Chapter 4
Symplectic Exponential Runge–Kutta Methods for Solving Nonlinear Hamiltonian Systems

Symplecticity is an important property for exponential Runge–Kutta (ERK) methods when the underlying problem $y'(t) = My(t) + f(y(t))$ is a Hamiltonian system. The main theme of this chapter is to present symplectic exponential Runge–Kutta methods. Using the fundamental analysis of geometric integrators, we first derive and analyse the symplectic conditions for ERK methods. These conditions reduce to the conventional ones when $M \to \mathbf{0}$. Furthermore, revised stiff order conditions are proposed and investigated in detail. This chapter is also accompanied by numerical results that demonstrate the potential of the symplectic ERK methods.

4.1 Introduction

The purpose of this chapter is to explore the efficient computation of initial value problems expressed in the autonomous form

$$\begin{cases} y'(t) = My(t) + f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{4.1}$$

where the matrix $(-M)$ is symmetric positive definite or skew-Hermitian with eigenvalues of large modulus. Problems of the form (4.1) arise in a wide range of practical problems, such as fluid mechanics, quantum mechanics, electrodynamics, optics, and water waves. Among them, one typical problem originating from the mixed initial-boundary value problems of evolution PDEs, can be written in an abstract form as follows:

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t} = \mathscr{L}u + \mathscr{N}(u), \quad x \in D, \ t \in [t_0, T], \\ B(x)u(x,t) = 0, \quad x \in \partial D, \ t > t_0, \\ u(x,0) = g(x), \quad x \in D, \end{cases} \tag{4.2}$$

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where D is a spatial domain with boundary ∂D in $\mathbb{R}^d$, $\mathscr{L}$ and $\mathscr{N}$ represent respectively linear and nonlinear operators, and $B(x)$ denotes the boundary operator. Under appropriate discretisation by finite difference approximations, spectral methods or finite elements methods, the problem (4.2) can be converted into (4.1). Stiff problems also yield examples of this type.

It is always challenging to effectively solve the problem (4.1) numerically, since the stiffness occurs due to the linear term My. In light of this point, exponential Runge–Kutta (ERK) methods were proposed for solving this type of problems instead of classical Runge–Kutta (RK) methods. ERK methods have been studied by many authors (see, e.g. [1, 2, 5, 6, 10–13, 15, 17, 18, 20]), and detailed analysis such as the convergence and the construction of these methods can be found therein. It is noted that the extended Runge–Kutta–Nyström (ERKN) methods (see, e.g. [29–32]) can also be classified into the category of exponential integrators, since they are especially designed for efficiently solving second order oscillatory or highly oscillatory problems.

It is well known that both stiff problems and Hamiltonian systems are of prime importance in applications. Much effort has been made in developing a wide variety of approaches to solving each of them. However, it is very clear that problem (4.1) can become identical to a Hamiltonian system if

$$f(y(t)) = J^{-1}\nabla U(y(t))$$

and

$$M = J^{-1}Q,$$

for the skew-symmetric matrix

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

where $U(y)$ is a smooth potential function, Q is a symmetric matrix, and I is the identity matrix. This observation motivates the main theme in this chapter, because (4.1) may be a Hamiltonian system. As is known, in the case of Hamiltonian systems, symplectic ERK methods are strongly recommended to preserve the symplecticity of the original problem, since symplectic methods provide long time energy preservation and stability, based on backward error analysis for symplectic methods when applied to Hamiltonian systems [7, 8]. On account of this point, we make a further study on symplectic conditions for ERK methods. Moreover, using the obtained symplectic conditions, we also derive and analyse a class of ERK methods with the important structure-preserving property.

We also note that an important issue for the study of ERK methods is the so-called stiff order. Unfortunately, however, as claimed by Berland et al. in [1], the stiff order conditions are rather restrictive in practice, e.g., the fifth-order ERK method recently constructed by Luan and Ostermann [20] has eight stages provided the full stiff order conditions are considered. Therefore, in this chapter, we deal with the stiff order conditions in a weak form, under which the revised stiff order conditions can be naturally derived from the classical (nonstiff) ones. This process is reasonable based on the fact that no order reduction has been observed, as shown in [15], where ERK methods only need classical (nonstiff) order.

The plan of this chapter is as follows. In Sect. 4.2, we investigate and present sufficient conditions for symplectic ERK methods. In Sect. 4.3, the revised stiff order conditions are investigated and a class of special and important ERK methods are considered, which share the same structure-preserving property as their corresponding RK methods (those corresponding to the underlying ERK methods when $M \to \mathbf{0}$). Section 4.4 is concerned with numerical results to illustrate the efficiency of the symplectic ERK methods. The last section is concerned with conclusions and discussions.

4.2 Symplectic Conditions for ERK Methods

In the study of structure-preserving algorithms, it is an important principle that the construction of numerical schemes for the initial value problem (4.1) should incorporate the structure of the original continuous system in an appropriate way. Taking this point into account, instead of (4.1), we directly consider the following variation-of-constants formula (or the Volterra integral equation) corresponding to (4.1):

$$y(t) = e^{(t-t_0)M} y_0 + \int_{t_0}^{t} e^{(t-\xi)M} f(y(\xi))d\xi. \tag{4.3}$$

It follows from (4.3) that, for any $t, \mu, h \in \mathbb{R}$ with $t, t + \mu h \in [t_0, T]$, the solution to (4.1) satisfies the following integral equation:

$$y(t + \mu h) = e^{\mu h M} y_0 + h \int_{0}^{\mu} e^{(\mu - z)hM} f(y(t + hz))dz, \tag{4.4}$$

which clearly shows the structure of the internal stages and update of an RK-type integrator for solving (4.1). In fact, the case of $0 < \mu < 1$ in (4.4) gives the structure of the internal stages, and $\mu = 1$ in (4.4) presents the structure of the updates of ERK methods. The integral in (4.4) will be approximated by a suitable quadrature formula once the numerical simulation is required for the underlying problem. From this point of view, therefore, ERK methods are generated quite naturally and fundamentally.

It is now easy to formulate ERK methods from the integral equation (4.4). An s-stage ERK method, especially for the stiff problem (4.1), can be written as (see, e.g. [12])

$$\begin{cases} Y_i = e^{c_i hM} y_0 + h \displaystyle\sum_{j=1}^{s} \bar{a}_{ij}(hM) f(Y_j), \quad i = 1, \ldots, s, \\ y_1 = e^{hM} y_0 + h \displaystyle\sum_{i=1}^{s} \bar{b}_i(hM) f(Y_i), \end{cases} \tag{4.5}$$

where $\bar{a}_{ij}(hM)$ and $\bar{b}_i(hM)$ are matrix-valued functions of hM. It is worth mentioning that an ERK method (4.5) reduces to a classical RK method if $M \to \mathbf{0}$. In this sense, the latter is called the *RK method corresponding* to the ERK method (4.5) in this chapter.

It is very clear that (4.1) becomes a Hamiltonian system if $f(y(t)) = J^{-1}\nabla U(y(t))$ and $M = J^{-1}Q$, where $U(y(t))$ is a smooth potential function and Q is a symmetric matrix. With this premise, in the remainder of this chapter we will consider the following Hamiltonian system

$$\begin{cases} y'(t) = J^{-1}Qy(t) + J^{-1}\nabla U(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0. \end{cases} \tag{4.6}$$

Hence, the existence of symplectic ERK methods is of great importance for (4.6), but has not received much attention yet in the literature. Consequently, in what follows, we will present and prove the symplectic conditions for ERK methods rigorously. The construction of symplectic ERK methods for solving (4.6) will be analysed in detail in the next section, which definitely confirms the existence of symplectic ERK methods.

Theorem 4.1 *If the coefficients of an s-stage ERK method satisfy the following conditions:*

$$\begin{cases} \bar{b}_i^{\intercal} JSS_i^{-1} = S_i^{-\intercal} S^{\intercal} J\bar{b}_i = \gamma J, \qquad \gamma \in \mathbb{R}, i = 1, \dots, s, \\ \bar{b}_i^{\intercal} J\bar{b}_j = \bar{b}_i^{\intercal} JSS_i^{-1}\bar{a}_{ij} + \bar{a}_{ji}^{\intercal} S_j^{-\intercal} S^{\intercal} J\bar{b}_j, \qquad i, j = 1, \dots, s, \end{cases} \tag{4.7}$$

where $S = e^{hM}$ and $S_i = e^{c_i hM}$ for $i = 1, \dots, s$, then the ERK method is symplectic. Here, γ is an arbitrary real number (independent of i).

Proof We first denote

$$D_i = \frac{\partial f(Y_i)}{\partial y}, \quad X_i = \frac{\partial Y_i}{\partial y_0},$$

for $i = 1, \dots, s$. If $f = J^{-1}\nabla U(y)$, $M = J^{-1}Q$ in (4.1), then (4.1) is a Hamiltonian system. Thus, M is the infinitesimal symplectic matrix. This leads to the symplecticity of S and S_i as they are exponential forms of λM for some $\lambda \in \mathbb{R}$. Differentiating the scheme (4.5) yields

$$X_i = \frac{\partial Y_i}{\partial y_0} = S_i + h\sum_{j=1}^{s} \bar{a}_{ij} D_j X_j, \tag{4.8}$$

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

$$\frac{\partial y_1}{\partial y_0} = S + h\sum_{i=1}^{s} \bar{b}_i D_i X_i. \tag{4.9}$$

We then have

$$\Big(\frac{\partial y_1}{\partial y_0}\Big)^{\intercal} J\Big(\frac{\partial y_1}{\partial y_0}\Big) = S^{\intercal} J S + h\sum_{i=1}^{s}\big(\bar{b}_i D_i X_i\big)^{\intercal} J S$$

$$+\,h\sum_{i=1}^{s} S^{\intercal} J\bar{b}_i D_i X_i + h^2\Big(\sum_{i=1}^{s}\bar{b}_i D_i X_i\Big)^{\intercal} J\Big(\sum_{i=1}^{s}\bar{b}_i D_i X_i\Big)$$

$$= J + h\sum_{i=1}^{s}\big(\bar{b}_i D_i X_i\big)^{\intercal} J S + h\sum_{i=1}^{s} S^{\intercal} J\bar{b}_i D_i X_i + h^2\sum_{i=1}^{s}\sum_{j=1}^{s}\big(\bar{b}_i D_i X_i\big)^{\intercal} J\big(\bar{b}_j D_j X_j\big). \quad (4.10)$$

Using Eq. (4.8), we obtain

$$\big(\bar{b}_i D_i X_i\big)^{\intercal} J S S_i^{-1} X_i = \big(\bar{b}_i D_i X_i\big)^{\intercal} J S + h\sum_{j=1}^{s}\big(\bar{b}_i D_i X_i\big)^{\intercal} J S S_i^{-1}\bar{a}_{ij} D_j X_j, \quad (4.11)$$

$$(X_i)^{\intercal} S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i X_i = S^{\intercal} J\bar{b}_i D_i X_i + h\sum_{j=1}^{s}\big(\bar{a}_{ij} D_j X_j\big)^{\intercal} S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i X_i, \quad (4.12)$$

which respectively give

$$\big(\bar{b}_i D_i X_i\big)^{\intercal} J S = \big(\bar{b}_i D_i X_i\big)^{\intercal} J S S_i^{-1} X_i - h\sum_{j=1}^{s}\big(\bar{b}_i D_i X_i\big)^{\intercal} J S S_i^{-1}\bar{a}_{ij} D_j X_j, \quad (4.13)$$

$$S^{\intercal} J\bar{b}_i D_i X_i = (X_i)^{\intercal} S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i X_i - h\sum_{j=1}^{s}\big(\bar{a}_{ij} D_j X_j\big)^{\intercal} S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i X_i. \quad (4.14)$$

Substituting the new expressions of $\big(\bar{b}_i D_i X_i\big)^{\intercal} J S$ and $S^{\intercal} J\bar{b}_i D_i X_i$ in Eqs. (4.13) and (4.14) into (4.10) yields

$$\Big(\frac{\partial y_1}{\partial y_0}\Big)^{\intercal} J\Big(\frac{\partial y_1}{\partial y_0}\Big) = J + h\sum_{i=1}^{s}\Big(X_i^{\intercal} D_i^{\intercal}\bar{b}_i^{\intercal} J S S_i^{-1} X_i + X_i^{\intercal} S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i X_i\Big)$$

$$-\,h^2\sum_{i=1}^{s}\sum_{j=1}^{s}\Big(X_i^{\intercal} D_i^{\intercal}\bar{b}_i^{\intercal} J S S_i^{-1}\bar{a}_{ij} D_j X_j\Big) - h^2\sum_{i=1}^{s}\sum_{j=1}^{s}\Big(X_j^{\intercal} D_j^{\intercal}\bar{a}_{ij}^{\intercal} S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i X_i\Big)$$

$$+\,h^2\sum_{i=1}^{s}\sum_{j=1}^{s} X_i^{\intercal} D_i^{\intercal}\bar{b}_i^{\intercal} J\bar{b}_j D_j X_j = J + h\sum_{i=1}^{s} X_i^{\intercal}\Big(D_i^{\intercal}\bar{b}_i^{\intercal} J S S_i^{-1} + S_i^{-\intercal} S^{\intercal} J\bar{b}_i D_i\Big) X_i$$

$$+\,h^2\sum_{i=1}^{s}\sum_{j=1}^{s} X_i^{\intercal} D_i^{\intercal}\Big(\bar{b}_i^{\intercal} J\bar{b}_j - \bar{b}_i^{\intercal} J S S_i^{-1}\bar{a}_{ij} - \bar{a}_{ji}^{\intercal} S_j^{-\intercal} S^{\intercal} J\bar{b}_j\Big) D_j X_j\,. \quad (4.15)$$

Since $f = J^{-1}\nabla U(y)$ and $D_i = \dfrac{\partial f(Y_i)}{\partial y}$, a direct calculation gives

$$J D_i + D_i^{\intercal} J = 0, \quad i = 1, \ldots, s,$$

on noticing that the Hessian $\dfrac{\partial^2 U}{\partial y^2}$ of U at Y_i is symmetric for $i = 1, \ldots, s$. It then follows from the conditions (4.7) that

$$\Big(\frac{\partial y_1}{\partial y_0}\Big)^{\intercal} J \Big(\frac{\partial y_1}{\partial y_0}\Big) = J.$$

Therefore, the method with coefficients satisfying (4.7) is symplectic. □

Remark 4.1 Here, Theorem 4.1 actually provides a class of sufficient conditions for symplectic ERK methods. Moreover, it can be easily verified that the proposed conditions will reduce to the classical symplectic conditions for RK methods when $M \to \mathbf{0}$. The details are analysed as follows. When $M \to \mathbf{0}$, the matrices $S = e^{hM}$ and $S_i = e^{c_i hM}$ for $i = 1, \ldots, s$ become identity matrices, and $\bar{a}_{ij}, \bar{b}_i$ for $i, j = 1, \ldots, s$ are scalars (more precisely, they are products of the scalars and the identity matrix). In this sense, the first equation of (4.7) holds automatically. The second one is then identical to

$$\bar{b}_i \bar{b}_j J = \bar{b}_i \bar{a}_{ij} J + \bar{a}_{ji} \bar{b}_j J.$$

Hence

$$\bar{b}_i \bar{b}_j = \bar{b}_i \bar{a}_{ij} + \bar{b}_j \bar{a}_{ji},$$

which is exactly the classical symplectic conditions of RK methods [7, 8, 22].

4.3 Symplectic ERK Methods

The direct construction of symplectic ERK methods based on the order conditions accompanying the symplectic conditions is always of high complexity. In spite of this, we make an effort to find a class of ERK methods with the important structure-preserving property. To achieve this goal, the "generalized Runge–Kutta methods", proposed in [17], are helpful and we are hopeful of obtaining some symplectic ERK methods. We first introduce the following theorem, which can be found in [1, 17].

Theorem 4.2 *If* $\boldsymbol{c} = (c_1, \ldots, c_s)^{\intercal}$, $\boldsymbol{b} = (b_1, \ldots, b_s)^{\intercal}$ *and* $A = (a_{i,j})_{s\times s}$ *are coefficients of an s-stage RK method of order p, then the ERK method with the same nodes* $\boldsymbol{c}$*, whose coefficients are defined by*

$$\bar{a}_{ij} = a_{ij} e^{(c_i - c_j)hM}, \qquad \bar{b}_i = b_i e^{(1-c_i)hM}, \quad i, j = 1, \ldots, s, \tag{4.16}$$

is also of order p when applied to the stiff problem (4.1).

The mapping (4.16) actually gives an effective approach for constructing ERK methods based on classical RK methods. It is rather attractive since RK methods have already been well developed in the literature. It is noted that the order is obtained in the sense of the classical (nonstiff) order. However, we will show below that the classical (nonstiff) order conditions are sufficient for the convergence order provided a class of modified stiff order conditions is admitted.

As claimed by Berland et al. [1], the stiff order conditions are rather restrictive. Here, we reconsider the stiff order conditions in a revised version, which does not affect the convergence order of the ERK methods. In fact, the stiff order conditions are derived from the estimation of the global error bound (see [10] for details). Using the explicit form of (4.24) in [10], the expression of the global errors e_n for ERK methods (4.5) can be written as

$$\begin{aligned} e_{n+1} =& e^{hM} e_n + h\mathscr{N}(e_n)e_n - h^2\psi_2(hM)f'(t_n) \\ & - h^3\psi_3(hM)f''(t_n) - h^3\sum_{i=1}^{s}\bar{b}_i(hM)J_n\psi_{2,i}(hM)f'(t_n) \\ & - h^4\psi_4(hM)f'''(t_n) - h^4\sum_{i=1}^{s}\bar{b}_i(hM)J_n\psi_{3,i}(hM)f''(t_n) \\ & - h^4\sum_{i=1}^{s}\bar{b}_i(hM)J_n\sum_{j=1}^{s}\bar{a}_{ij}J_n\psi_{2,j}(hM)f'(t_n) \\ & - h^4\sum_{i=1}^{s}\bar{b}_i(hM)c_iK_n\psi_{2,j}(hM)f'(t_n) + h^5\mathscr{R}_n, \end{aligned} \tag{4.17}$$

where J_n and K_n denote arbitrary square matrices, $\psi_i(hM)$ and $\psi_{i,j}(hM)$ are matrix-valued functions of hM respectively defined by

$$\psi_i(hM) = \varphi_i(hM) - \sum_{k=1}^{s}\bar{b}_k(hM)\frac{c_k^{i-1}}{(i-1)!}, \tag{4.18}$$

$$\psi_{j,i}(hM) = \varphi_j(c_ihM)c_i^j - \sum_{k=1}^{s}\bar{a}_{ik}(hM)\frac{c_k^{j-1}}{(j-1)!}, \tag{4.19}$$

and $\varphi_k(z)$ is defined by

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z}\frac{\theta^{k-1}}{(k-1)!}d\theta, \quad k \geq 1, \tag{4.20}$$

which has the recurrence relation

$$\varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z}, \quad \varphi_0(z) = e^z. \tag{4.21}$$

By setting some terms in (4.17) as zero, the stiff order conditions can be derived accordingly, just as the authors did in [10]. However, this results in restrictive algebraic conditions which are very difficult to satisfy in practice. Fortunately, a careful observation from (4.17) can help us deal with the stiff order in a modified version, in which the stiff order conditions are approximated satisfactorily by the required order of the underlying integrator instead of the stiff order conditions. In light of this approach, the revised stiff order conditions up to order four are obtained and listed in Table 4.1. It is quite reasonable in applications to admit the new revised stiff order conditions which can be thought of an extension of the conventional ones. With the revised stiff order conditions, (4.17) can be simplified as

$$e_{n+1} = e^{hM}e_n + h\mathscr{N}(e_n)e_n + h^5\widetilde{\mathscr{R}}_n, \tag{4.22}$$

which has no obvious reduction effect on the convergence order. This approach also can be found in determining the order conditions for ERKN methods [30, 32].

The most important advantage of admitting the revised stiff order conditions is that these conditions can be naturally deduced from the classical order conditions. Here, we give an example to show how to achieve the fifth condition in Table 4.1, based on the fourth (classical) order conditions. For convenience, we formally express $\bar{a}_{ij}(hM)$ and $\bar{b}_i(hM)$ as

$$\bar{a}_{ij}(hM) = \sum_{k=0}^{\infty} \bar{a}_{ij}^{(k)} \cdot (hM)^k, \quad \bar{b}_i(hM) = \sum_{k=0}^{\infty} \bar{b}_i^{(k)} \cdot (hM)^k, \quad i, j = 1, \dots, s, \tag{4.23}$$

where the coefficients $\bar{a}_{ij}^{(k)}$ and $\bar{b}_i^{(k)}$ are real numbers. Moreover, it can be derived from the recurrence relation (4.21) that

$$\varphi_k(V) = \sum_{j=0}^{\infty} \frac{V^j}{(j+k)!}, \tag{4.24}$$

for any matrix V and $k \geq 0$. Hence, taking (4.19), (4.23) and (4.24) into account, we have

$$\sum_{i=0}^{s} \bar{b}_i(hM)J_n\psi_{2,i}(hM) = \sum_{\mu=0}^{\infty}\sum_{\nu=0}^{\mu}\sum_{i=1}^{s} \bar{b}_i^{(\nu)} \left(\frac{c_i^{2+\mu-\nu}}{(2+\mu-\nu)!} - \sum_{k=1}^{s} \bar{a}_{ik}^{(\mu-\nu)} c_k \right) \cdot h^{\mu}(M^{\nu}J_nM^{\mu-\nu}). \tag{4.25}$$

The fifth condition $\sum_{i=0}^{s} \bar{b}_i(hM)J_n\psi_{2,i}(hM) = \mathscr{O}(h^2)$ in Table 4.1 then becomes identical to

$$\sum_{i=1}^{s} \bar{b}_i^{(0)} \left(\frac{c_i^2}{2!} - \sum_{k=1}^{s} \bar{a}_{ik}^{(0)} c_k \right) = 0, \tag{4.26}$$

Table 4.1 The revised stiff order conditions up to order four

No.	*Order*	*Order conditions*
1	1	$\psi_1(hM) = \mathcal{O}(h^4)$
2	2	$\psi_2(hM) = \mathcal{O}(h^3)$
3	2	$\psi_{1,i}(hM) = \mathcal{O}(h^3)$
4	3	$\psi_3(hM) = \mathcal{O}(h^2)$
5	3	$\sum_{i=0}^{s} \bar{b}_i(hM)J_n\psi_{2,i}(hM) = \mathcal{O}(h^2)$
6	4	$\psi_4(hM) = \mathcal{O}(h)$
7	4	$\sum_{i=1}^{s} \bar{b}_i(hM)J_n\psi_{3,i}(hM) = \mathcal{O}(h)$
8	4	$\sum_{i=1}^{s} \bar{b}_i(hM)J_n \sum_{j=1}^{s} \bar{a}_{ij} J_n\psi_{2,j}(hM) = \mathcal{O}(h)$
9	4	$\sum_{i=1}^{s} \bar{b}_i(hM)c_i K_n\psi_{2,j}(hM) = \mathcal{O}(h)$

$$\sum_{\nu=0}^{1}\sum_{i=1}^{s}\bar{b}_i^{(\nu)}\left(\frac{c_i^{3-\nu}}{(3-\nu)!}-\sum_{k=1}^{s}\bar{a}_{ik}^{(1-\nu)}c_k\right)=\sum_{i=1}^{s}\bar{b}_i^{(0)}\left(\frac{c_i^3}{3!}-\sum_{k=1}^{s}\bar{a}_{ik}^{(1)}c_k\right)$$
$$+\bar{b}_i^{(1)}\left(\frac{c_i^2}{2!}-\sum_{k=1}^{s}\bar{a}_{ik}^{(0)}c_k\right)=0. \tag{4.27}$$

In can be easily verified that the two Eqs. (4.26) and (4.27) are satisfied, based on the following conditions of order four [1, 10]:

$$\sum_{i=1}^{s}\bar{b}_i^{(0)}c_i^2=\frac{1}{3},\quad \sum_{i=1}^{s}\sum_{k=1}^{s}\bar{b}_i^{(0)}\bar{a}_{ik}^{(0)}c_k=\frac{1}{6},\quad \sum_{i=1}^{s}\bar{b}_i^{(0)}c_i^3=\frac{1}{4},$$
$$\sum_{i=1}^{s}\sum_{k=1}^{s}\bar{b}_i^{(0)}\bar{a}_{ik}^{(1)}c_k=\frac{1}{24},\quad \sum_{i=1}^{s}\bar{b}_i^{(1)}c_i^2=\frac{1}{12},\quad \sum_{i=1}^{s}\sum_{k=1}^{s}\bar{b}_i^{(1)}\bar{a}_{ik}^{(0)}c_k=\frac{1}{24}.$$

The other conditions in Table 4.1 can be verified in a similar way and the details are omitted here.

The discussions about the stiff order conditions is not pursued further here, since we are mainly devoted to investigating the symplectic conditions for ERK methods, and developing symplectic ERK integrators in this chapter. In the sequel, we will denote the coefficients of classical RK methods by $\mathbf{c} = (c_1, \ldots, c_s)^\intercal$, $\mathbf{b} = (b_1, \ldots, b_s)^\intercal$ and $A = (a_{ij})_{s\times s}$ for convenience. The following theorem states the main result of this chapter.

Theorem 4.3 *If an s-stage RK method is symplectic, then the ERK method yielded by (4.16) is also symplectic.*

Proof Inserting (4.16) into each term in (4.7) yields

$$\begin{cases} \bar{b}_i^\top JSS_i^{-1} = \big(b_i e^{(1-c_i)hM}\big)^\top J\big(e^{(1-c_i)hM}\big), \\ S_i^{-\top} S^\top J\bar{b}_i = \big(e^{(1-c_i)hM}\big)^\top J\big(b_i e^{(1-c_i)hM}\big), \\ \bar{b}_i^\top J\bar{b}_j = \big(b_i e^{(1-c_i)hM}\big)^\top J\big(b_j e^{(1-c_j)hM}\big), \\ \bar{b}_i^\top JSS_i^{-1}\bar{a}_{ij} + \bar{a}_{ji}^\top S_j^{-\top} S^\top J\bar{b}_j = \big(b_i e^{(1-c_i)hM}\big)^\top J\big(e^{(1-c_i)hM}\big)\big(a_{ij} e^{(c_i-c_j)hM}\big) \\ \qquad\qquad + \big(a_{ji} e^{(c_j-c_i)hM}\big)^\top \big(e^{(1-c_j)hM}\big)^\top J\big(b_j e^{(1-c_j)hM}\big). \end{cases} \tag{4.28}$$

Noting that the following identity holds

$$P^\top JP = J, \tag{4.29}$$

provided P is symplectic, and that $e^{\beta hM}$ is symplectic for any real β and infinitesimal symplectic matrix M, it follows from (4.28) that

$$\begin{cases} \bar{b}_i^\top JSS_i^{-1} = S_i^{-\top} S^\top J\bar{b}_i = b_i\big(e^{(1-c_i)hM}\big)^\top J\big(e^{(1-c_i)hM}\big) = b_i J, \\ \bar{b}_i^\top J\bar{b}_j = \big(b_i e^{(1-c_i)hM}\big)^\top J\big(b_j e^{(1-c_j)hM}\big) = b_i b_j\big(e^{-c_i hM}\big)^\top J\big(e^{-c_j hM}\big) = b_i b_j J\big(e^{(c_i-c_j)hM}\big), \\ \bar{b}_i^\top JSS_i^{-1}\bar{a}_{ij} + \bar{a}_{ji}^\top S_j^{-\top} S^\top J\bar{b}_j = (b_i a_{ij} + b_j a_{ji})J\big(e^{(c_i-c_j)hM}\big), \end{cases} \tag{4.30}$$

which immediately leads to the satisfaction of the symplectic conditions (4.7) based on those conditions for RK methods, i.e.,

$$b_i b_j = b_i a_{ij} + b_j a_{ji}.$$

This completes the proof. □

Another interesting result about the "generalized Runge–Kutta methods" of [17] is that if the corresponding RK method is symmetric, i.e., the coefficients of an s-stage ERK method satisfy the following conditions

$$\begin{cases} 1 - c_{s+1-i} = c_i, \quad i = 1, \ldots, s, \\ \bar{b}_i(hM) = e^{hM}\bar{b}_{s+1-i}(-hM), \quad i = 1, \ldots, s, \\ e^{(1-c_{s+1-i})hM}\bar{b}_{s+1-j}(-hM) = \bar{a}_{ij}(hM) + \bar{a}_{s+1-i,s+1-j}(-hM), \quad i, j = 1, \ldots, s, \end{cases} \tag{4.31}$$

then the ERK method yielded by (4.16) is symmetric as well. We refer the reader to [3] for more details on this result.

Theorem 4.4 *If the coefficients of an s-stage ERK method satisfy both the symplectic conditions (4.7) and symmetric conditions (4.31), then the ERK method is symplectic and symmetric.*

Proof Under the assumptions of the theorem, the conclusion is quite clear. We therefore omit the details of the proof here. □

4.4 Numerical Experiments

In this section, we implement some numerical experiments to show the high accuracy and good energy preservation of symplectic ERK methods stated in the previous section. In our experiments, the corresponding RK methods are selected as follows:

- RK2: the implicit midpoint method of order two;
- RK4: the Legendre-Gauss collocation method of order four [8].

It should be noted here that both RK2 and RK4 are symplectic, and then ERK2 and ERK4 obtained by the formula (4.16) share the same order as them by Theorem 4.2 and the same symplecticity as their corresponding RK methods by Theorem 4.3. Since all these underlying methods are implicit, iterations are required in the implementation of these methods. The study of existence and uniqueness of numerical solutions of ERK methods is entirely similar to that of implicit RK methods (see, e.g. [4, 16]), and we shall therefore assume unique existence of solution in the remainder of this chapter. As recommended by Hairer et al. (see VIII.6 in [8]), fixed-point iteration is used for the solution of the implicit RK methods, whereas the Newton iteration should be considered for the two implicit ERK methods (see, e.g. [24, 27]). The iteration will be stopped once the norm of the difference of two successive approximations is smaller than 10^{-16}. In all the experiments, the maximum norm is used for both the global errors (GE) and the difference of two successive approximations during the iterations. Throughout the numerical experiments, we point out that the matrix-valued functions $\varphi_k(V)$ ($k \geq 0$) are exactly evaluated. For larger problems, the Krylov subspace method is well known, and recommended in this case due to its fast convergence. The details about Krylov subspace methods can be found in [9, 13].

As emphasised by the authors in [9, 12, 13], we are hopeful of showing higher accuracy for the ERK methods than their corresponding RK methods in numerical experiments, since they can exactly solve the homogeneous equation $y'(t) = My$, and M always has eigenvalues of large modulus. Meanwhile, good energy preservation is also expected due to the symplecticity of the underlying ERK methods. Another point is that the convergence of iterations for the implicit ERK methods is much better than that for the corresponding RK methods. The main reason is that the occurrence of My in the RK methods when applied to system (4.1) will obviously decrease the convergence due to the large norm of M. Consequently, the faster convergence for the ERK methods results in less consumed CPU time. On the basis of the analysis stated above, we will focus on the previously mentioned advantages of the symplectic ERK methods over their corresponding traditional symplectic RK methods during our numerical experiments.

Problem 4.1 Consider the Duffing equation (see, e.g. [19])

$$\begin{cases} \ddot{q} + \omega^2 q = k^2(2q^3 - q), \\ q(0) = 0, \quad \dot{q}(0) = \omega, \end{cases}$$

with $0 \leq k < \omega$.

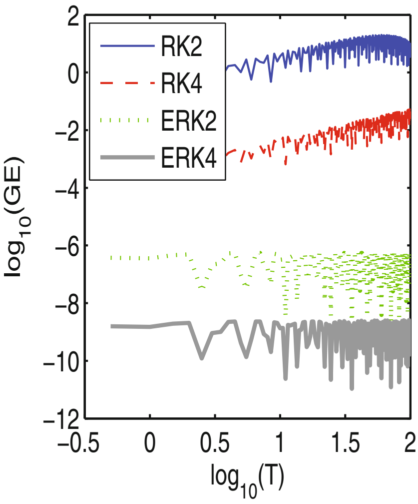

Fig. 4.1 Results for Problem 4.1: the global errors with $h = 1/40$

Let $p = q',\ z = (p, q)^{\intercal}$. Then the Duffing equation can be rewritten as

$$z'(t) = Mz + f(z),$$

where

$$M = \begin{pmatrix} 0 & -\omega^2 \\ 1 & 0 \end{pmatrix},$$

and

$$f = \Big(k^2(2q^3 - q),\ 0\Big)^{\intercal}.$$

This is a Hamiltonian system with the Hamiltonian

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

The analytic solution is given by

$$q(t) = sn(\omega t, k/\omega),$$

where *sn* is the Jacobian elliptic function.

This problem is solved on the interval [0, 100] with $\omega = 10$, $k = 0.03$ and the stepsize $h = 1/40$. The global errors for these methods are shown in Fig. 4.1. It can be observed from Fig. 4.1 that these two ERK methods significantly display better numerical behaviour in terms of accuracy than their corresponding RK methods.

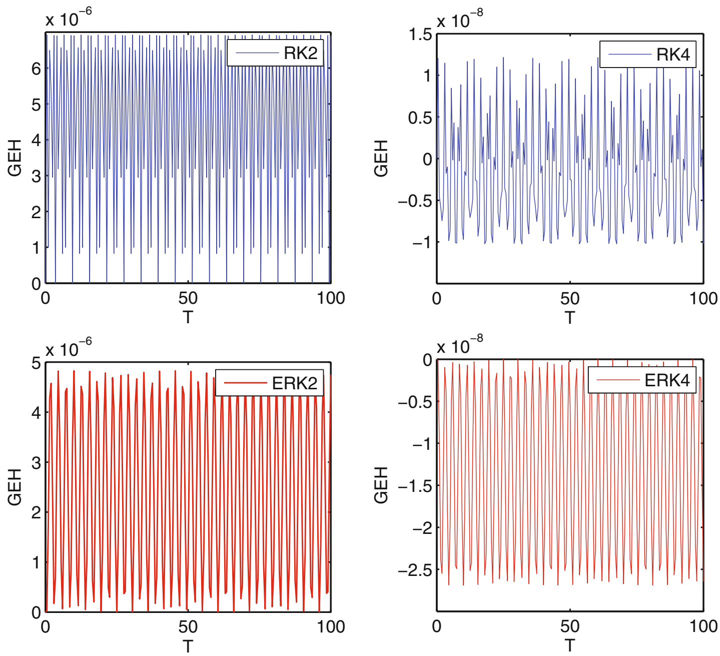

Fig. 4.2 Results for Problem 4.1: the energy preservation

Energy preservation behaviour is shown in Fig. 4.2, from which it can be observed that the obtained ERK methods show comparable energy preservation in comparison with their corresponding RK methods. The CPU times (in seconds) are 0.52, 0.91, 3.26 and 3.34, respectively, for ERK2, ERK4, RK2 and RK4. This shows the faster convergence and higher efficiency of ERK methods than the corresponding RK methods. This also indicates the superiority of the two symplectic ERK methods.

Problem 4.2 Consider the Fermi–Pasta–Ulam problem (see, e.g. [8]) which is an important nonlinear model for research on nonlinear dynamical systems in physics:

$$x''(t) + Ax(t) = -\nabla_x U(x(t)), \tag{4.32}$$

where

$$A = \begin{pmatrix} \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times m} & \omega^2 I_{m\times m} \end{pmatrix},$$

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

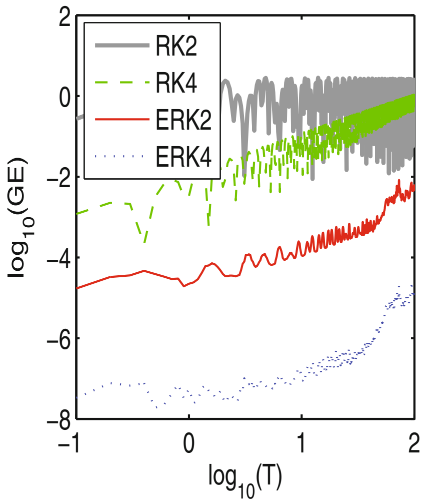

Fig. 4.3 Results for Problem 4.2: the global errors with $h = 1/200$

With $y = x'$, this problem can be expressed by the following Hamiltonian system:

$$z'(t) = Mz(t) + f(z(t)),$$

where $z = (y^\intercal, x^\intercal)^\intercal$,

$$M = \begin{pmatrix} \mathbf{0} & -A \\ E & \mathbf{0} \end{pmatrix},$$

and

$$f = \Big(-\big(\nabla_x U(x)\big)^\intercal,\ 0^\intercal \Big)^\intercal,$$

with the Hamiltonian

$$H(z) = \frac{1}{2}\sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{m+i}^2 + U(x). \tag{4.33}$$

Here, E is the identity matrix.

In this experiment, we choose

$$m = 3,\ x_1(0) = 1,\ y_1(0) = 1,\ x_4(0) = \frac{1}{\omega},\ y_1(0) = 1,\ \omega = 100,$$

and zero for the remaining initial data. This problem is integrated on the interval $[0, 100]$ with the stepsize $h = 1/200$. As shown in Fig. 4.3, the ERK methods give much better accuracy than their corresponding RK methods in global errors. Good

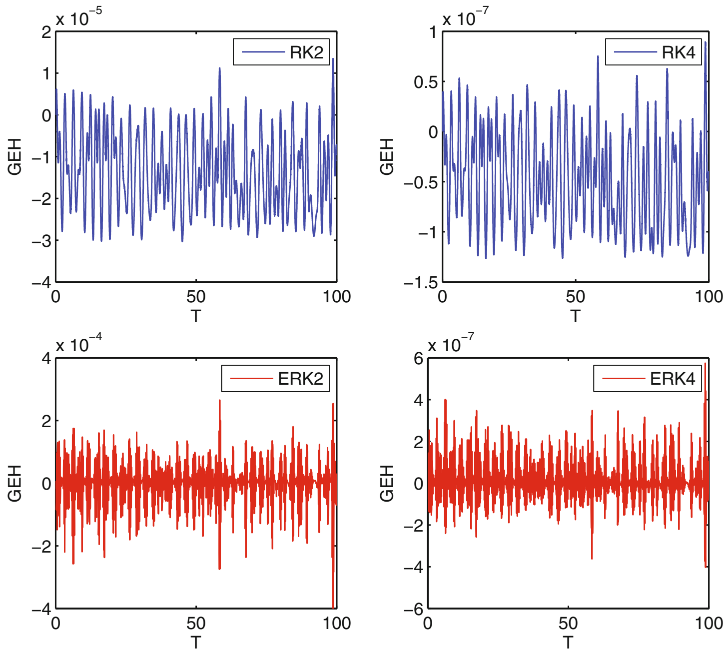

Fig. 4.4 Results for Problem 4.2: the energy preservation

energy preservation behaviour is also displayed by ERK2 and ERK4 in Fig. 4.4. The higher efficiency of the symplectic ERK methods than RK methods is supported by their smaller CPU times (seconds), which are 2.09, 8.43, 29.20 and 30.20, respectively, for ERK2, ERK4, RK2, and RK4.

Problem 4.3 Consider the sine-Gordon equation with the periodic boundary conditions (see, e.g. [23])

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial^2 u}{\partial x^2} - \sin u, \ -5 \le x \le 5, \ t \ge 0, \\ u(-5, t) = u(5, t). \end{cases} \tag{4.34}$$

Here, we use the Fourier pseudo-spectral discretisation (see e.g. [26]) for the spatial derivative. Then it can be converted into the following ordinary differential equations:

$$\frac{d}{dt}\begin{pmatrix} U' \\ U \end{pmatrix} = \begin{pmatrix} \mathbf{0} & M \\ E & \mathbf{0} \end{pmatrix}\begin{pmatrix} U' \\ U \end{pmatrix} + \begin{pmatrix} -\sin(U) \\ 0 \end{pmatrix}, \tag{4.35}$$

where $U(t) = (u_1(t), \dots, u_N(t))^\intercal$ with $u_i(t) \approx u(x_i, t)$, $x_i = -5 + i\Delta x$ for $i = 1, \dots, N$, $\Delta x = 10/N$, E is the identity matrix and the second-order spectral differentiation matrix M can be found in [26]. It can be verified that $-M$ is symmetric positive semi-definite. The Hamiltonian corresponding to (4.35) is given by

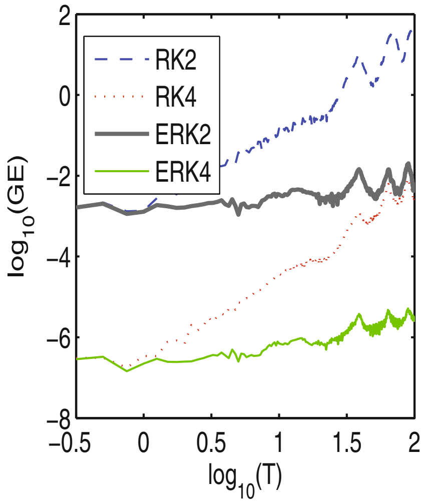

Fig. 4.5 Results for Problem 4.3: the global errors with $h = 1/40$

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

For this problem, we set the initial conditions as

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

with $N = 64$. Again, Fig. 4.5 shows the much better accuracy of the two ERK methods than their corresponding RK methods. The detailed behaviour of energy conservation for each method is shown in Fig. 4.6, which clearly displays comparable performance in qualitative behaviour between the ERK integrators and their corresponding RK methods. The CPU times (in seconds) are 0.86, 3.77, 5.59 and 6.50, respectively, for ERK2, ERK4, RK2 and RK4.

Problem 4.4 Consider the nonlinear Klein–Gordon equation with the periodic boundary condition (see, e.g. [14, 28])

$$\begin{cases} u_{tt} + u_{xx} + u + u^3 = 0, \quad 0 < x < L, \quad t \in (0, T), \\ u(0, t) = u(L, t). \end{cases}$$

The initial conditions are given by

$$u(x, 0) = A\left[1 + \cos\left(\frac{2\pi}{L}x\right)\right], \quad u_t(x, 0) = 0,$$

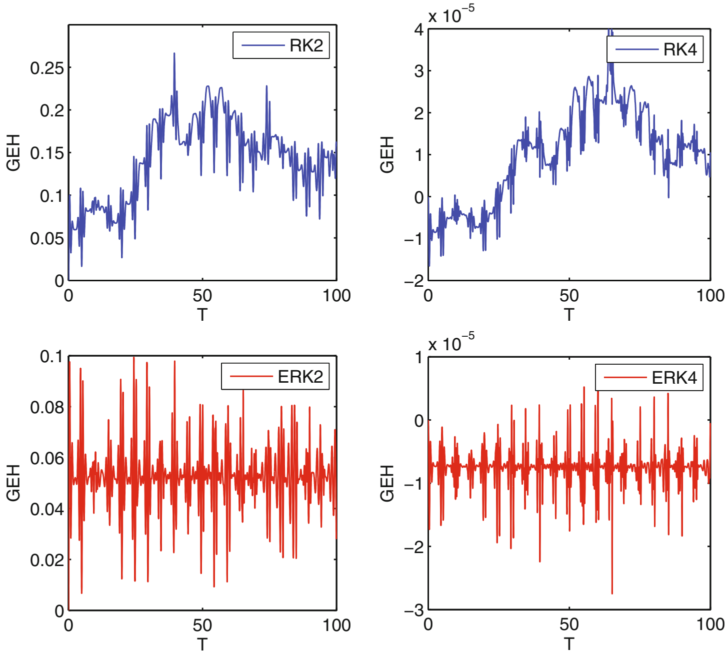

Fig. 4.6 Results for Problem 4.3: the energy preservation

where $L = 1.28$ and A is the amplitude. Similarly to Problem 4.3, if the Fourier pseudo-spectral discretisation is applied to this problem, the semi-discrete ODEs can be obtained:

$$\frac{d}{dt}\begin{pmatrix} U' \\ U \end{pmatrix} = \begin{pmatrix} \mathbf{0} & M \\ E & \mathbf{0} \end{pmatrix}\begin{pmatrix} U' \\ U \end{pmatrix} + \begin{pmatrix} -U - U^3 \\ 0 \end{pmatrix}, \tag{4.36}$$

whose Hamiltonian is given by

$$H(U', U) = \frac{1}{2}U'^{\intercal}U' + \frac{1}{2}U^{\intercal}(-M)U + \frac{1}{2}U^2 + \frac{1}{4}U^4.$$

For this problem, we set $A = 20$. As claimed in [14, 28], this equation is challenging for numerical methods, since the solution shows abrupt changes in both time and space directions with a large amplitude. Similarly to [28], we also carry out numerical simulations with the space stepsize $\Delta x = 0.02$ and the time stepsize $h = 0.01$. The good energy preservation for the two symplectic ERK methods is shown in Fig. 4.7, where the relative errors $RGEH = \frac{GEH}{H_0}$ are plotted for the large value of $H_0 = 1.14 \times 10^7$ and amplitude $A = 20$. Moreover, we display the numerical wave forms from the two ERK methods in Figs. 4.8 and 4.9, respectively. It is shown that both the two ERK methods perform very well, since they preserve

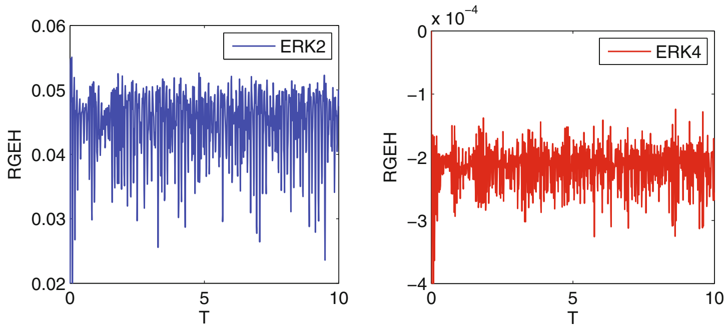

Fig. 4.7 Results for Problem 4.4: the energy preservation

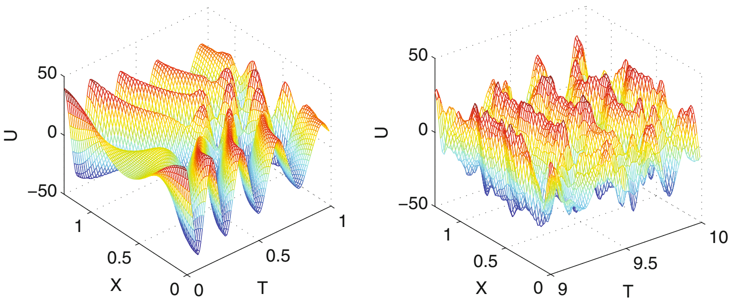

Fig. 4.8 Results for Problem 4.4: the numerical wave forms of ERK2 on different time intervals: the left $t \in [0, 1]$ and the right $t \in [9, 10]$

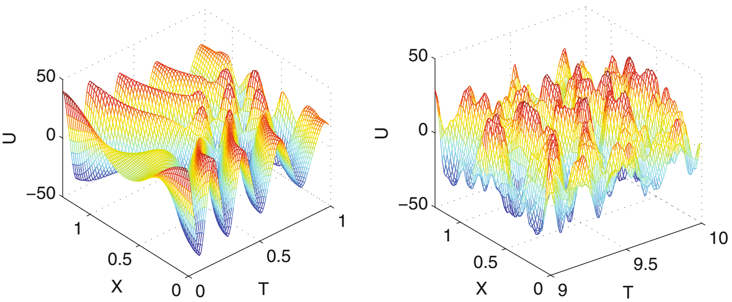

Fig. 4.9 Results for Problem 4.4: the numerical wave forms of ERK4 on different time intervals: the left $t \in [0, 1]$ and the right $t \in [9, 10]$

spatial symmetry as well as the continuity of the solution. Unfortunately, however, the two corresponding RK methods cannot give effective numerical results, since the iterations in the case of $\Delta x = 0.02$ and $h = 0.01$ are not convergent for both RK2 and RK4. The CPU times (in seconds) are 0.23 and 2.37, respectively, for ERK2 and ERK4.

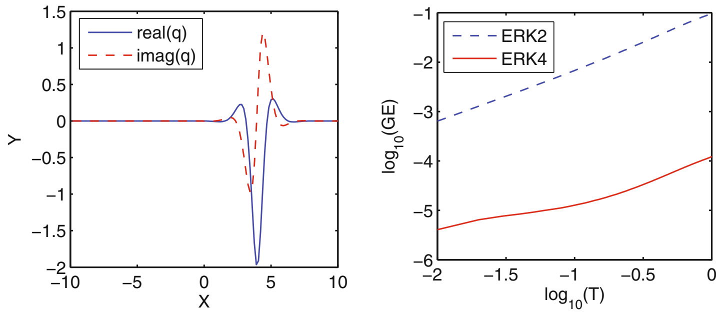

Fig. 4.10 Results for Problem 4.5: exact solutions and the global errors with $h = 0.01$ at $T = 1$

Finally, we turn to the important nonlinear Schrödinger (NLS) equations.

Problem 4.5 Consider the nonlinear Schrödinger (NLS) equation (see, e.g. [25])

$$iq_t = q_{xx} + 2|q|^2 q, \quad t \in (0, T),$$

on the interval $x \in [-10, 10]$ with periodic boundary conditions. The exact solution is given by

$$q(x,t) = 2\eta e^{-i[2\zeta x - 4(\zeta^2 - \eta^2)t + (\Phi_0 + \frac{\pi}{2})]} \mathrm{sech}(2\eta x - 8\zeta\eta t - x_0),$$

where x_0, Φ_0, ζ and η are some constants.

For this problem, we respectively denote u and v as the real and imaginary parts of q. If the Fourier pseudo-spectral method is used for the spatial discretization, this problem can be converted into the Hamiltonian system of the form

$$\frac{d}{dt}\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} \mathbf{0} & M \\ -M & \mathbf{0} \end{pmatrix}\begin{pmatrix} U \\ V \end{pmatrix} + \begin{pmatrix} 2(U^2 + V^2)V \\ -2(U^2 + V^2)U \end{pmatrix}, \tag{4.37}$$

whose Hamiltonian reads

$$H(U, V) = \frac{1}{2}U^{\intercal}(-M)U + \frac{1}{2}V^{\intercal}(-M)V - \frac{1}{2}\big(U^{\intercal}U + V^{\intercal}V\big)^2, \tag{4.38}$$

where M is the second-order spectral differentiation matrix approximating the spatial derivative, $U(t) = (u_1(t), \ldots, u_N(t))^{\intercal}$, and $V(t) = (v_1(t), \ldots, v_N(t))^{\intercal}$. Note that the multiplication of two vectors occurring in (4.37) is in the componentwise sense.

This problem is numerically solved with the given parameters $x_0 = 0$, $\Phi_0 = 0$, $\zeta = 1$, $\eta = 1$, $N = 128$ and $T = 1$. The real and imaginary parts of the exact solution and the global errors for ERK2 and ERK4 with $h = 0.01$ at the endpoint are plotted in Fig. 4.10. It is worth mentioning that only numerical results for ERK methods are plotted in Fig. 4.10, as their corresponding RK methods do not work due

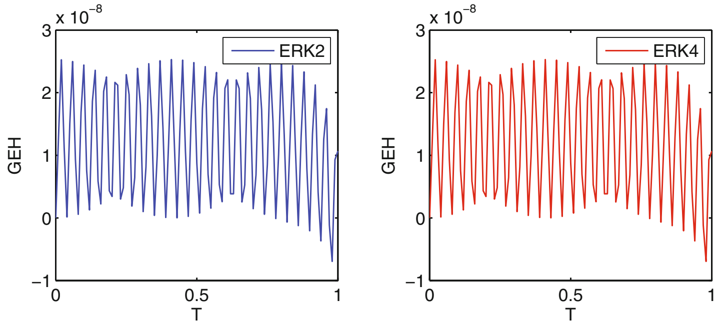

Fig. 4.11 Results for Problem 4.5: the energy preservation

to the appearance of non-convergence during the interactive process. This shows the better performance and broader applicability of symplectic ERK methods over their corresponding symplectic RK methods. Moreover, it can be observed from Fig. 4.11 that both ERK methods show good energy preservation behaviour as well. The CPU times (in seconds) are 0.20 and 0.57, respectively, for ERK2 and ERK4.

4.5 Conclusions and Discussions

Exponential Runge–Kutta methods are very attractive and practical in applications since they always show better performance than classical RK methods in dealing with stiff problems. However, when the underlying problem (4.1) is a Hamiltonian system, the research work has not received much attention up to now. This motivates the main theme of this work: *effective integrators for this kind of Hamiltonian systems using ERK integrators*. With respect to the construction of effective high-order ERK methods, we investigated the structure-preserving property of the novel ERK integrators such as the symplecticity in this chapter. To this end, sufficient conditions for symplecticity were derived by a fundamental analysis of geometric integrators. Furthermore, we presented a novel class of *structure-preserving ERK methods*; that is the structure-preserving "generalized Runge–Kutta methods" (see Lawson [17]), which can preserve symplecticity in the same way as their corresponding RK methods. In order to dispose of the restriction of the conventional stiff order conditions, revised stiff conditions were proposed and investigated in detail. After the establishment of the associated theory for structure-preserving ERK methods, we derived a class of symplectic ERK methods. We took ERK2 and ERK4 as examples in this chapter. Finally, we conducted some numerical experiments, including the approximation of a nonlinear Schrödinger equation, in comparison with the corresponding symplectic Gauss-Legendre RK methods: RK2 and RK4, and the numerical results (both the accuracy and behaviour of energy preservation) are quite promising, and strongly support our theoretical analysis in this chapter. The numerical experiments demonstrate that our symplectic ERK methods are more efficient in many settings than classical methods for the computation of nonlinear Hamiltonian systems.

It is noted that a new exponential scheme EAVF was proposed in the recent paper [18] and summarised in Chap. 2, which preserves the first integral or the Lyapunov function for the conservative or dissipative system. Therefore, it seems that the other properties of structure preservation such as energy preservation and symmetry should be investigated further for the development of ERK integrators. This is the point we also wish to emphasise here.

In the previous four chapters we paid attention to first-order differential equations. In the next four chapters, we will turn to structure-preserving algorithms for multi-frequency and multi-dimensional highly oscillatory second-order differential equations which frequently occur in a wide variety of science and engineering applications.

The material of this chapter is based on the work by Mei and Wu [21].

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