The trigonometric collocation (denoted by TCr) method for (5.17) is defined as:

$$\begin{cases} \tilde{q}(\tau) = \phi_0(K)q_0 + \tau h \phi_1(K)p_0 - \tau^2 h^2 \int_0^1 \mathcal{A}_{\tau,\sigma}(K) f(\tilde{q}(\sigma)) d\sigma, & q_1 = \tilde{q}(1), \\ \tilde{p}(\tau) = -\tau h \Upsilon \phi_1(K)q_0 + \phi_0(K)p_0 - \tau h \int_0^1 \mathcal{B}_{\tau,\sigma}(K) f(\tilde{q}(\sigma)) d\sigma, & p_1 = \tilde{p}(1), \end{cases} \quad (5.18)$$

where $K = \tau^2 h^2 \Upsilon$, $f(q) = \nabla U(q)$,

$$\phi_i(K) := \sum_{l=0}^{\infty} \frac{(-1)^l K^l}{(2l+i)!},$$

for $i = 0, 1, \dots$, and

$$\begin{aligned} \mathcal{A}_{\tau,\sigma}(K) &= \sum_{i=0}^{r-1} \int_0^1 (1-\xi) \phi_i((1-\xi)^2 K) \tilde{\psi}_i(\xi\tau) d\xi \tilde{\psi}_i(\sigma), \\ \mathcal{B}_{\tau,\sigma}(K) &= \sum_{i=0}^{r-1} \int_0^1 \phi_i((1-\xi)^2 K) \tilde{\psi}_i(\xi\tau) d\xi \tilde{\psi}_i(\sigma). \end{aligned} \quad (5.19)$$

Remark 5.4 In [59], the authors developed and researched a type of trigonometric Fourier collocation methods for second-order ODEs $q''(t) + Mq(t) = f(q(t))$. However, as shown in [59], those methods cannot preserve the energy exactly. From the analysis to be presented in this chapter, it turns out that the trigonometric collocation scheme (5.18) derived here can attain arbitrary algebraic order and can preserve the energy of (5.16) exactly or approximately.

Remark 5.5 It is remarked that the multi-frequency highly oscillatory Hamiltonian system (5.5) is a kind of second-order system $q''(t) + \bar{M}^{-1} \bar{K} q(t) = -\bar{M}^{-1} \nabla U(q(t))$ and applying the ECr method (5.12) to it leads to the TCr method (5.18) with $K = \tau^2 h^2 \bar{M}^{-1} \bar{K}$ and $f(q) = \bar{M}^{-1} \nabla U(q)$.

In the special case where $N = 0$ and $\Upsilon = 0$, the system (5.14) reduces to the conventional second-order ODEs

$$q''(t) = -\nabla U(q(t)), \quad q(0) = q_0, \quad q'(0) = q'_0, \quad t \in [0, T]. \quad (5.20)$$

Then the TCr method has the following form.

Definition 5.3 A TCr method for solving (5.20) is defined as

$$\begin{cases} \tilde{q}(\tau) = q_0 + \tau h p_0 - \tau^2 h^2 \int_0^1 \bar{\mathcal{A}}_{\tau,\sigma} \nabla U(\tilde{q}(\sigma)) d\sigma, & q_1 = \tilde{q}(1), \\ \tilde{p}(\tau) = p_0 - \tau h \int_0^1 \bar{\mathcal{B}}_{\tau,\sigma} \nabla U(\tilde{q}(\sigma)) d\sigma, & p_1 = \tilde{p}(1), \end{cases} \quad (5.21)$$

where

$$\bar{\mathcal{A}}_{\tau,\sigma} = \sum_{i=0}^{r-1} \int_0^1 (1-\xi) \tilde{\psi}_i(\xi\tau) d\xi \tilde{\psi}_i(\sigma), \quad \bar{\mathcal{B}}_{\tau,\sigma} = \sum_{i=0}^{r-1} \int_0^1 \tilde{\psi}_i(\xi\tau) d\xi \tilde{\psi}_i(\sigma). \quad (5.22)$$

This scheme looks like a continuous-stage RKN method, and is denoted by RKNCr in this chapter.

5.4 Energy-Preserving Analysis

In this section, we analyse the energy-preserving property of the ECr methods.

Theorem 5.1 *If Q is skew symmetric and $\tilde{u}(\tau) \in X_h$, the first integral H determined by (5.2) of the conservative system (5.1) can be preserved exactly by the ECr method (5.12): i.e., $H(y_1) = H(y_0)$. If $\tilde{u}(\tau) \notin X_h$, the ECr method (5.12) approximately preserves the energy H with the following accuracy $H(y_1) = H(y_0) + \mathcal{O}(h^{2r+1})$.*

Proof We begin with the first part of this proof under the assumption that Q is skew symmetric and $\tilde{u}(\tau) \in X_h$. It follows from $\tilde{u}(\tau) \in X_h$ that $\tilde{u}'(\tau) \in Y_h$ and $Q^{-1}\tilde{u}'(\tau) \in Y_h$. Then, in the light of (5.8), we obtain

$$\begin{aligned} \int_0^1 \tilde{u}'(\tau)^\top (Q^{-1})^\top \tilde{u}'(\tau) d\tau &= \int_0^1 \tilde{u}'(\tau)^\top (Q^{-1})^\top (A\tilde{u}(\tau) + \mathcal{P}_h g(\tilde{u}(\tau))) d\tau \\ &= \int_0^1 \tilde{u}'(\tau)^\top (Q^{-1})^\top (A\tilde{u}(\tau) + g(\tilde{u}(\tau))) d\tau. \end{aligned}$$

Here Q is skew symmetric, so is Q^{-1} . We then have

$$0 = \int_0^1 \tilde{u}'(\tau)^\top (Q^{-1})^\top \tilde{u}'(\tau) d\tau = - \int_0^1 \tilde{u}'(\tau)^\top Q^{-1} (A\tilde{u}(\tau) + g(\tilde{u}(\tau))) d\tau.$$

On the other hand, it is clear that

$$H(y_1) - H(y_0) = \int_0^1 \frac{d}{d\tau} H(\tilde{u}(\tau)) d\tau = h \int_0^1 \tilde{u}'(\tau)^\top \nabla H(\tilde{u}(\tau)) d\tau.$$

It follows from (5.1) and (5.3) that

$$\nabla H(\tilde{u}(\tau)) = Q^{-1} (A\tilde{u}(\tau) + g(\tilde{u}(\tau))).$$

Therefore, we obtain

$$H(y_1) - H(y_0) = h \int_0^1 \tilde{u}'(\tau)^\top Q^{-1} (A\tilde{u}(\tau) + g(\tilde{u}(\tau))) d\tau = h \cdot 0 = 0.$$

We next prove the second part of this theorem under the assumption that $\tilde{u}(\tau) \notin X_h$. With the above analysis for the first part of the proof, we have

$$\begin{aligned}
& H(y_1) - H(y_0) \\
&= h \int_0^1 \tilde{u}'(\tau)^\top Q^{-1} (A\tilde{u}(\tau) + g(\tilde{u}(\tau))) d\tau \\
&= h \int_0^1 \tilde{u}'(\tau)^\top Q^{-1} (A\tilde{u}(\tau) + \mathcal{P}_h g(\tilde{u}(\tau)) + g(\tilde{u}(\tau)) - \mathcal{P}_h g(\tilde{u}(\tau))) d\tau \\
&= -h \int_0^1 \tilde{u}'(\tau)^\top (Q^{-1})^\top \tilde{u}'(\tau) d\tau + h \int_0^1 \tilde{u}'(\tau)^\top Q^{-1} (g(\tilde{u}(\tau)) - \mathcal{P}_h g(\tilde{u}(\tau))) d\tau \\
&= h \int_0^1 \tilde{u}'(\tau)^\top Q^{-1} (g(\tilde{u}(\tau)) - \mathcal{P}_h g(\tilde{u}(\tau))) d\tau.
\end{aligned}$$

Exploiting Lemma 3.4 presented in [34] and Lemma 5.2 proved in Sect. 5.6, we obtain $\tilde{u}'(\tau) = \mathcal{P}_h \tilde{u}'(\tau) + \mathcal{O}(h^r)$. Therefore, one arrives at

$$\begin{aligned}
& H(y_1) - H(y_0) \\
&= h \int_0^1 (\mathcal{P}_h \tilde{u}'(\tau) + \mathcal{O}(h^r))^\top Q^{-1} (g(\tilde{u}(\tau)) - \mathcal{P}_h g(\tilde{u}(\tau))) d\tau \\
&= h \int_0^1 (\mathcal{P}_h \tilde{u}'(\tau))^\top Q^{-1} (g(\tilde{u}(\tau)) - \mathcal{P}_h g(\tilde{u}(\tau))) d\tau + \mathcal{O}(h^{2r+1}) \\
&= h \int_0^1 (\mathcal{P}_h \tilde{u}'(\tau))^\top Q^{-1} (g(\tilde{u}(\tau)) - g(\tilde{u}(\tau))) d\tau + \mathcal{O}(h^{2r+1}) = \mathcal{O}(h^{2r+1}),
\end{aligned}$$

where the result (5.28) in Sect. 5.6 is used.

The proof is complete. \square

Remark 5.6 It is noted that for the special case $g(y) = 0$ or $A = 0$, it is easy to choose Y_h and X_h such that $\tilde{u}(\tau) \in X_h$. For the case $A \neq 0$ and $g(y) \equiv C$, if we consider $Y_h = \text{span}\{1, e^{\tau h A}\}$ and $X_h = \text{span}\{1, \tau h, e^{\tau h A}\}$, it follows from (5.12) that $\tilde{u}(\tau) = e^{\tau h A} y_0 + A^{-1}(e^{\tau h A} - I)C$. This also leads to $\tilde{u}(\tau) \in X_h$. However, for the general situation, it is usually not easy to check whether the fact $\tilde{u}(\tau) \in X_h$ is true or not for the considered Y_h and X_h . Therefore, we present the results for two different cases $\tilde{u}(\tau) \in X_h$ and $\tilde{u}(\tau) \notin X_h$ in Theorem 5.1.

Remark 5.7 For the result of $\tilde{u}(\tau) \notin X_h$, we only present the local error of the energy conservation, which is a direct consequence of Theorem 5.4. For the long-time energy conservation, we have proved the result for exponential integrators in [60]. It is possible to perform the long-time analysis for the methods presented in this chapter by using modulated Fourier expansions.

Theorem 5.2 *If Q is negative semi-definite and $\tilde{u}(\tau) \in X_h$, then H , the Lyapunov function of the dissipative system (5.1), given by (5.2), can be preserved by the ECr method (5.12); i.e., $H(y_1) \leq H(y_0)$. If $\tilde{u}(\tau) \notin X_h$, it is true that $H(y_1) \leq H(y_0) + \mathcal{O}(h^{2r+1})$.*

Proof Applying the fact that $\int_0^1 \tilde{u}'(\tau)^\top Q^{-1} \tilde{u}'(\tau) d\tau \leq 0$, this theorem can be proved in a similar way to the proof of Theorem 5.1. \square

5.5 Existence, Uniqueness and Smoothness of the Solution

In this section, we focus on the study of the existence and uniqueness of $\tilde{u}(\tau)$ associated with the ECr method (5.12).

According to Lemma 3.1 given in [50], it is easily verified that the coefficients $e^{\tau h A}$ and $\bar{A}_{\tau, \sigma}(A)$ of the methods for $0 \leq \tau \leq 1$ and $0 \leq \sigma \leq 1$ are uniformly bounded. We begin by assuming that

$$M_k = \max_{\tau, \sigma, h \in [0, 1]} \left\| \frac{\partial^k \bar{A}_{\tau, \sigma}}{\partial h^k} \right\|, \quad C_k = \max_{\tau, h \in [0, 1]} \left\| \frac{\partial^k e^{\tau h A}}{\partial h^k} y_0 \right\|, \quad k = 0, 1, \dots$$

Furthermore, denoting n -th-order derivative of g at y by $g^{(n)}(y)$, we then have the following result about the existence and uniqueness of the methods.

Theorem 5.3 *Let $B(\bar{y}_0, R) = \{y \in \mathbb{R}^d : \|y - \bar{y}_0\| \leq R\}$ and*

$$D_n = \max_{y \in B(\bar{y}_0, R)} \|g^{(n)}(y)\|, \quad n = 0, 1, \dots,$$

where R is a positive constant, $\bar{y}_0 = e^{\tau h A} y_0$, $\|\cdot\| = \|\cdot\|_\infty$ is the maximum norm for vectors in \mathbb{R}^d or the corresponding induced norm for the multilinear maps $g^{(n)}(y)$. If h satisfies

$$0 \leq h \leq \kappa < \min \left\{ \frac{1}{M_0 D_1}, \frac{R}{M_0 D_0}, 1 \right\}, \quad (5.23)$$

then the ECr method (5.12) has a unique solution $\tilde{u}(\tau)$ which is smoothly dependent on h .

Proof Set $\tilde{u}_0(\tau) = \bar{y}_0$ and define

$$\tilde{u}_{n+1}(\tau) = e^{\tau h A} y_0 + \tau h \int_0^1 \bar{A}_{\tau, \sigma}(A) g(\tilde{u}_n(\sigma)) d\sigma, \quad n = 0, 1, \dots, \quad (5.24)$$

which leads to a function sequence $\{\tilde{u}_n(\tau)\}_{n=0}^\infty$. We note that $\lim_{n \rightarrow \infty} \tilde{u}_n(\tau)$ is a solution of the TCr method (5.12) if $\{\tilde{u}_n(\tau)\}_{n=0}^\infty$ is uniformly convergent, which will

be shown by proving the uniform convergence of the infinite series $\sum_{n=0}^{\infty} (\tilde{u}_{n+1}(\tau) - \tilde{u}_n(\tau))$.

By induction and according to (5.23) and (5.24), we obtain $\|\tilde{u}_n(\tau) - \bar{y}_0\| \leq R$ for $n = 0, 1, \dots$. It then follows from (5.24) that

$$\begin{aligned} & \|\tilde{u}_{n+1}(\tau) - \tilde{u}_n(\tau)\| \\ & \leq \tau h \int_0^1 M_0 D_1 \|\tilde{u}_n(\sigma) - \tilde{u}_{n-1}(\sigma)\| d\sigma \\ & \leq h \int_0^1 M_0 D_1 \|\tilde{u}_n(\sigma) - \tilde{u}_{n-1}(\sigma)\| d\sigma \leq \beta \|\tilde{u}_n - \tilde{u}_{n-1}\|_c, \quad \beta = \kappa M_0 D_1, \end{aligned}$$

where $\|\cdot\|_c$ is the maximum norm for continuous functions defined as $\|w\|_c = \max_{\tau \in [0,1]} \|w(\tau)\|$ for a continuous \mathbb{R}^d -valued function w on $[0, 1]$. Hence, we obtain

$$\|\tilde{u}_{n+1} - \tilde{u}_n\|_c \leq \beta \|\tilde{u}_n - \tilde{u}_{n-1}\|_c$$

and

$$\|\tilde{u}_{n+1} - \tilde{u}_n\|_c \leq \beta^n \|\tilde{u}_1 - y_0\|_c \leq \beta^n R, \quad n = 0, 1, \dots$$

It then immediately follows from Weierstrass M -test and the fact of $\beta < 1$ that $\sum_{n=0}^{\infty} (\tilde{u}_{n+1}(\tau) - \tilde{u}_n(\tau))$ is uniformly convergent.

If the ECr method (5.12) has another solution $\tilde{v}(\tau)$, we obtain the following inequalities

$$\|\tilde{u}(\tau) - \tilde{v}(\tau)\| \leq h \int_0^1 \|\bar{A}_{\tau,\sigma}(A)(g(\tilde{u}(\sigma)) - g(\tilde{v}(\sigma)))\| d\sigma \leq \beta \|\tilde{u} - \tilde{v}\|_c,$$

and $\|\tilde{u} - \tilde{v}\|_c \leq \beta \|\tilde{u} - \tilde{v}\|_c$. This yields $\|\tilde{u} - \tilde{v}\|_c = 0$ and $\tilde{u}(\tau) \equiv \tilde{v}(\tau)$. The existence and uniqueness have been proved.

With respect to the result that $\tilde{u}(\tau)$ is smoothly dependent of h , since each $\tilde{u}_n(\tau)$ is a smooth function of h , we need only to prove that the sequence $\left\{ \frac{\partial^k \tilde{u}_n(\tau)}{\partial h^k} \right\}_{n=0}^{\infty}$ is uniformly convergent for $k \geq 1$. Differentiating (5.24) with respect to h gives

$$\begin{aligned} \frac{\partial \tilde{u}_{n+1}}{\partial h}(\tau) &= \tau A e^{\tau h A} y_0 + \tau \int_0^1 \left(\bar{A}_{\tau,\sigma}(A) + h \frac{\partial \bar{A}_{\tau,\sigma}}{\partial h} \right) g(\tilde{u}_n(\sigma)) d\sigma \\ &+ \tau h \int_0^1 \bar{A}_{\tau,\sigma}(A) g^{(1)}(\tilde{u}_n(\sigma)) \frac{\partial \tilde{u}_n}{\partial h}(\sigma) d\sigma, \end{aligned} \quad (5.25)$$

which yields

$$\left\| \frac{\partial \tilde{u}_{n+1}}{\partial h} \right\|_c \leq \alpha + \beta \left\| \frac{\partial \tilde{u}_n}{\partial h} \right\|_c, \quad \alpha = C_1 + (M_0 + \kappa M_1)D_0.$$

By induction, it is easy to show that $\left\{ \frac{\partial \tilde{u}_n}{\partial h}(\tau) \right\}_{n=0}^{\infty}$ is uniformly bounded:

$$\left\| \frac{\partial \tilde{u}_n}{\partial h} \right\|_c \leq \alpha(1 + \beta + \cdots + \beta^{n-1}) \leq \frac{\alpha}{1 - \beta} = C^*, \quad n = 0, 1, \dots \quad (5.26)$$

It follows from (5.25)–(5.26) that

$$\begin{aligned} & \left\| \frac{\partial \tilde{u}_{n+1}}{\partial h} - \frac{\partial \tilde{u}_n}{\partial h} \right\|_c \\ & \leq \tau \int_0^1 (M_0 + hM_1) \|g(\tilde{u}_n(\sigma)) - g(\tilde{u}_{n-1}(\sigma))\| d\sigma \\ & \quad + \tau h \int_0^1 M_0 \left(\left\| (g^{(1)}(\tilde{u}_n(\sigma)) - g^{(1)}(\tilde{u}_{n-1}(\sigma))) \frac{\partial \tilde{u}_n}{\partial h}(\sigma) \right\| \right. \\ & \quad \left. + \left\| g^{(1)}(\tilde{u}_{n-1}(\sigma)) \left(\frac{\partial \tilde{u}_n}{\partial h}(\sigma) - \frac{\partial \tilde{u}_{n-1}}{\partial h}(\sigma) \right) \right\| \right) d\sigma \leq \gamma \beta^{n-1} + \beta \left\| \frac{\partial \tilde{u}_n}{\partial h} - \frac{\partial \tilde{u}_{n-1}}{\partial h} \right\|_c, \end{aligned}$$

where $\gamma = (M_0 D_1 + \kappa M_1 D_1 + \kappa M_0 L_2 C^*)R$, and L_2 is a constant satisfying

$$\|g^{(1)}(y) - g^{(1)}(z)\| \leq L_2 \|y - z\|, \quad \text{for } y, z \in B(\bar{y}_0, R).$$

Therefore, the following result is obtained by induction

$$\left\| \frac{\partial \tilde{u}_{n+1}}{\partial h} - \frac{\partial \tilde{u}_n}{\partial h} \right\|_c \leq n\gamma \beta^{n-1} + \beta^n C^*, \quad n = 1, 2, \dots$$

This shows the uniform convergence of $\sum_{n=0}^{\infty} \left(\frac{\partial \tilde{u}_{n+1}}{\partial h}(\tau) - \frac{\partial \tilde{u}_n}{\partial h}(\tau) \right)$ and then

$\left\{ \frac{\partial \tilde{u}_n}{\partial h}(\tau) \right\}_{n=0}^{\infty}$ is uniformly convergent.

Likewise, it can be shown that other function series $\left\{ \frac{\partial^k \tilde{u}_n}{\partial h^k}(\tau) \right\}_{n=0}^{\infty}$ for $k \geq 2$ are uniformly convergent as well. Therefore, $\tilde{u}(\tau)$ is smoothly dependent on h . \square

5.6 Algebraic Order

In this section, we analyse the algebraic order of the ECr method (5.12). To express the dependence of the solutions of $y'(t) = Ay(t) + g(y(t))$ on the initial values, we denote by $y(\cdot, \tilde{t}, \tilde{y})$ the solution satisfying the initial condition $y(\tilde{t}, \tilde{t}, \tilde{y}) = \tilde{y}$ for any given $\tilde{t} \in [0, h]$ and set $\Phi(s, \tilde{t}, \tilde{y}) = \frac{\partial y(s, \tilde{t}, \tilde{y})}{\partial \tilde{y}}$. Recalling the elementary theory of ODEs, we have the following standard result

$$\frac{\partial y(s, \tilde{t}, \tilde{y})}{\partial \tilde{t}} = -\Phi(s, \tilde{t}, \tilde{y})(A\tilde{y} + g(\tilde{y})).$$

Throughout this section, for convenience, an h -dependent function $w(\tau)$ is called regular if it can be expanded as $w(\tau) = \sum_{n=0}^{r-1} w^{[n]}(\tau)h^n + \mathcal{O}(h^r)$, where $w^{[n]}(\tau) = \frac{1}{n!} \frac{\partial^n w(\tau)}{\partial h^n} |_{h=0}$ is a vector-valued function with polynomial entries of degrees $\leq n$.

It can be deduced from Proposition 3.3 in [34] that $P_{\tau, \sigma}$ is regular. Moreover, we can prove the following result.

Lemma 5.2 *The ECr method (5.12) generates a regular h -dependent function $\tilde{u}(\tau)$.*

Proof By the result given in [34], we know that $P_{\tau, \sigma}$ can be smoothly extended to $h = 0$ by setting $P_{\tau, \sigma} |_{h=0} = \lim_{h \rightarrow 0} P_{\tau, \sigma}(h)$. Furthermore, it follows from Theorem 5.3 that $\tilde{u}(\tau)$ is smoothly dependent on h . Therefore, $\tilde{u}(\tau)$ and $\bar{A}_{\tau, \sigma}(A)$ can be expanded with respect to h at zero as follows:

$$\tilde{u}(\tau) = \sum_{m=0}^{r-1} \tilde{u}^{[m]}(\tau)h^m + \mathcal{O}(h^r), \quad \bar{A}_{\tau, \sigma}(A) = \sum_{m=0}^{r-1} \bar{A}_{\tau, \sigma}^{[m]}(A)h^m + \mathcal{O}(h^r).$$

Then let $\delta = \tilde{u}(\sigma) - y_0$ and we have

$$\delta = \tilde{u}^{[0]}(\sigma) - y_0 + \mathcal{O}(h) = y_0 - y_0 + \mathcal{O}(h) = \mathcal{O}(h).$$

We expand $f(\tilde{u}(\sigma))$ at y_0 and insert the above equalities into the first equation of the ECr method (5.12). This manipulation yields

$$\begin{aligned} \sum_{m=0}^{r-1} \tilde{u}^{[m]}(\tau)h^m &= \sum_{m=0}^{r-1} \frac{\tau^m A^m y_0}{m!} h^m \\ + \tau h \int_0^1 \sum_{k=0}^{r-1} \bar{A}_{\tau, \sigma}^{[k]}(A) h^k \sum_{n=0}^{r-1} \frac{1}{n!} g^{(n)}(y_0) (\underbrace{\delta, \dots, \delta}_{n\text{-fold}}) d\sigma &+ \mathcal{O}(h^r). \end{aligned} \quad (5.27)$$

In order to show that $\tilde{u}(\tau)$ is regular, we need only to prove that

$$\tilde{u}^{[m]}(\tau) \in P_m^d = \underbrace{P_m([0, 1]) \times \cdots \times P_m([0, 1])}_{d\text{-fold}} \quad \text{for } m = 0, 1, \dots, r-1,$$

where $P_m([0, 1])$ consists of polynomials of degree $\leq m$ on $[0, 1]$. This can be confirmed by induction as follows.

Firstly, it is clear that $\tilde{u}^{[0]}(\tau) = y_0 \in P_0^d$. We assume that $\tilde{u}^{[n]}(\tau) \in P_n^d$ for $n = 0, 1, \dots, m$. Comparing the coefficients of h^{m+1} on both sides of (5.27) and using (5.13) lead to

$$\begin{aligned} & \tilde{u}^{[m+1]}(\tau) \\ &= \frac{\tau^{m+1} A^{m+1}}{(m+1)!} y_0 + \sum_{k+n=m} \tau \int_0^1 \bar{A}_{\tau, \sigma}^{[k]}(A) h_n(\sigma) d\sigma \\ &= \frac{\tau^{m+1} A^{m+1}}{(m+1)!} y_0 + \sum_{k+n=m} \tau \int_0^1 \int_0^1 \left[e^{(1-\xi)\tau h A} P_{\xi\tau, \sigma} \right]^{[k]} h_n(\sigma) d\sigma d\xi, \\ & \quad h_n(\sigma) \in P_n^d. \end{aligned}$$

Since $P_{\xi\tau, \sigma}$ is regular, it is easy to check that $e^{(1-\xi)\tau h A} P_{\xi\tau, \sigma}$ is also regular. Thus, under the condition $k+n=m$, we have

$$\int_0^1 \left[e^{(1-\xi)\tau h A} P_{\xi\tau, \sigma} \right]^{[k]} h_n(\sigma) d\sigma := \check{p}_m^k(\xi\tau) \in P_m^d([0, 1]).$$

Then, the above result can be simplified as

$$\begin{aligned} \tilde{u}^{[m+1]}(\tau) &= \frac{\tau^{m+1} A^{m+1}}{(m+1)!} y_0 + \sum_{k+n=m} \tau \int_0^1 \check{p}_m^k(\xi\tau) d\xi \\ &= \frac{\tau^{m+1} A^{m+1}}{(m+1)!} y_0 + \sum_{k+n=m} \int_0^\tau \check{p}_m^k(\alpha) d\alpha \in P_{m+1}^d. \end{aligned}$$

□

According to Lemma 3.4 presented in [34] and the above lemma, we obtain

$$\mathcal{P}_h g(\tilde{u}(\tau)) - g(\tilde{u}(\tau)) = \mathcal{O}(h^r), \quad (5.28)$$

which will be used in the analysis of algebraic order. We are now ready to present the result about the algebraic order of the ECr method (5.12).

Theorem 5.4 *About the stage order and order of the ECr method (5.12), we have*

$$\begin{aligned}\tilde{u}(\tau) - y(t_0 + \tau h) &= \mathcal{O}(h^{r+1}), \quad 0 < \tau < 1, \\ \tilde{u}(1) - y(t_0 + h) &= \mathcal{O}(h^{2r+1}).\end{aligned}$$

Proof According to the previous preliminaries, we obtain

$$\begin{aligned}& \tilde{u}(\tau) - y(t_0 + \tau h) \\ &= y(t_0 + \tau h, t_0 + \tau h, \tilde{u}(\tau)) - y(t_0 + \tau h, t_0, y_0) \\ &= \int_0^\tau \frac{d}{d\alpha} y(t_0 + \tau h, t_0 + \alpha h, \tilde{u}(\alpha)) d\alpha \\ &= \int_0^\tau \left(h \frac{\partial y}{\partial t} (t_0 + \tau h, t_0 + \alpha h, \tilde{u}(\alpha)) + \frac{\partial y}{\partial \tilde{y}} (t_0 + \tau h, t_0 + \alpha h, \tilde{u}(\alpha)) h \tilde{u}'(\alpha) \right) d\alpha \\ &= \int_0^\tau \left(-h \frac{\partial y}{\partial \tilde{y}} (t_0 + \tau h, t_0 + \alpha h, \tilde{u}(\alpha)) (A \tilde{u}(\alpha) + g(\tilde{u}(\alpha))) \right. \\ &\quad \left. + \frac{\partial y}{\partial \tilde{y}} (t_0 + \tau h, t_0 + \alpha h, \tilde{u}(\alpha)) (h A \tilde{u}(\alpha) + h \langle P_{\tau, \sigma}, g(\tilde{u}(\alpha)) \rangle_\alpha) \right) d\alpha \\ &= -h \int_0^\tau \Phi^\tau(\alpha) (g(\tilde{u}(\alpha)) - \mathcal{P}_h(g \circ \tilde{u})(\alpha)) d\alpha = \mathcal{O}(h^{r+1}),\end{aligned}\tag{5.29}$$

where $\Phi^\tau(\alpha) = \frac{\partial y}{\partial \tilde{y}}(t_0 + \tau h, t_0 + \alpha h, \tilde{u}(\alpha))$. Letting $\tau = 1$ in (5.29) yields

$$\tilde{u}(1) - y(t_0 + h) = -h \int_0^1 \Phi^1(\alpha) (g(\tilde{u}(\alpha)) - \mathcal{P}_h(g \circ \tilde{u})(\alpha)) d\alpha.\tag{5.30}$$

We partition the matrix-valued function $\Phi^1(\alpha)$ as $\Phi^1(\alpha) = (\Phi_1^1(\alpha), \dots, \Phi_d^1(\alpha))^\top$. It follows from Lemma 5.2 that

$$\Phi_i^1(\alpha) = \mathcal{P}_h \Phi_i^1(\alpha) + \mathcal{O}(h^r), \quad i = 1, \dots, d.\tag{5.31}$$

On the other hand, we have

$$\int_0^1 (\mathcal{P}_h \Phi_i^1(\alpha))^\top g(\tilde{u}(\alpha)) d\alpha = \int_0^1 (\mathcal{P}_h \Phi_i^1(\alpha))^\top \mathcal{P}_h(g \circ \tilde{u})(\alpha) d\alpha, \quad i = 1, \dots, d.\tag{5.32}$$

Therefore, it follows from (5.30), (5.31) and (5.32) that

$$\begin{aligned}
 & \tilde{u}(1) - y(t_0 + h) \\
 &= -h \int_0^1 \left(\begin{pmatrix} (\mathcal{P}_h \Phi_1^1(\alpha))^\top \\ \vdots \\ (\mathcal{P}_h \Phi_d^1(\alpha))^\top \end{pmatrix} + \mathcal{O}(h^r) \right) (g(\tilde{u}(\alpha)) - \mathcal{P}_h(g \circ \tilde{u})(\alpha)) d\alpha \\
 &= -h \int_0^1 \begin{pmatrix} (\mathcal{P}_h \Phi_1^1(\alpha))^\top (g(\tilde{u}(\alpha)) - \mathcal{P}_h(g \circ \tilde{u})(\alpha)) \\ \vdots \\ (\mathcal{P}_h \Phi_d^1(\alpha))^\top (g(\tilde{u}(\alpha)) - \mathcal{P}_h(g \circ \tilde{u})(\alpha)) \end{pmatrix} d\alpha - h \int_0^1 \mathcal{O}(h^r) \times \mathcal{O}(h^r) d\alpha \\
 &= 0 + \mathcal{O}(h^{2r+1}) = \mathcal{O}(h^{2r+1}).
 \end{aligned}$$

□

5.7 Application in Stiff Gradient Systems

When the matrix Q in (5.1) is the identity matrix, the system (5.1) is a stiff gradient system as follows:

$$y' = -\nabla U(y), \quad y(0) = y_0 \in \mathbb{R}^d, \quad t \in [0, T], \quad (5.33)$$

where the potential U has the form

$$U(y) = \frac{1}{2} y^\top M y + V(y). \quad (5.34)$$

Such problems arise from the spatial discretisation of Allen–Cahn and Cahn–Hilliard PDEs (see, e.g. [61]). Along every exact solution, it is true that

$$\frac{d}{dt} U(y(t)) = \nabla U(y(t))^\top y'(t) = -y'(t)^\top y'(t) \leq 0,$$

which implies that $U(y(t))$ is monotonically decreasing.

For solving this stiff gradient system, it follows from Theorem 5.2 that the practical ECr method (5.40) is unconditionally energy-diminishing. For a quadratic potential (i.e., $V(y) = 0$ in (5.34)), the numerical solution of the method is given by

$$y_1 = R(-hA)y_0 = e^{-hA}y_0.$$

The importance of the damping property $|R(\infty)| < 1$ for the approximation properties of Runge–Kutta methods has been studied and well understood in

[62, 63] for solving semilinear parabolic equations. The role of the condition $|R(\infty)| < 1$ in the approximation of stiff differential equations has been researched in Chapter VI of [64]. It has been shown in [39] that for each Runge–Kutta method the energy decreases once the stepsize satisfies some conditions. Discrete-gradient methods, AVF methods and AVF collocation methods derived in [39] are unconditionally energy-diminishing methods but they show no damping for very stiff gradient systems. However, it is clear that the methods are unconditionally energy-diminishing methods and they have

$$|R(\infty)| = |e^{-\infty}| = 0.$$

This implies that the methods are strongly damped even for very stiff gradient systems and this is a significant feature.

5.8 Practical Examples of Exponential Collocation Methods

In this section, we present practical examples of exponential collocation methods. Choosing $\tilde{\varphi}_k(\tau) = (\tau h)^k$ for $k = 0, 1, \dots, r-1$ and using the Gram–Schmidt process, we obtain the standard orthonormal basis of Y_h as follows:

$$\hat{p}_j(\tau) = (-1)^j \sqrt{2j+1} \sum_{k=0}^j \binom{j}{k} \binom{j+k}{k} (-\tau)^k,$$

$$j = 0, 1, \dots, r-1, \quad \tau \in [0, 1],$$

which are the shifted Legendre polynomials on $[0, 1]$. Therefore, $P_{\tau, \sigma}$ can be determined by (5.10) as follows $P_{\tau, \sigma} = \sum_{i=0}^{r-1} \hat{p}_i(\tau) \hat{p}_i(\sigma)$.

5.8.1 An Example of ECr Methods

For the ECr method (5.12), we need to calculate $\bar{A}_{\tau, \sigma}(A)$ appearing in the methods. It follows from (5.13) that

$$\begin{aligned} \bar{A}_{\tau, \sigma}(A) &= \int_0^1 e^{(1-\xi)\tau h A} P_{\xi\tau, \sigma} d\xi = \sum_{i=0}^{r-1} \int_0^1 e^{(1-\xi)\tau h A} \hat{p}_i(\xi\tau) d\xi \hat{p}_i(\sigma) \\ &= \sum_{i=0}^{r-1} \int_0^1 e^{(1-\xi)\tau h A} (-1)^i \sqrt{2i+1} \sum_{k=0}^i \binom{i}{k} \binom{i+k}{k} (-\xi\tau)^k d\xi \hat{p}_i(\sigma) \\ &= \sum_{i=0}^{r-1} \sqrt{2i+1} \sum_{k=0}^i (-1)^{i+k} \frac{(i+k)!}{k!(i-k)!} \bar{\varphi}_{k+1}(\tau h A) \hat{p}_i(\sigma). \end{aligned} \quad (5.35)$$

Here the $\bar{\varphi}$ -functions (see, e.g. [2, 14, 49, 50]) are defined by:

$$\bar{\varphi}_0(z) = e^z, \quad \bar{\varphi}_k(z) = \int_0^1 e^{(1-\sigma)z} \frac{\sigma^{k-1}}{(k-1)!} d\sigma, \quad k = 1, 2, \dots$$

It is noted that a number of approaches have been developed which work with the application of the φ -functions on a vector (see [2, 65, 66], for example).

5.8.2 An Example of TCr Methods

For the TCr method (5.18) solving $q''(t) + \Omega q(t) = -\nabla U(q(t))$, we need to compute $\mathcal{A}_{\tau,\sigma}$ and $\mathcal{B}_{1,\sigma}$. It follows from (5.19) that

$$\begin{aligned} & \mathcal{A}_{\tau,\sigma}(K) \\ &= \sum_{j=0}^{r-1} \int_0^1 (1-\xi)\phi_1((1-\xi)^2 K) \hat{p}_j(\xi\tau) d\xi \hat{p}_j(\sigma) \\ &= \sum_{j=0}^{r-1} \sqrt{2j+1} \sum_{l=0}^{\infty} (-1)^j \sum_{k=0}^j \binom{j}{k} \binom{j+k}{k} \int_0^1 (-\xi)^k (1-\xi)^{2l+1} d\xi \frac{(-1)^l K^l}{(2l+1)!} \tau^k \hat{p}_j(\sigma) \\ &= \sum_{j=0}^{r-1} \sqrt{2j+1} \sum_{l=0}^{\infty} \sum_{k=0}^j (-1)^{j+k} \binom{j}{k} \binom{j+k}{k} \frac{k!(2l+1)!}{(2l+k+2)!} \frac{(-1)^l K^l}{(2l+1)!} \tau^k \hat{p}_j(\sigma) \\ &= \sum_{j=0}^{r-1} \sqrt{2j+1} \hat{p}_j(\sigma) \sum_{l=0}^{\infty} \sum_{k=0}^j \frac{(-1)^{j+k+l} (j+k)!}{k!(j-k)!(2l+k+2)!} \tau^k K^l. \end{aligned}$$

Recall that the generalised hypergeometric function ${}_mF_n$ is defined by

$${}_mF_n \left[\begin{matrix} \alpha_1, \alpha_2, \dots, \alpha_m; \\ \beta_1, \beta_2, \dots, \beta_n; \end{matrix} x \right] = \sum_{l=0}^{\infty} \frac{\prod_{i=1}^m (\alpha_i)_l}{\prod_{i=1}^n (\beta_i)_l} \frac{x^l}{l!}, \quad (5.36)$$

where α_i and β_i are arbitrary complex numbers, except that β_i can be neither zero nor a negative integer, and $(z)_l$ is the Pochhammer symbol which is defined as

$$(z)_0 = 1, \quad (z)_l = z(z+1)\cdots(z+l-1), \quad l \in \mathbb{N}.$$

Then, $\mathcal{A}_{\tau,\sigma}$ can be expressed by

$$\mathcal{A}_{\tau,\sigma}(K) = \sum_{j=0}^{r-1} \sqrt{2j+1} \hat{p}_j(\sigma) \sum_{l=0}^{\infty} \frac{(-1)^{j+l}}{(2l+2)!} {}_2F_1 \left[\begin{matrix} -j, j+1; \\ 2l+3; \end{matrix} \tau \right] K^l. \quad (5.37)$$

Likewise, we can obtain

$$\mathcal{B}_{1,\sigma}(K) = \sum_{j=0}^{r-1} \sqrt{2j+1} \hat{p}_j(\sigma) S_j(K), \quad (5.38)$$

where $S_j(K)$ are

$$\begin{aligned} S_{2j}(K) &= (-1)^j \frac{(2j)!}{(4j+1)!} K^j {}_0F_1 \left[\begin{matrix} -; \\ \frac{1}{2}; \end{matrix} -\frac{K}{16} \right] {}_0F_1 \left[\begin{matrix} -; \\ 2j + \frac{3}{2}; \end{matrix} -\frac{K}{16} \right], \\ S_{2j+1}(K) &= (-1)^j \frac{(2j+2)!}{(4j+4)!} K^{j+1} {}_0F_1 \left[\begin{matrix} -; \\ \frac{3}{2}; \end{matrix} -\frac{K}{16} \right] {}_0F_1 \left[\begin{matrix} -; \\ 2j + \frac{5}{2}; \end{matrix} -\frac{K}{16} \right], \quad j=0, 1, \dots \end{aligned} \quad (5.39)$$

5.8.3 An Example of RKNCr Methods

By letting $K = 0$ in the above analysis, we obtain an example of RKNCr methods for solving the general second-order ODEs (5.20) as

$$\left\{ \begin{aligned} q_{d_i} &= q_0 + d_i h p_0 - d_i^2 h^2 \int_0^1 \bar{\mathcal{A}}_{d_i,\sigma} \nabla U \left(\sum_{m=1}^r q_{d_m} l_m(\sigma) \right) d\sigma, \quad i = 1, \dots, r, \\ q_1 &= q_0 + h p_0 - h^2 \int_0^1 \bar{\mathcal{A}}_{1,\sigma} \nabla U \left(\sum_{m=1}^r q_{d_m} l_m(\sigma) \right) d\sigma, \\ p_1 &= p_0 - h \int_0^1 \bar{\mathcal{B}}_{1,\sigma} \nabla U \left(\sum_{m=1}^r q_{d_m} l_m(\sigma) \right) d\sigma, \end{aligned} \right.$$

where $\bar{\mathcal{A}}_{\tau,\sigma} = \sum_{i=0}^{r-1} \int_0^1 (1-\xi) \hat{p}_i(\xi \tau) d\xi \hat{p}_i(\sigma)$ and $\bar{\mathcal{B}}_{1,\sigma} = \sum_{i=0}^{r-1} \int_0^1 \hat{p}_i(\xi) d\xi \hat{p}_i(\sigma)$.

Remark 5.8 It is noted that one can make different choices of Y_h and X_h and the whole analysis presented in this chapter still holds. Different choices will produce different practical methods, and in this chapter, we do not pursue this point for brevity.

5.9 Numerical Experiments

Applying the r -point Gauss–Legendre quadrature to the integral of (5.12) yields

$$\begin{cases} y_{c_i} = e^{c_i h A} y_0 + c_i h \sum_{j=1}^r b_j \bar{A}_{c_i, c_j}(A) g(y_{c_j}), & i = 1, \dots, r, \\ y_1 = e^{h A} y_0 + h \sum_{j=1}^r b_j \bar{A}_{1, c_j}(A) g(y_{c_j}), \end{cases} \quad (5.40)$$

where c_j and b_j for $j = 1, \dots, r$ are the nodes and weights of the quadrature, respectively. It is shown that the quadrature formula used here is not exact in general for arbitrary g . According to Theorem 5.4 and the order of Gauss–Legendre quadrature, it is obtained that this scheme approximately preserves the energy H with the accuracy $H(y_1) = H(y_0) + \mathcal{O}(h^{2r+1})$.

In this section, we use fixed-point iteration in practical computation. Concerning the convergence of the fixed-point iteration for the above scheme (5.40), we have the following result.

Theorem 5.5 *Assume that g satisfies a Lipschitz condition in the variable y , i.e., there exists a constant L with the property that $\|g(y_1) - g(y_2)\| \leq L \|y_1 - y_2\|$. If the stepsize h satisfies*

$$0 < h < \frac{1}{LC \max_{i=1, \dots, r} c_i \max_{j=1, \dots, r} |b_j|}, \quad (5.41)$$

then the fixed-point iteration for the scheme (5.40) is convergent, where the constant C depends on r but is independent of A .

Proof We rewrite the first formula of (5.40) as

$$Y = e^{chA} y_0 + h \bar{K}(A) g(Y), \quad (5.42)$$

where $c = (c_1, c_2, \dots, c_r)^\top$, $Y = (y_1, y_2, \dots, y_r)^\top$, $\bar{K}(A) = (\bar{K}_{ij}(A))_{r \times r}$ and $\bar{K}_{ij}(A)$ are defined by

$$\bar{K}_{ij}(A) := c_i b_j \bar{A}_{c_i, c_j}(A).$$

It then follows from (5.35) that

$$\|\bar{K}_{ij}(A)\| \leq c_i |b_j| \sum_{l=0}^{r-1} \sqrt{2l+1} \sum_{k=0}^l \frac{(l+k)!}{k!(l-k)!} \|\bar{\varphi}_{k+1}(c_i h A)\| |\hat{\rho}_l(c_j)| \leq C c_i |b_j|,$$

where the constant C depends on r but is independent of A . It then follows that $\|\bar{K}(A)\| \leq C \max_{i=1, \dots, r} c_i \max_{j=1, \dots, r} |b_j|$. Letting

$$\varphi(x) = e^{chA} y_0 + h \bar{K}(A) g(x),$$

we obtain that

$$\begin{aligned} \|\varphi(x) - \varphi(y)\| &= \|h \bar{K}(A) g(x) - h \bar{K}(A) g(y)\| \leq hL \|\bar{K}(A)\| \|x - y\| \\ &\leq hLC \max_{i=1, \dots, r} c_i \max_{j=1, \dots, r} |b_j| \|x - y\|. \end{aligned}$$

The proof is complete by the Contraction Mapping Theorem. \square

Remark 5.9 It can be concluded from this theorem that the convergence of the method (5.40) is independent of $\|A\|$. However, it can be checked easily that the convergence of some other methods such as RKEPC methods given in [30] depends on $\|A\|$. This fact confirms the efficiency of the method (5.40) and is demonstrated numerically by the experiments presented in this section. This is also a reason why the RKEPC2 formula does not precisely conserve the energy of Problem 5.1.

In order to show the efficiency and robustness of the methods, we take $r = 2$ and denote the corresponding method by EC2P. Then we choose the same Y_h and X_h for the functionally fitted energy-preserving method developed in [34], and by this choice, the method becomes the 2 r th order RKEPC method given in [30]. For this method, we choose $r = 2$ and approximate the integral by the Lobatto quadrature of order eight, which is precisely the “extended Labatto IIIA method of order four” in [67]. We denote this corresponding method as RKEPC2. Another integrator we select for comparison is the explicit three-stage exponential integrator of order four derived in [14] which is denoted by EEI3s4. It is noted that the first two methods

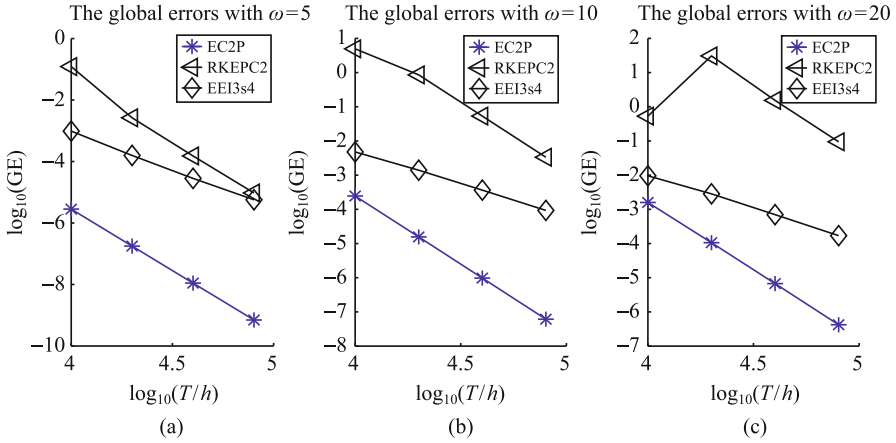


Fig. 5.1 The logarithm of the global error against the logarithm of T/h

are implicit and we set 10^{-16} as the error tolerance and 5 as the maximum number¹ demonstrate the efficiency of ECr methods when applied to first-order systems, for brevity.

Problem 5.1 Consider the Duffing equation defined by

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -\omega^2 - k^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ 2k^2q^3 \end{pmatrix}, \quad \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = \begin{pmatrix} 0 \\ \omega \end{pmatrix}.$$

It is a Hamiltonian system with the Hamiltonian:

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

The exact solution of this system is $q(t) = sn(\omega t; k/\omega)$ with the Jacobi elliptic function sn . Choose $k = 0.07$, $\omega = 5, 10, 20$ and solve the problem on the interval $[0, 1000]$ with different stepsizes $h = 0.1/2^i$ for $i = 0, \dots, 3$. The global errors are presented in Fig. 5.1. Then, we integrate this problem with the stepsize $h = 1/100$ on the interval $[0, 10000]$. See Fig. 5.2 for the energy conservation for different methods. Finally, we solve this problem on the interval $[0, 10]$ with $\omega = 20$, $h = 0.01$ and different error tolerances in the fixed-point iteration. See Table 5.1 for the total numbers of iterations for the implicit methods EC2P and RKEPC2.

¹It is noted that in order to show that the methods can perform well even for few iterations, a low maximum number 5 of fixed-point iterations is used in this section. It is possible to increase to other bigger maximum number of fixed-point iterations, but we do not go further here for brevity.

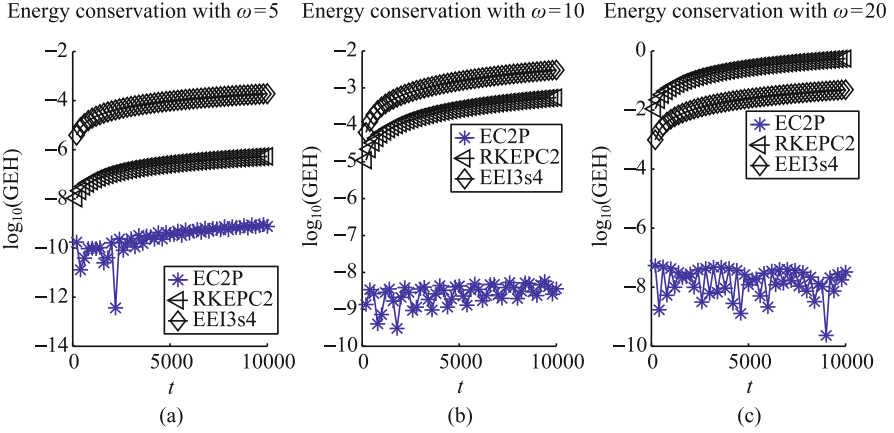


Fig. 5.2 The logarithm of the error of Hamiltonian against t

Table 5.1 Results for Problem 5.1: the total numbers of iterations for different error tolerances (tol)

Methods	tol = 1.0×10^{-6}	tol = 1.0×10^{-8}	tol = 1.0×10^{-10}	tol = 1.0×10^{-12}
EC2P	859	992	1000	1651
RKEPC2	6886	8907	10, 647	11, 899

Problem 5.2 Consider the following averaged system in wind-induced oscillation (see [40])

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}' = \begin{pmatrix} -\zeta & -\lambda \\ \lambda & -\zeta \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} x_1 x_2 \\ \frac{1}{2}(x_1^2 - x_2^2) \end{pmatrix},$$

where $\zeta \geq 0$ is a damping factor and λ is a detuning parameter. By setting

$$\zeta = r \cos \theta, \quad \lambda = r \sin \theta, \quad r \geq 0, \quad 0 \leq \theta \leq \pi/2,$$

this system can be transformed into the scheme (5.1) with

$$Q = \begin{pmatrix} -\cos \theta & -\sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}, \quad M = \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix},$$

$$V = -\frac{1}{2} \sin \theta \left(x_1 x_2^2 - \frac{1}{3} x_1^3 \right) + \frac{1}{2} \cos \theta \left(-x_1^2 x_2 + \frac{1}{3} x_2^3 \right).$$

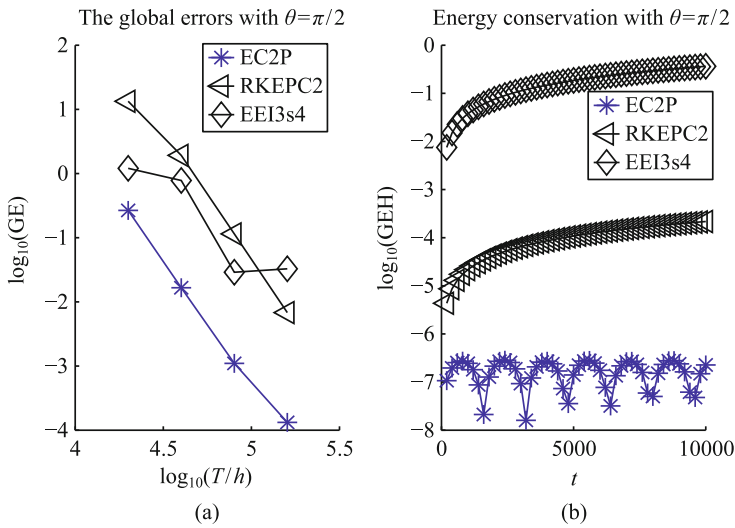


Fig. 5.3 (a) The logarithm of the global error against the logarithm of T/h . (b) The logarithm of the error of Hamiltonian against t

Its first integral (conservative case, when $\theta = \pi/2$) or Lyapunov function (dissipative case, when $\theta < \pi/2$) is

$$H = \frac{1}{2}r(x_1^2 + x_2^2) - \frac{1}{2} \sin \theta \left(x_1 x_2^2 - \frac{1}{3} x_1^3 \right) + \frac{1}{2} \cos \theta \left(-x_1^2 x_2 + \frac{1}{3} x_2^3 \right).$$

The initial values are given by $x_1(0) = 0, x_2(0) = 1$. Firstly we consider the conservative case and choose $\theta = \pi/2, r = 20$. The problem is integrated on $[0, 1000]$ with the stepsize $h = 0.1/2^i$ for $i = 1, \dots, 4$ and the global errors are given in Fig. 5.3a. Then we solve this system with the stepsize $h = 1/200$ on the interval $[0, 10000]$ and Fig. 5.3b shows the results of the energy preservation. Secondly we choose $\theta = \pi/2 - 10^{-4}$ and this gives a dissipative system. The system is solved on $[0, 1000]$ with $h = 0.1/2^i$ for $i = 1, \dots, 4$ and the errors are presented in Fig. 5.4a. See Fig. 5.4b for the results of the Lyapunov function with $h = 1/20$. Here we consider the results given by EC2P with a smaller stepsize $h = 1/1000$ as the ‘exact’ values of the Lyapunov function. Table 5.2 gives the total numbers of iterations when applying the methods to this problem on $[0, 10]$ with $\theta = \pi/2, r = 20, h = 0.01$ and different error tolerances.

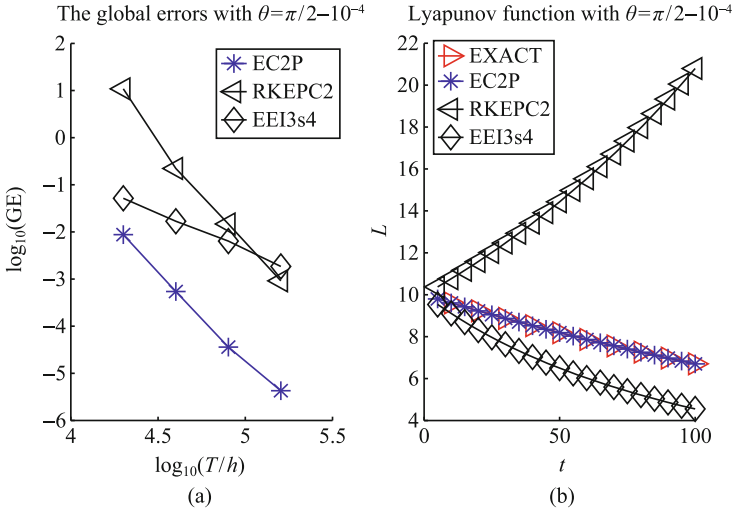


Fig. 5.4 (a) The logarithm of the global error against the logarithm of T/h . (b) The results for the Lyapunov function against t

Table 5.2 Results for Problem 5.2: the total number of iterations for different error tolerances (tol)

Methods	tol = 1.0×10^{-6}	tol = 1.0×10^{-8}	tol = 1.0×10^{-10}	tol = 1.0×10^{-12}
EC2P	2000	3000	3434	4000
RKEPC2	6000	8000	9999	11,000

Problem 5.3 Consider the nonlinear Schrödinger equation (see [68])

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0, \quad \psi(x, 0) = 0.5 + 0.025 \cos(\mu x),$$

with the periodic boundary condition $\psi(0, t) = \psi(L, t)$. Following [68], we choose $L = 4\sqrt{2}\pi$ and $\mu = 2\pi/L$. The initial condition chosen here is in the vicinity of the homoclinic orbit. Using $\psi = p + iq$, this equation can be rewritten as a pair of real-valued equations

$$\begin{aligned} p_t + q_{xx} + 2(p^2 + q^2)q &= 0, \\ q_t - p_{xx} - 2(p^2 + q^2)p &= 0. \end{aligned}$$

Discretising the spatial derivative ∂_{xx} by the pseudospectral method given in [68], this problem is converted into the following system:

$$\begin{pmatrix} p \\ q \end{pmatrix}' = \begin{pmatrix} 0 & -D_2 \\ D_2 & 0 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} + \begin{pmatrix} -2(p^2 + q^2) \cdot q \\ 2(p^2 + q^2) \cdot p \end{pmatrix}, \tag{5.43}$$

where $p = (p_0, p_1, \dots, p_{N-1})^\top$, $q = (q_0, q_1, \dots, q_{N-1})^\top$ and $D_2 = (D_2)_{0 \leq j, k \leq N-1}$ is the pseudospectral differentiation matrix defined by:

$$(D_2)_{jk} = \begin{cases} \frac{1}{2} \mu^2 (-1)^{j+k+1} \frac{1}{\sin^2(\mu(x_j - x_k)/2)}, & j \neq k, \\ -\mu^2 \frac{2(N/2)^2 + 1}{6}, & j = k, \end{cases}$$

with $x_j = j \frac{L}{N}$ for $j = 0, 1, \dots, N - 1$. The Hamiltonian of (5.43) is

$$H(p, q) = \frac{1}{2} p^\top D_2 p + \frac{1}{2} q^\top D_2 q + \frac{1}{2} \sum_{i=0}^{N-1} (p_i^2 + q_i^2)^2.$$

We choose $N = 128$ and first solve the problem on the interval $[0, 10]$ with $h = 0.1/2^i$ for $i = 3, \dots, 6$. See Fig. 5.5a for the global errors. Then, this problem is integrated with $h = 1/200$ on $[0, 1000]$ and the energy conservation is presented in Fig. 5.5b. The total numbers of iterations when solving this problem on $[0, 10]$ with $N = 32$, $h = 0.1$ and different error tolerances are shown in Table 5.3.

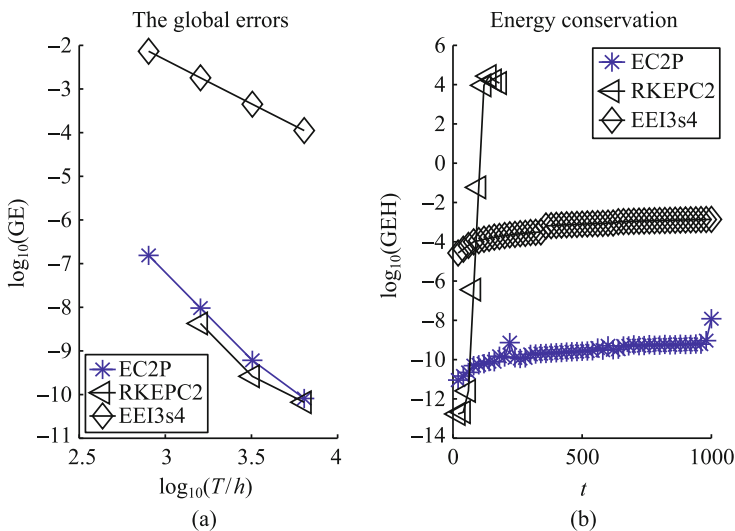


Fig. 5.5 (a) The logarithm of the global error against the logarithm of T/h . (b) The logarithm of the Hamiltonian error against t

Table 5.3 Results for Problem 5.3: the total number of iterations for different error tolerances (tol)

Methods	tol = 1.0×10^{-6}	tol = 1.0×10^{-8}	tol = 1.0×10^{-10}	tol = 1.0×10^{-12}
EC2P	488	632	796	963
RKEPC2	2558	4229	6991	8551

It can be concluded from these numerical experiments that the EC2P method definitely shows higher accuracy, better invariant-preserving property, and good long-term behaviour in the numerical simulations, compared to the other effective methods in the literature.

5.10 Concluding Remarks and Discussions

For several decades, exponential integrators have constituted an important class of methods for the numerical simulation of first-order ODEs, including the semi-discrete nonlinear Schrödinger equation etc. Finite element methods for ODEs can be traced back to the early 1960s and they have been investigated by many researchers. In this chapter, combining the ideas of these two types of effective methods, we derived and analysed a type of exponential collocation method for the conservative or dissipative system (5.1). We have also rigorously analysed its properties including existence and uniqueness, and algebraic order. It has been proved that the exponential collocation methods can achieve an arbitrary order of accuracy as well as preserve first integrals or Lyapunov functions exactly or approximately. The application of the methods to stiff gradient systems was discussed. The efficiency and superiority of exponential collocation methods were demonstrated by numerical results. By the analysis of this chapter, arbitrary-order energy-preserving methods were presented for second-order highly oscillatory/general systems.

Last, but not least, it is noted that the application of the methodology presented in this chapter to other ODEs such as general gradient systems (see [69]) and Poisson systems (see [70]) has been presented recently. We also note that there are some further issues of these methods to be considered.

- The error bounds and convergence properties of exponential collocation methods can be investigated.
- Another issue for exploration is the application of the methodology to PDEs such as nonlinear Schrödinger equations and wave equations (see, e.g. [71]).
- The long-time energy conservation of exponential collocation methods as well as its analysis by modulated Fourier expansion is another point which can be researched.

The material in this chapter is based on the work by Wang and Wu [72].

References

1. Hairer E, Lubich C, Wanner G. Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. 2nd ed. Berlin, Heidelberg: Springer-Verlag, 2006.
2. Hochbruck M, Ostermann A. Exponential integrators. *Acta Numer.*, 2010, 19: 209–286.
3. Wu X, Wang B. Recent Developments in Structure-Preserving Algorithms for Oscillatory Differential Equations. Singapore: Springer Nature Singapore Pte Ltd., 2018.
4. Wu X, You X, Wang B. Structure-preserving Algorithms for Oscillatory Differential Equations. Berlin, Heidelberg: Springer-Verlag, 2013.
5. Berland H, Owren B, Skaflestad B. B-series and order conditions for exponential integrators. *SIAM J. Numer. Anal.*, 2005, 43: 1715–1727.
6. Butcher J C. Trees, B-series and exponential integrators. *IMA J. Numer. Anal.*, 2009, 30: 131–140.
7. Caliarì M, Ostermann A. Implementation of exponential Rosenbrock-type integrators. *Appl. Numer. Math.*, 2009, 59: 568–581.
8. Calvo M, Palencia C. A class of explicit multistep exponential integrators for semilinear problems. *Numer. Math.*, 2006, 102: 367–381.
9. Cano B, Gonzalez-Pachon A. Projected explicit Lawson methods for the integration of Schrödinger equation. *Numer. Methods Partial Differ. Eq.*, 2015, 31: 78–104.
10. Celledoni E, Cohen D, Owren B. Symmetric exponential integrators with an application to the cubic Schrödinger equation. *Found. Comput. Math.*, 2008, 8: 303–317.
11. Einkemmer L, Tokman M, Loffeld J. On the performance of exponential integrators for problems in magnetohydrodynamics. *J. Comput. Phys.*, 2017, 330: 550–565.
12. Grimm V, Hochbruck M. Error analysis of exponential integrators for oscillatory second order differential equations. *J. Phys. A: Math. Gen.*, 2006, 39: 5495–5507.
13. Hochbruck M, Ostermann A. Exponential Runge–Kutta methods for parabolic problems. *Appl. Numer. Math.*, 2005, 53: 323–339.
14. Hochbruck M, Ostermann A, Schweitzer J. Exponential rosenbrock-type methods. *SIAM J. Numer. Anal.*, 2009, 47: 786–803.
15. Ostermann A, Thalhammer M, Wright W M. A class of explicit exponential general linear methods. *BIT Numer. Math.*, 2006, 46: 409–431.
16. Wang B, Wu X, Meng F, et al. Exponential Fourier collocation methods for solving first-order differential equations. *J. Comput. Math.*, 2017, 35: 711–736.
17. Wu X, Wang B, Xia J. Explicit symplectic multidimensional exponential fitting modified Runge–Kutta–Nyström methods. *BIT Numer. Math.*, 2012, 52: 773–795.
18. Mei L, Wu X. Symplectic exponential Runge–Kutta methods for solving nonlinear Hamiltonian systems. *J. Comput. Phys.*, 2017, 338: 567–584.
19. Celledoni E, McLachlan R I, Owren B, et al. Energy-preserving integrators and the structure of B-series. *Found. Comput. Math.*, 2010, 10: 673–693.
20. Celledoni E, Owren B, Sun Y. The minimal stage, energy preserving Runge–Kutta method for polynomial Hamiltonian systems is the averaged vector field method. *Math. Comput.*, 2014, 83: 1689–1700.
21. Quispel G R W, McLaren D I. A new class of energy-preserving numerical integration methods. *J. Phys. A: Math. Theor.*, 2008, 41: 045206.
22. McLachlan R I, Quispel G R W. Discrete gradient methods have an energy conservation law. *Disc. Contin. Dyn. Syst.*, 2014, 34: 1099–1104.
23. McLachlan, R.I., Quispel, G.R.W., Robidoux, N.: Geometric integration using discrete gradient. *Philos. Trans. R. Soc. Lond. A* **357**, 1021–1045 (1999)
24. Wang, B., Wu, X.: The formulation and analysis of energy-preserving schemes for solving high-dimensional nonlinear Klein-Gordon equations. *SIMA J. Numer. Anal.* **39**, 2016–2044 (2019)

25. Brugnano, L., Iavernaro, F.: *Line Integral Methods for Conservative Problems*. Chapman and Hall/CRC Press, Boca Raton (2016)
26. Brugnano, L., Iavernaro, F., Trigiante, D.: Hamiltonian boundary value methods (energy preserving discrete line integral methods). *J. Numer. Anal. Ind. Appl. Math.* **5**, 13–17 (2010)
27. Brugnano, L., Iavernaro, F., Trigiante, D.: A simple framework for the derivation and analysis of effective one-step methods for ODEs. *Appl. Math. Comput.* **218**, 8475–8485 (2012)
28. Brugnano, L., Iavernaro, F., Trigiante, D.: Energy- and quadratic invariants-preserving integrators based upon Gauss-collocation formulae. *SIAM J. Numer. Anal.* **50**, 2897–2916 (2012)
29. Cohen, D., Hairer, E.: Linear energy-preserving integrators for Poisson systems. *BIT Numer. Math.* **51**, 91–101 (2011)
30. Hairer, E.: Energy-preserving variant of collocation methods. *J. Numer. Anal. Ind. Appl. Math.* **5**, 73–84 (2010)
31. Betsch, P., Steinmann, P.: Inherently energy conserving time finite elements for classical mechanics. *J. Comput. Phys.* **160**, 88–116 (2000)
32. Betsch, P., Steinmann, P.: Conservation properties of a time FE method, I. Time-stepping schemes for N-body problems. *Int. J. Numer. Meth. Eng.* **49**, 599–638 (2000)
33. Hansbo, P.: A note on energy conservation for Hamiltonian systems using continuous time finite elements. *Commun. Numer. Methods Eng.* **7**, 863–869 (2001)
34. Li, Y.W., Wu, X.: Functionally fitted energy-preserving methods for solving oscillatory nonlinear Hamiltonian systems. *SIAM J. Numer. Anal.* **54**, 2036–2059 (2016)
35. Tang, W., Sun, Y.: Time finite element methods: a unified framework for the numerical discretizations of ODEs. *Appl. Math. Comput.* **219**, 2158–2179 (2012)
36. Miyatake, Y.: An energy-preserving exponentially-fitted continuous stage Runge–Kutta method for Hamiltonian systems. *BIT Numer. Math.* **54**, 777–799 (2014)
37. Miyatake, Y.: A derivation of energy-preserving exponentially-fitted integrators for Poisson systems. *Comput. Phys. Commun.* **187**, 156–161 (2015)
38. Calvo, M., Laburta, M.P., Montijano, J.I., et al.: Projection methods preserving Lyapunov functions. *BIT Numer. Math.* **50**, 223–241 (2010)
39. Hairer, E., Lubich, C.: Energy-diminishing integration of gradient systems. *IMA J. Numer. Anal.* **34**, 452–461 (2014)
40. McLachlan, R.I., Quispel, G.R.W., Robidoux, N.: A unified approach to Hamiltonian systems, Poisson systems, gradient systems, and systems with Lyapunov functions or first integrals. *Phys. Rev. Lett.* **81**, 2399–2411 (1998)
41. Wang, B., Wu, X.: A new high precision energy-preserving integrator for system of oscillatory second-order differential equations. *Phys. Lett. A* **376**, 1185–1190 (2012)
42. Wu, X., Wang, B., Shi, W.: Efficient energy preserving integrators for oscillatory Hamiltonian systems. *J. Comput. Phys.* **235**, 587–605 (2013)
43. Li, Y.W., Wu, X.: Exponential integrators preserving first integrals or Lyapunov functions for conservative or dissipative systems. *SIAM J. Sci. Comput.* **38**, 1876–1895 (2016)
44. Brugnano, L., Gurioli, G., Sun, Y.: Energy-conserving Hamiltonian boundary value methods for the numerical solution of the Korteweg-de Vries equation. *J. Comput. Appl. Math.* **351**, 117–135 (2019)
45. Brugnano, L., Gurioli, G., Zhang, C.: Spectrally accurate energy-preserving methods for the numerical solution of the “Good” Boussinesq equation. *Numer. Methods Partial Differ. Eq.* **35**, 1343–1362 (2019)
46. Brugnano, L., Iavernaro, F., Montijano, J.I., et al.: Spectrally accurate space-time solution of Hamiltonian PDEs. *Numer. Algor.* **81**, 1183–1202 (2019)
47. Brugnano, L., Montijano, J.I., Rández, L.: On the effectiveness of spectral methods for the numerical solution of multi-frequency highly-oscillatory Hamiltonian problems. *Numer. Algor.* **81**, 345–376 (2019)
48. Brugnano, L., Zhang, C., Li, D.: A class of energy-conserving Hamiltonian boundary value methods for nonlinear Schrödinger equation with wave operator. *Commun. Nonlinear Sci. Numer. Simul.* **60**, 33–49 (2018)

49. Hochbruck, M., Lubich, C., Selhofer, H.: Exponential integrators for large systems of differential equations. *SIAM J. Sci. Comput.* **19**, 1552–1574 (1998)
50. Hochbruck, M., Ostermann, A.: Explicit exponential Runge–Kutta methods for semilinear parabolic problems. *SIAM J. Numer. Anal.* **43**, 1069–1090 (2005)
51. Cohen, D., Hairer, E., Lubich, C.: Numerical energy conservation for multi-frequency oscillatory differential equations. *BIT Numer. Math.* **45**, 287–305 (2005)
52. Franco, J.M.: New methods for oscillatory systems based on ARKN methods. *Appl. Numer. Math.* **56**, 1040–1053 (2006)
53. García-Archilla, B., Sanz-Serna, J.M., Skeel, R.D.: Long-time-step methods for oscillatory differential equations. *SIAM J. Sci. Comput.* **20**, 930–963 (1999)
54. Hochbruck, M., Lubich, C.: A Gautschi-type method for oscillatory second-order differential equations. *Numer. Math.* **83**, 403–426 (1999)
55. Iserles, A.: Think globally, act locally: solving highly-oscillatory ordinary differential equations. *Appl. Numer. Math.* **43**, 145–160 (2002)
56. Wang, B., Meng, F., Fang, Y.: Efficient implementation of RKN-type Fourier collocation methods for second-order differential equations. *Appl. Numer. Math.* **119**, 164–178 (2017)
57. Wang, B., Wu, X., Meng, F.: Trigonometric collocation methods based on Lagrange basis polynomials for multi-frequency oscillatory second-order differential equations. *J. Comput. Appl. Math.* **313**, 185–201 (2017)
58. Wu, X., You, X., Shi, W., et al.: ERKN integrators for systems of oscillatory second-order differential equations. *Comput. Phys. Commun.* **181**, 1873–1887 (2010)
59. Wang, B., Iserles, A., Wu, X.: Arbitrary-order trigonometric Fourier collocation methods for multi-frequency oscillatory systems. *Found. Comput. Math.* **16**, 151–181 (2016)
60. Wang, B., Li, J., Fang, Y.: Long-term analysis of exponential integrators for highly oscillatory conservative systems (2018). arXiv: 1809. 07268
61. Barrett, J., Blowey, J.: Finite element approximation of an Allen-Cahn/Cahn-Hilliard system. *IMA J. Numer. Anal.* **22**, 11–71 (2002)
62. Lubich, C., Ostermann, A.: Runge–Kutta methods for parabolic equations and convolution quadrature. *Math. Comput.* **60**, 105–131 (1993)
63. Lubich, C., Ostermann, A.: Runge–Kutta time discretization of reaction-diffusion and Navier Stokes equations: nonsmooth-data error estimates and applications to long-time behaviour. *Appl. Numer. Math.* **22**, 279–292 (1996)
64. Hairer, E., Wanner, G.: Solving ordinary differential equations II. Stiff and Differential Algebraic Problems, Springer Series in Computational Mathematics 14, 2nd edn. Springer, Berlin (1996)
65. Al-Mohy, A.H., Higham, N.J.: Computing the action of the matrix exponential, with an application to exponential integrators. *SIAM J. Sci. Comput.* **33**, 488–511 (2011)
66. Hochbruck, M., Lubich, C.: On Krylov subspace approximations to the matrix exponential operator. *SIAM J. Numer. Anal.* **34**, 1911–1925 (1997)
67. Iavernaro, F., Trigiante, D.: High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems. *J. Numer. Anal. Ind. Appl. Math.* **4**, 87–101 (2009)
68. Chen, J.B., Qin, M.Z.: Multi-symplectic Fourier pseudospectral method for the nonlinear Schrödinger equation. *Electron. Trans. Numer. Anal.* **12**, 193–204 (2001)
69. Wang, B., Li, T., Wu, Y.: Arbitrary-order functionally fitted energy-diminishing methods for gradient systems. *Appl. Math. Lett.* **83**, 130–139 (2018)
70. Wang, B., Wu, X.: Functionally-fitted energy-preserving integrators for Poisson systems. *J. Comput. Phys.* **364**, 137–152 (2018)
71. Wang, B., Wu, X.: Exponential collocation methods based on continuous finite element approximations for efficiently solving the cubic Schrödinger equation. *Numer. Methods Partial Differ. Eq.* **36**, 1735–1757 (2020)
72. Wang, B., Wu, X.: Exponential collocation methods for conservative or dissipative systems. *J. Comput. Appl. Math.* **360**, 99–116 (2019)