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Exponentially fitted symmetric and symplectic DIRK methods for oscillatory Hamiltonian systems

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Abstract The order conditions for modified Runge–Kutta methods are derived via the rooted trees. Symmetry and symplecticity conditions and exponential fitting conditions for modified diagonally implicit Runge–Kutta (DIRK) are considered. Three new exponentially fitted symmetric and symplectic diagonally implicit Runge–Kutta (EFSSDIRK) methods of respective second order and fourth order are constructed. Phase properties of the new methods are analyzed. The new EFSSDIRK methods are applied to several Hamiltonian problems and compared to the results obtained by the existing symplectic DIRK methods in the literature.

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1 Introduction

In this paper, we are concerned with effective integration of initial value problems of the system of first order differential equations in the form

$$y' = f(x, y), \quad y(x_0) = y_0, \tag{1}$$

where $y \in \mathbb{R}^d$, $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth function. Such problems arise frequently in applied sciences such as celestial mechanics, chemistry, molecular dynamics and systems biology. More than often, the exact solution to the problem (1) is not available, therefore highly accurate numerical solution is of great importance. Runge–Kutta type methods constitute a category of most widely used integrators for the numerical solution of the problem (1) (see [1–4]).

Implicit RK methods have been designed for stiff differential equations [1,5]. Besides, implicit methods usually possess large stability regions, which means less limitation in stepsizes. Unfortunately, to integrate a system of d differential equations, an s-stage implicit method with a full coefficient matrix requires the solution of $d \times s$ simultaneous implicit (in general nonlinear) equations at each time step. But for an s-stage diagonally implicit RK (DIRK) method with a lower triangular matrix, each internal stages can be computed by solving an d-dimensional system (see [6]). This saves computational cost dramatically. Al-Rabeh [7] examined the optimal order of non-confluent DIRK methods with non-zero weights. Faragó et al. [8] investigated the convergence of the combination of any of the diagonally implicit (including also the explicit) Runge–Kutta methods with active Richardson extrapolation and showed that the numerical solution obtained converges under rather natural conditions.

In many cases, the problem (1) takes the form of a Hamiltonian system with the differential equations (see Hairer et al. [9], Feng and Qin [10])

$$\dot{y} = -J \nabla H(y) \tag{2}$$

where $y = (p^T, q^T)^T$, $p = (p_1, \ldots, p_N)^T$ is the generalized momenta, $q = (q_1, \ldots, q_N))^T$ is the generalized coordinates, $J = \begin{pmatrix} \mathbf{0} & I_N \\ -I_N & \mathbf{0} \end{pmatrix}$ and $H = H(p, q)$ is the Hamiltonian energy. As typical examples of Hamiltonian systems, we mention the Kepler problem, the mathematical pendulum, the Fermi-Pasta-Ulam and the Lotka–Volterra oscillator (see [9,11,12]).

The problem (2) calls for some special class of numerical integrators, namely, *symplectic integrators*. Many numerical analysts in this area attest to the fact that symplectic integrators for the numerical solution of (2) have great advantages because of the preservation of the qualitative (geometric) properties of the flow over classical

integrators. The symplecticity conditions for Runge–Kutta were discovered by Sanz-Serna [13]. Among pioneers in this area are Forest and Ruth [14], Yoshida [15], Feng and Qin [16] and McLachlan and Atela [17]. Some symplectic diagonally implicit methods (DIRK) were proposed by Cooper [18], Sanz-Serna and Calvo [19] and Feng and Qin [10].

On the other hand, as Hairer et al. [9] pointed out, symmetric methods show better long time behaviour than non-symmetric methods when applied to reversible systems. Earlier work on the numerical solution of the system (2) with the Runge–Kutta type method seldom considered the symmetry property of the method. Sanz-Serna and Abia [20] proposed to construct symplecitc and symmetric DIRK methods. J.M. Franco and I. Gómez [21] derived fourth-order symmetric DIRK methods for periodic stiff problems.

In applications, the solution to the IVP (1) can often be expressed primarily as a linear combination of functions $\{\exp(\pm\lambda x)\}$ for some complex number λ with perhaps a small perturbation. This motives the attempt to design RK methods that can integrate without truncation error differential equations with solution of the form $\{\exp(\pm\lambda x)\}$. These methods are named exponentially fitted methods. Calvo et al. [22] investigated the structure (linear and quadratic invariants) preservation of exponentially fitted Runge–Kutta methods and derived a family of symplectic two-stage and fourth order EFRK methods.

In the particular case that $\lambda = i\omega$ where $\omega > 0$, $i^2 = -1$, the previous exponentially fitted methods are called trigonometrically fitted methods. Gautschi [23] and Bettis [24] constructed linear multistep methods and Runge–Kutta methods respectively which are exact if the solution is a trigonometric polynomial in ωt of a prescribed degree. A survey of exponentially fitted methods can be found in the monograph by Ixaru and Vanden Berghe [25] and the monograph by Wu et al. [26].

The combination of symplecticity with the exponential/trigonometric fitting was first proposed by Simos and Vigo-Aguiar [27] where a two-stage Runge–Kutta–Nyström method was derived for second order differential equations. Recently, Vanden Berghe and Van Daele [28] have derived trigonometrically fitted RK methods. Unfortunately explicit Runge–Kutta methods cannot be symplectic [10] or symmetric. Calvo et al. [29] constructed sixth-order symmetric and symplectic exponentially fitted Runge–Kutta methods of the Gauss type. Very recently, Kalogiratou [30] derived a three-stage trigonometrically fitted DIRK method which is shown to be very effective when applied to oscillatory Hamiltonian systems.

The purpose of this paper is to investigate the symmetry and symplecticity conditions for modified exponentially fitted DIRK methods when they are applied to Hamiltonian systems in the form (1) or (2). The remainder of this paper is organized as follows. In Sect. 2 we introduce a new type of imaginary trees to derive the order conditions for modified DIRK methods followed by symmetry, symplecticity and exponentially fitting conditions. In Sect. 3, we derive two practical symmetric and symplectic exponentially fitted RK methods. Phase properties of the new EFSSDIRK methods are analyzed in Sect. 4. Numerical experiments are carried out in Sect. 5 to illustrate the effectiveness of the new methods. Conclusive remarks are given in Sect. 6.

2 Modified RK methods with order conditions, symmetry, symplecticity and exponential fitting conditions

Suppose the IVP (1) has oscillatory solution of the principal frequency ω. The idea of a fitted type Runge–Kutta method is to introduce coefficients depending on $z = i\omega h$ and the method is referred to as a modified Runge–Kutta method.

Definition 2.1 An s-stage *modified Runge–Kutta (RK) method* for solving the system (1) has the scheme

$$Y_i = \eta_i(z)y_n + h\sum_{j=1}^{s} a_{ij}(z)f(x_n + c_j(z)h, Y_j), \quad i = 1, \ldots, s,$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i(z)f(x_n + c_i(z)h, Y_i), \tag{3}$$

where h is the stepsize, $\eta_i(z), b_i(z), a_{ij}(z), c_i(z), 1 \leq j \leq i, i = 1, \ldots, s$ are assumed to be even functions of $z = \omega h$.

It is usually assumed that $\lim_{z \to 0} \eta_i(z) = 1$ so that as $z \to 0$, the scheme (3) reduces to a traditional Runge–Kutta method.

The scheme (3) can be briefly expressed by the Butcher tableau of coefficients

$$\frac{c(z) \quad \eta(z) \quad A(z)}{\qquad\qquad b^T} = \begin{array}{ccc|c|ccc}
c_1(z) & \eta_1(z) & a_{11}(z) & \ldots & a_{1s}(z) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
c_s(z) & \eta_s(z) & a_{s1}(z) & \ldots & a_{ss}(z) \\
\hline
 & & b_1(z) & \ldots & b_s(z)
\end{array}.$$

The purpose of this section is to present the algebraic order conditions, symmetric conditions and exponential fitting conditions for the modified RK method (3).

2.1 Order conditions

A modified Runge–Kutta method of the form (3) has order p if for any sufficiently smooth function $f(x, y)$ in Problem (1), under the assumption that $y(x_0) = y_0$, the local truncation error of the solution satisfies

$$LTE = y(x_0 + h) - y_1 = \mathcal{O}(h^{p+1}) \quad \text{as} \quad h \to 0.$$

The order conditions can be obtained by comparing the series expansion of the numerical solution with that of the exact solution. The exact solution can be expanded into series of the time step in terms of the rooted tree (see Butcher [4], Hairer et al. [9])

$$y(x_n + h) = y_n + \sum_{\tau \in \mathcal{T}} \frac{h^{\rho(\tau)}}{\rho(\tau)!}\alpha(\tau)\mathcal{F}(\tau)(y_n),$$

where $\mathcal{T}$ is the set of (modified) rooted trees, $\mathcal{F}(\tau)(y_n)$ is the elementary differential of f associated to $\tau \in \mathcal{T}$ at y_n, $\rho(\tau)$ is the order of the tree τ, $\gamma(\tau)$ is the density of τ, $\alpha(\tau)$ is the number of monotonic labellings of τ and $\Phi(\tau)$ is the elementary weight coefficient which depends on $A(z)$.

On the other hand, the numerical solution of the modifed RK method (3)

$$
\begin{aligned}
y_{n+1} = {} & y_n + h \sum_{i=1}^{s} b_i(z) f\left(\eta_i(z) y_n + h \sum_{j=1}^{s} a_{ij}(z) f(Y_j) \right) \\
= {} & y_n + h \sum_{i=1}^{s} b_i(z) \left[f(y_n) + f'(y_n) \left((\eta_i(z) - 1) y_n + h \sum_{j=1}^{s} a_{ij}(z) f(Y_j) \right) \right. \\
& + \frac{1}{2!} f''(y_n) \left((\eta_i(z) - 1) y_n + h \sum_{j=1}^{s} a_{ij}(z) f(Y_j) \right)^2 \\
& \left. + \frac{1}{3!} f^{(3)}(y_n) \left((\eta_i(z) - 1) y_n + h \sum_{j=1}^{s} a_{ij}(z) f(Y_j) \right)^3 + \cdots \right].
\end{aligned}
$$

Further expanding $f(Y_j)$ at y_n we have

$$
\begin{aligned}
y_{n+1} = {} & y_n + \sum_{\tau \in \mathcal{T}} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \gamma(\tau) b(z)^T \Phi(\tau) \alpha(\tau) \mathcal{F}(\tau)(y_n) \\
& + \sum_{\tau \in \widetilde{\mathcal{T}}} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \widetilde{\gamma}(\tau) b(z)^T \widetilde{\Phi}(\tau) \widetilde{\alpha}(\tau) \widetilde{\mathcal{F}}(\tau)(y_n),
\end{aligned}
$$

where $\widetilde{\mathcal{T}}$ is the set of *complex rooted trees* (also called *imaginary rooted trees, or imaginary trees*), for $\tau \in \widetilde{\mathcal{T}}$, the order $\rho(\tau)$, the function $\widetilde{\alpha}(\tau)$ and the density $\widetilde{\gamma}(\tau)$ are defined in the same way as those for traditional trees $\tau \in \mathcal{T}$, $\widetilde{\mathcal{F}}(\tau)(y_n)$ is the elementary differential of f associated to τ at y_n and $\widetilde{\Phi}(\tau)$ is the vector of elementary weight coefficients which depends on $A(z)$ and $\eta(z)$. The first imaginary trees with the corresponding vector of elementary weight coefficients and elementary differentials are presented in Table 1.

Thus the local truncation error of the modified RK method (3) can be expressed as

$$
\begin{aligned}
LTE = {} & \sum_{\tau \in \mathcal{T}} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \left(\gamma(\tau) b(z)^T \Phi(\tau) - 1 \right) \alpha(\tau) \mathcal{F}(\tau)(y_n) \\
& + \sum_{\tau \in \widetilde{\mathcal{T}}} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \widetilde{\gamma}(\tau) b(z)^T \widetilde{\Phi}(\tau) \widetilde{\alpha}(\tau) \widetilde{\mathcal{F}}(\tau)(y_n, y_n'), \quad (4)
\end{aligned}
$$

By the independence of the elementary differentials, it follows from (4) that the method (3) is of order p if

$$b(z)^T \Phi(\tau) - \frac{1}{\gamma(\tau)} = \mathcal{O}\left(h^{p+1-\rho(\tau)}\right) \quad \text{for all } \tau \in \mathcal{T} \text{ with order } \rho(\tau) \leq p,$$

and

$$b(z)^T \widetilde{\Phi}(\tau) = \mathcal{O}\left(h^{p+1-\rho(\tau)}\right) \quad \text{for all } \tau \in \widetilde{\mathcal{T}} \text{ with order } \rho(\tau) \leq p.$$

To be specific, the p-th order conditions are listed in two groups as follows:

(i) For traditional trees

$$b(z)^T e = 1 + \mathcal{O}(z^p), \quad b(z)^T A(z)e = \frac{1}{2} + \mathcal{O}(z^{p-1}),$$

$$b(z)^T (A(z)e)^2 = \frac{1}{3} + \mathcal{O}(z^{p-2}), \quad b(z)^T A^2(z)e = \frac{1}{6} + \mathcal{O}(z^{p-2}),$$

$$b(z)^T (A(z)e)^3 = \frac{1}{4} + \mathcal{O}(z^{p-3}), \quad b(z)^T \left(A(z)e \cdot \left(A(z)^2 e\right)\right) = \frac{1}{12} + \mathcal{O}(z),$$

$$b(z)^T A(z)\left(A(z)e\right)^2 = \frac{1}{8} + \mathcal{O}(z^{p-3}), \quad b(z)^T A^3(z)e = \frac{1}{24} + \mathcal{O}(z^{p-3}),$$

$$\cdots \tag{5}$$

(ii) For imaginary trees

$$b(z)^T \left(\eta(z) - e\right)^k = \mathcal{O}(z^p), \quad 1 \leq k < p/2,$$

$$b(z)^T \left(\left(\eta(z) - e\right)^k \cdot A(z)\left(\eta(z) - e\right)^l\right) = \mathcal{O}(z^{p-1}), \quad 1 < k + l < p/2,$$

$$b(z)^T \left(\left(\eta(z) - e\right)^k \cdot A(z)\left(\eta(z) - e\right)^l \cdot A(z)\left(\eta(z) - e\right)^m\right) = \mathcal{O}(z^{p-2}),$$
$$1 \leq k + l + m < p/2,$$

$$b(z)^T \left(\left(\eta(z) - e\right)^k \cdot A(z)\left(\left(\eta(z) - e\right)^l \cdot A(z)\left(\eta(z) - e\right)^m\right)\right) = \mathcal{O}(z^{p-2}),$$
$$1 \leq k + l + m < p/2,$$

$$b(z)^T \left(\eta(z) - e\right)^k \cdot \left(A(z)(\eta(z) - e)^l \cdot A(z)(\eta(z) - e)^m \cdot A(z)(\eta(z) - e)^n\right)$$
$$= \mathcal{O}(z^{p-3}), \quad 1 \leq k + l + m + n < p/2,$$

$$b(z)^T \left(\left(\eta(z) - e\right)^k \cdot A(z)(\eta(z) - e)^l \cdot A(z)\left(\left(\eta(z) - e\right)^m \cdot A(z)(\eta(z) - e)^n\right)\right)$$
$$= \mathcal{O}(z^{p-3}), \quad 1 \leq k + l + m + n < p/2,$$

$$b(z)^T \left(\left(\eta(z) - e\right)^k \cdot A(z)(\eta(z) - e)^l \cdot \left(A(z)(\eta(z) - e)^m \cdot A(z)(\eta(z) - e)^n\right)\right)$$
$$= \mathcal{O}(z^{p-3}), \quad 1 \leq k + l + m + n < p/2,$$

$$b(z)^T \left(\left(\eta(z) - e\right)^k \cdot A(z)\left(\left(\eta(z) - e\right)^l \cdot A(z)\left(\left(\eta(z) - e\right)^m \cdot A(z)(\eta(z) - e)^n\right)\right)\right)$$
$$= \mathcal{O}(z^{p-3}), \quad 1 \leq k + l + m + n < p/2,$$

$$\cdots \tag{6}$$

where $e = (1, \ldots, 1)^T, k, l, m, n$ are non-negative integers and a dot "·" between two vectors indicates componentwise multiplication. The first set of conditions (5) can be used to simplify successively the second set (6). For example, for $k = 2, l = 1$ and $p = 7$, if the conditions

$$b(z)^T A(z)e = \frac{1}{2} + \mathcal{O}(z^6), \quad b(z)^T (\eta(z) \cdot A(z)e) = \frac{1}{2} + \mathcal{O}(z^6),$$

$$b(z)^T (\eta(z)^2 \cdot A(z)e) = \frac{1}{2} + \mathcal{O}(z^6), \quad b(z)^T A(z)\eta(z) = \frac{1}{2} + \mathcal{O}(z^6),$$

$$b(z)^T (\eta(z) \cdot A(z)\eta(z)) = \frac{1}{2} + \mathcal{O}(z^6),$$

have been confirmed, then the second condition in (5) implies that

$$
\begin{aligned}
b(z)^T (\eta(z)^2 \cdot A(z)\eta(z)) &= 2b(z)^T (\eta(z) \cdot A(z)\eta(z)) \\
&\quad - b(z)^T A(z)\eta(z) + b(z)^T (\eta(z)^2 \cdot A(z)e) \\
&\quad - 2b(z)^T (\eta(z) \cdot A(z)e) + b(z)^T A(z)e + \mathcal{O}(z^6), \\
&= \frac{1}{2} + \mathcal{O}(z^6),
\end{aligned}
$$

which can be equivalently replaced by a simpler one

$$b(z)^T (\eta(z)^2 \cdot A(z)\eta(z)) = \frac{1}{2} + \mathcal{O}(z^6).$$

Keeping $\eta(z) - e = \mathcal{O}(z^2)$ in mind, the first to fourth conditions are listed as follows:

(i) First order conditions:
$$b(z)^T e = 1 + \mathcal{O}(z). \tag{7}$$

(ii) Second order conditions:

$$b(z)^T e = 1 + \mathcal{O}(z^2), \quad b(z)^T A(z)e = \frac{1}{2} + \mathcal{O}(z). \tag{8}$$

(iii) Third order conditions:

$$b(z)^T e = 1 + \mathcal{O}(z^3), \quad b(z)^T \eta(z) = 1 + \mathcal{O}(z^3), \quad b(z)^T A(z)e = \frac{1}{2} + \mathcal{O}(z^2),$$

$$b(z)^T (A(z)e)^2 = \frac{1}{3} + \mathcal{O}(z), \quad b(z)^T A(z)^2 e = \frac{1}{6} + \mathcal{O}(z). \tag{9}$$

(iv) Fourth order conditions:

$$b(z)^T e = 1 + \mathcal{O}(z^4), \quad b(z)^T \eta(z) = 1 + \mathcal{O}(z^4), \quad b(z)^T A(z)e = \frac{1}{2} + \mathcal{O}(z^3),$$

Table 1 Imaginary trees, vector of weight coefficients, elementary differentials

Graph of tree	Vector of weight coefficients $\widetilde{\Phi}(\tau)$	Elementary differential $\widetilde{\mathcal{F}}(\tau)(y)$
	$(\eta(z)-e)^k$	$f^{(k)}\,y^k$
	$(\eta(z)-e)^k \cdot A(z)(\eta(z)-e)^l$	$f^{(k+1)}(y^k,\, f^{(l)}y^l)$
	$(\eta(z)-e)^k \cdot A(z)(\eta(z)-e)^l \cdot A(z)(\eta(z)-e)^m$	$f^{(k+2)}(y^k,\, f^{(l)}y^l,\, f^{(m)}y^m)$
	$(\eta(z)-e)^k \cdot A(z)((\eta(z)-e)^l \cdot A(z)(\eta(z)-e)^m)$	$f^{(k+1)}(y^k,\, f^{(l+1)}(y^l,\, f^{(m)}y^m))$
	$(\eta(z)-e)^k \cdot A(z)(\eta(z)-e)^l \cdot A(z)(\eta(z)-e)^m \cdot A(z)(\eta(z)-e)^n$	$f^{(k+3)}(y^k,\, f^{(l)}y^l,\, f^{(m)}y^m,\, f^{(n)}y^n)$
	$(\eta(z)-e)^k \cdot A(z)(\eta(z)-e)^l \cdot A(z)((\eta(z)-e)^m \cdot A(z)(\eta(z)-e)^n)$	$f^{(k+2)}(y^k,\, f^{(l)}y^l,\, f^{(m+1)}(y^m,\, f^{(n)}y^n))$
	$(\eta(z)-e)^k \cdot A(z)((\eta(z)-e)^l \cdot A(z)(\eta(z)-e)^m \cdot A(z)(\eta(z)-e)^n)$	$f^{(k+1)}(y^k,\, f^{(l+2)}(y^l,\, f^{(m)}y^m,\, f^{(n)}y^n))$
	$(\eta(z)-e)^k \cdot A(z)((\eta(z)-e)^l \cdot A(z)((\eta(z)-e)^m \cdot A(z)(\eta(z)-e)^n))$	$f^{(k+1)}(y^k,\, f^{(l+1)}(y^l,\, f^{(m+1)}(y^m,\, f^{(n)}y^n)))$

$$b(z)^T A(z)\eta(z) = \frac{1}{2} + \mathcal{O}(z^3), \quad b(z)^T \big(\eta(z) \cdot A(z)e\big) = \frac{1}{2} + \mathcal{O}(z^3),$$

$$b(z)^T (A(z)e)^2 = \frac{1}{3} + \mathcal{O}(z^2), \quad b(z)^T A^2(z)e = \frac{1}{6} + \mathcal{O}(z^2),$$

$$b(z)^T (A(z)e)^3 = \frac{1}{4} + \mathcal{O}(z), \quad b(z)^T A(z)(A(z)e)^2 = \frac{1}{12} + \mathcal{O}(z),$$

$$b(z)^T \big(A(z)e \cdot A^2(z)e\big) = \frac{1}{8} + \mathcal{O}(z), \quad b(z)^T A^3(z)e = \frac{1}{24} + \mathcal{O}(z). \tag{10}$$

(iv) Fifth order conditions:

$$b(z)^T e = 1 + \mathcal{O}(z^5), \quad b(z)^T \eta(z) = 1 + \mathcal{O}(z^5), \quad b(z)^T \eta(z)^2 = 1 + \mathcal{O}(z^5),$$

$$b(z)^T A(z)e = \frac{1}{2} + \mathcal{O}(z^4), b(z)^T A(z)\eta(z) = \frac{1}{2} + \mathcal{O}(z^4),$$

$$b(z)^T \big(\eta(z) \cdot A(z)e\big) = \frac{1}{2} + \mathcal{O}(z^4), \quad b(z)^T (A(z)e)^2 = \frac{1}{3} + \mathcal{O}(z^3),$$

$$b(z)^T \big(\eta(z) \cdot (A(z)e)^2\big) = \frac{1}{3} + \mathcal{O}(z^3), \quad b(z)^T \big(A(z)\eta(z) \cdot (A(z)e)\big) = \frac{1}{3} + \mathcal{O}(z^3),$$

$$b(z)^T A^2(z)e = \frac{1}{6} + \mathcal{O}(z^3), \quad b(z)^T \big(\eta(z) \cdot A^2(z)e\big) = \frac{1}{6} + \mathcal{O}(z^3),$$

$$b(z)^T A(z)\big(\eta(z) \cdot A(z)e\big) = \frac{1}{6} + \mathcal{O}(z^3), \quad b(z)^T A^2(z)\eta(z) = \frac{1}{6} + \mathcal{O}(z^3),$$

$$b(z)^T (A(z)e)^3 = \frac{1}{4} + \mathcal{O}(z^2), \quad b(z)^T A(z)(A(z)e)^2 = \frac{1}{12} + \mathcal{O}(z^2),$$

$$b(z)^T \big(A(z)e \cdot A^2(z)e\big) = \frac{1}{8} + \mathcal{O}(z^2), \quad b(z)^T A^3(z)e = \frac{1}{24} + \mathcal{O}(z^2),$$

$$b(z)^T (A(z)e)^4 = \frac{1}{5} + \mathcal{O}(z),$$

$$b(z)^T \big((A(z)e)^2 \cdot A(z)^2 e\big) = \frac{1}{10} + \mathcal{O}(z), \quad b(z)^T \big(A(z)^2 e \cdot A(z)^2 e\big) = \frac{1}{20} + \mathcal{O}(z),$$

$$b(z)^T \big(A(z)e \cdot A(z)(A(z)e)^2\big) = \frac{1}{15} + \mathcal{O}(z), \quad b(z)^T \big(A(z)e \cdot A(z)^3 e\big) = \frac{1}{15} + \mathcal{O}(z),$$

$$b(z)^T A(z)\big(A(z)e\big)^3 = \frac{1}{20} + \mathcal{O}(z), \quad b(z)^T A(z)\big(A(z)e \cdot A(z)^2 e\big) = \frac{1}{10} + \mathcal{O}(z),$$

$$b(z)^T A(z)^2 \big(A(z)e\big)^2 = \frac{1}{40} + \mathcal{O}(z), \quad b(z)^T A(z)^4 e = \frac{1}{60} + \mathcal{O}(z).$$

2.2 Symmetry conditions

Definition 2.2 [9] The *adjoint method* Φ_h^* of a modified RK method Φ_h is the inverse map of the original method with reversed time step $-h$, i.e., $\Phi_h^* := \Phi_{-h}^{-1}$. A method for which $\Phi_h^* := \Phi_{-h}$ is called *symmetric*.

Theorem 2.1 *The adjoint method of a modified RK method* (3) *is again an s-stage modified RK method and its coefficients are given by*

$$c_i^*(z) = 1 - c_{s+1-i}(z), \quad \eta_i^*(z) = \eta_{s+1-i}(z), \quad b_i^*(z) = b_{s+1-i}(z), \quad i = 1, \ldots, s,$$

$$a_{ij}^*(z) = \eta_{s+1-i}(z)b_{s+1-j}(z) - a_{s+1-i,s+1-j}(z), \quad i, j = 1, \ldots, s, \tag{11}$$

If

$$c_i(z) = 1 - c_{s+1-i}(z), \quad \eta_i(z) = \eta_{s+1-i}(z), \quad b_i(z) = b_{s+1-i}(z), \quad i = 1, \dots, s,$$
$$a_{ij}(z) = \eta_{s+1-i}(z)b_{s+1-j}(z) - a_{s+1-i,s+1-j}(z), \quad i, j = 1, \dots, s, \tag{12}$$

then the modified RK method (3) *is symmetric.*

Proof Interchanging $y_{n+1} \leftrightarrow y_n$ and $h \leftrightarrow -h$ in (3) yields

$$Y_i = \eta_i(z)y_n + h \sum_{j=1}^{s} \big(\eta_i(z)b_j(z) - a_{ij}(z)\big) f\big(x_n + (1 - c_j(z))h, Y_j\big), \quad i = 1, \dots, s,$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i(z) f\big(x_n + (1 - c_i(z))h, Y_i\big).$$

Replacing i by $s + 1 - i$ and j by $s + 1 - j$ and denoting Y_{s+1-i} as Y_i^* gives

$$Y_i^* = \eta_{s+1-i}(z)y_n + h \sum_{j=1}^{s} \big(\eta_{s+1-i}(z)b_{s+1-j}(z) - a_{s+1-i,s+1-j}(z)\big)$$
$$f(x_n + (1 - c_{s+1-j}(z))h, Y_j^*), \quad i = 1, \dots, s,$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_{s+1-i}(z) f(x_n + (1 - c_{s+1-i}(z))h, Y_i^*). \tag{13}$$

The system (13) resprents a modified RK methods with coefficients given by (11). Comparing (11) and (12) implies that the adjoint coincides the original method if $c_i^*(z) = c_i(z)$, $a_{ij}^*(z) = a_{ij}(z)$ and $b_i^*(z) = b_i(z)$ and the result follows. The proof is complete. □

Remark 2.1 As $z \to 0$, the conditions (12) reduces to the symmetry conditions for traditional RK methods with constant coefficients.

In this paper we are mainly interested in modified diagonally implicit RK (DIRK) methods, that is, in the scheme (3), $a_{ij}(z) = 0$ for $i < j$.

Corollary 2.1 *Under the assumptions of* (11)*, the modified DIRK is symmetric if*

$$c_i(z) = 1 - c_{s+1-i}(z), \quad \eta_i(z) = \eta_{s+1-i}(z), \quad b_i(z) = b_{s+1-i}(z), \quad i = 1, \dots, s,$$
$$a_{ij}(z) = \eta_i(z)b_j(z), \quad 1 \le j < i \le s,$$
$$a_{jj}(z) + a_{s+1-j,s+1-j}(z) = \eta_j(z)b_j(z), \quad j = 1, \dots, s. \tag{14}$$

2.3 Symplecticity conditions

The flow of the Hamiltonian system (2) is the map $\varphi_t : U \subset \mathbb{R}^{2N} \to \mathbb{R}^{2N}$, $\varphi_t(p_0, q_0) = \big(p(t, p_0, q_0), q(t, p_0, q_0)\big)$, where $p(t, p_0, q_0), q(t, p_0, q_0)$ is the solution of the system with the initial values $p(0) = p_0, q(0) = q_0$. It is well-known that the flow φ_t satisfies

$$\left(\frac{\partial \varphi_t}{\partial (p_0, q_0)}\right)^T J \left(\frac{\partial \varphi_t}{\partial (p_0, q_0)}\right) = J.$$

Definition 2.3 A one-step method $\Phi_h : y_n \rightarrow y_{n+1}$ is symplectic if its Jacobian matrix $\dfrac{\partial y_{n+1}}{\partial y_n}$ is symplectic, that is, $\left(\dfrac{\partial y_{n+1}}{\partial y_n}\right)^T J \left(\dfrac{\partial y_{n+1}}{\partial y_n}\right) = J.$

Theorem 2.2 [31] *The modified RK method* (3) *is symplectic if its coefficients satisfy the following conditions*

$$m_{ij} := b_j(z)\frac{a_{ji}(z)}{\eta_j(z)} + b_i(z)\frac{a_{ij}(z)}{\eta_i(z)} - b_i(z)b_j(z) = 0, \quad i, j = 1, \ldots, s.$$

The proof is essentially the same as that of Theorem 2 in Sanz-Serna and Calvo [19].

For a DIRK method, it follows from the symplecticity condition (15) that

$$\begin{aligned}
a_{ii} &= \frac{1}{2}\eta_i(z)b_i(z), \\
a_{ij} &= \eta_i(z)b_j(z) \quad \text{for } i > j,
\end{aligned} \tag{15}$$

assuming that $b_i(z) \neq 0$ $(i = 1, \ldots, s)$.

Combining (15) with (14), the scheme of a symmetric and symplectic modified DIRK can written as

$$
\begin{array}{c|c|ccccc}
c_1(z) & \eta_1(z) & \frac{1}{2}\eta_1(z)b_1(z) & & & & \\
c_2(z) & \eta_2(z) & \eta_2(z)b_1(z) & \frac{1}{2}\eta_2(z)b_2(z) & & & \\
\vdots & \vdots & \vdots & \vdots & \ddots & & \\
c_2(z) & \eta_2(z) & \eta_2(z)b_1(z) & \eta_2(z)b_2(z) & \ldots & \frac{1}{2}\eta_2(z)b_2(z) & \\
c_1(z) & \eta_1(z) & \eta_1(z)b_1(z) & \eta_1(z)b_2(z) & \ldots & \eta_1(z)b_2(z) & \frac{1}{2}\eta_1(z)b_1(z) \\
\hline
& & b_1(z) & b_2(z) & \ldots & b_2(z) & b_1(z)
\end{array}
\tag{16}
$$

2.4 Exponentially fitting conditions

The basic idea of exponential fitting is to introduce fitting coefficients to the scheme of a traditional Runge–Kutta method so that the method can integrate without truncation error differential equations with solution of a exponential function $\exp(\lambda x)$, $\lambda \in \mathbb{C}$. Exponentially fitted (EF) algorithms have been systematically studied by Ixaru and Vanden Berghe [25]. Vanden Berghe et al. [32] presented the exponential fitting conditions for the Runge–Kutta methods and derived some practical explicit EFRK methods. We follow the approach of Albrecht [33] and view each internal stage of the scheme (3) as a linear multistep method on a non-equidistant grid. In what follows,

- to the internal stages of (3), we associate the linear operators

$$
\mathcal{L}_i[A(z), h]y(x) = y(x + c_i(z)h) - \eta_i(z)y(x)
$$

$$
- h \sum_{j=1}^{s} a_{ij}(z)y'(x + c_j h), \quad i = 1, \ldots, s;
$$

- to the update of (3), we associate a linear operator

$$
\mathcal{L}[b(z), h]y(x) = y(x + h) - y(x) - h \sum_{i=1}^{s} b_i(z)y'(x + c_i h).
$$

Requiring that the operators $\mathcal{L}_i$ and $\mathcal{L}$ to vanish for the functions $\{\exp(\pm\lambda x)\}$ leads to the following equations:

$$
\sum_{j=1}^{s} a_{ij}(z)\sinh(c_j(z)z) = \frac{\cosh(c_i(z)z) - \eta_i(z)}{z}, \quad i = 1, \ldots, s,
$$

$$
\sum_{j=1}^{s} a_{ij}(z)\cosh(c_j(z)z) = \frac{\sinh(c_i(z)z)}{z}, \quad i = 1, \ldots, s,
$$

$$
\sum_{i=1}^{s} b_i(z)\sinh(c_i(z)z) = \frac{\cosh(z) - 1}{z},
$$

$$
\sum_{i=1}^{s} b_i(z)\cosh(c_i(z)z) = \frac{\sinh(z)}{z}, \tag{17}
$$

where $z = \lambda h$. Equations (17) are called the *exponential fitting conditions*.

If the coefficients of a modified diagonally implicit Runge–Kutta method satisfy the conditions (14), (15) and (17), then the method is referred to as an EFSSDIRK method.

3 Construction of new EFSSDIRK methods

The purpose of this section is to construct one to three-stage practical EFSSDIRK methods of order two and order four, respectively.

3.1 A one-stage EFSSDIRK method of order two

For $s = 1$, the scheme (16) becomes

$$
\begin{array}{c|c|c}
1/2 & \eta_1(z) & \frac{1}{2}\eta_1(z)b_1(z) \\
\hline
 & & b_1(z)
\end{array}
\tag{18}
$$

For this scheme, the exponentially fitting conditions (17) imply that

$$\cosh(c_1(z)z) - \eta_1(z) - za_{11}(z)\sinh(c_1(z)z) = 0,$$
$$\sinh(c_1(z)z) - za_{11}(z)\cosh(c_1(z)z) = 0,$$
$$\cosh(z) - zb_1(z)\sinh(c_1(z)z) - zb_2(z)\sinh(c_2(z)z) = 1,$$
$$\sinh(z) - zb_1(z)\cosh(c_1(z)z) - zb_2(z)\cosh(c_2(z)z) = 0. \tag{19}$$

Solving the system (19) with $c_1(z) = 1/2$, $a_{11}(z) = \frac{1}{2}\eta_1(z)b_1(z)$, we obtain

$$\eta_1(z) = \operatorname{sech}(z/2), \quad a_{11}(z) = \frac{\tanh(z/2)}{z}, \quad b_1(z) = \frac{2\sinh(z/2)}{z}. \tag{20}$$

It is easy to check that

$$b_1(z) = 1 + \frac{z^2}{24} + \mathcal{O}(z^4), \quad b_1(z)a_{11}(z) = \frac{1}{2} - \frac{z^2}{48} + \mathcal{O}(z^4).$$

Thus the method defined by (18) and (20) has order two and we denote the method as EFSSDIRK1s2. Note that as the frequency $\omega \to 0$ ($z \to 0$), this method reduces to a one-stage symmetric and symplectic DIRK method of order two

$$
\begin{array}{c|c}
1/2 & 1/2 \\
\hline
 & 1
\end{array}
$$

which is denoted as SSDIRK1s2 (Alexander [6]).

3.2 A two-stage EFSSDIRK method of order two

For $s = 2$, the scheme (16) becomes

$$
\begin{array}{c|cc}
c_1(z) & \eta_1(z) & \frac{1}{2}\eta_1(z)b_1(z) \\
1 - c_1(z) & \eta_1(z) & \eta_1(z)b_1(z) & \frac{1}{2}\eta_1(z)b_1(z) \\
\hline
 & & b_1(z) & b_1(z)
\end{array} \tag{21}
$$

For this scheme, the exponentially fitting conditions (17) imply that

$$\cosh(c_1(z)z) - \eta_1(z) - \frac{z}{2}\eta_1(z)b_1(z))\sinh(c_1(z)z) = 0,$$
$$\sinh(c_1(z)z) - \frac{z}{2}\eta_1(z)b_1(z)\cosh(c_1(z)z) = 0,$$
$$\cosh((1 - c_2(z))z) - \eta_2(z) - z\eta_1(z)b_1(z)\sinh(c_1(z)z)$$
$$\quad - \frac{z}{2}\eta_1(z)b_1(z)\sinh((1 - c_2(z))z) = 0,$$
$$\sinh(c_2(z)z) - z\eta_1(z)b_1(z)\cosh(c_1(z)z) - \frac{z}{2}\eta_1(z)b_1(z)\cosh((1 - c_2(z))z) = 0,$$

$$\cosh(z) - zb_1(z)\sinh(c_1(z)z) - zb_1(z)\sinh((1 - c_2(z))z) = 1,$$
$$\sinh(z) - zb_1(z)\cosh(c_1(z)z) - zb_1(z)\cosh((1 - c_2(z))z) = 0. \qquad (22)$$

Taking $c_1(z)$ as constant we solve the system (22) and obtain

$$c_1 = 1/4, \quad \eta_1(z) = \operatorname{sech}\left(\frac{z}{4}\right), \quad b_1(z) = 2\sinh\left(\frac{z}{4}\right)/z. \qquad (23)$$

It is easily checked that the method defined by (21) and (23) has order two and we denote the method as EFSSDIRK2s2.

We note that as $z \to 0$, the EFSSDIRK2 method reduces to a classical two-stage SSDIRK, which first appeared in Cooper [18] and we denote the method by SSDIRK2s2.

3.3 A three-stage EFSSDIRK method

Now we proceed to construct a three-stage method. For $s = 3$, the scheme (16) becomes

$$\begin{array}{c|c|ccc}
c_1(z) & \eta_1(z) & \frac{1}{2}\eta_1(z)b_1(z) & & \\
1/2 & \eta_2(z) & \eta_2(z)b_1(z) & \frac{1}{2}\eta_2(z)b_2(z) & \\
1 - c_1(z) & \eta_1(z) & \eta_1(z)b_1(z) & \eta_1(z)b_2(z) & \frac{1}{2}\eta_1(z)b_1(z) \\
\hline
 & & b_1(z) & b_2(z) & b_1(z)
\end{array} \qquad (24)$$

The exponentially fitting conditions for a three-stage modified DIRK method are given by

$$\cosh(c_1(z)z) - \eta_1(z) - za_{11}(z)\sinh(c_1(z)z) = 0,$$
$$\sinh(c_1(z)z) - za_{11}(z)\cosh(c_1(z)z) = 0,$$
$$\cosh(c_2(z)z) - \eta_2(z) - za_{21}(z)\sinh(c_1(z)z) - za_{22}(z)\sinh(c_2(z)z) = 0,$$
$$\sinh(c_2(z)z) - za_{21}(z)\cosh(c_1(z)z) - za_{22}(z)\cosh(c_2(z)z) = 0,$$
$$\cosh(c_3(z)z) - \eta_3(z) - za_{31}(z)\sinh(c_1(z)z) - za_{32}(z)\sinh(c_2(z)z)$$
$$\quad - za_{33}(z)\sinh(c_3(z)z) = 0,$$
$$\sinh(c_3(z)z) - za_{31}(z)\cosh(c_1(z)z) - za_{32}(z)\cosh(c_2(z)z) - za_{33}(z)$$
$$\quad \cosh(c_3(z)z) = 0,$$
$$\cosh(z) - 1 - zb_1(z)\sinh(c_1(z)z) - zb_2(z)\sinh(c_2(z)z) - zb_3(z)\sinh(c_3(z)z) = 0,$$
$$\sinh(z) - zb_1(z)\cosh(c_1(z)z) - zb_2(z)\cosh(c_2(z)z) - zb_3(z)\cosh(c_3(z)z) = 0,$$
$$(25)$$

where $c_2(z) = 1/2, c_3(z) = 1 - c_1(z), \eta_3(z) = \eta_1(z), a_{11}(z) = \frac{1}{2}\eta_1(z)b_1(z), a_{21}(z) = \eta_2(z)b_1(z), a_{22}(z) = \frac{1}{2}\eta_2(z)b_2(z), a_{31}(z) = \eta_1(z)b_1(z), a_{31}(z) = \eta_1(z)b_2(z), a_{33} = \frac{1}{2}\eta_1(z)b_1(z), b_3(z) = b_1(z)$.

We solve the system (25) for $\eta_1(z)$, $\eta_2(z)$, $b_1(z)$ and $b_2(z)$ expressed in terms of $c_1(z)$ as follows

$$\eta_1(z) = \operatorname{sech}(c_1(z)z), \quad \eta_2(z) = \operatorname{sech}((1 - 4c_1(z))z/2),$$
$$b_1(z) = \frac{2\sinh(c_1(z)z)}{z}, \quad b_2(z) = \frac{2\sinh((1 - 4c_1(z))z/2)}{z}. \tag{26}$$

Substituting the above coefficients into the order four conditions (10) with the node $c_1(z)$ expanded as

$$c_1(z) = c_{10} + c_{12}z^2 + c_{14}z^4 + c_{16}z^6 + c_{18}z^8 + \cdots \tag{27}$$

we obtain

$$
\begin{aligned}
c_{10} &= \frac{1}{3} + \frac{1}{12}\sqrt[3]{4} + \frac{1}{6}\sqrt[3]{2}, \quad c_{12} = -\frac{1}{576} - \frac{1}{960}\sqrt[3]{4} - \frac{1}{720}\sqrt[3]{2}, \\
c_{14} &= \frac{1}{11{,}520} + \frac{11}{201{,}600}\sqrt[3]{4} + \frac{37}{537{,}600}\sqrt[3]{2}, \\
c_{16} &= -\frac{43}{7{,}741{,}440} - \frac{4063}{1{,}161{,}216{,}000}\sqrt[3]{4} - \frac{5119}{1{,}161{,}216{,}000}\sqrt[3]{2} \\
c_{18} &= \frac{1201}{2{,}972{,}712{,}960} + \frac{2{,}184{,}631}{8{,}583{,}708{,}672{,}000}\sqrt[3]{4} + \frac{2{,}752{,}457}{8{,}583{,}708{,}672{,}000}\sqrt[3]{2}.
\end{aligned}
\tag{28}
$$

The fourth-order method by defined (24), (26), (27) and (28) is denoted by EFSS-DIRK3s4. We note that as $z \to 0$, the EFSSDIRK3s4 method reduces to a classical three-stage symmetric and symplectic DIRK with constant coefficients. This method first appeared in Sans-Serna and Abia [20] and was also presented in Feng and Qin [10]. We denote the method by SSDIRK3s4S.

4 Phase properties of the new EFSSDIRK methods

The dispersion and dissipation are important properties which give an idea of the numerical behaviour of methods constructed for oscillatory problems. This section is devoted to the phase-lag and the amplification errors of the methods derived in Sect. 3. Applying the modified RK method (3) to the linear scalar test equation

$$y' = i\lambda y$$

gives the recurrence

$$y_{n+1} = R(i\mu, z)y_n$$

where $\mu = h\lambda$ and

$$R(i\mu, z) = 1 + i\mu b(z)^T (I - i\mu A(z))^{-1}\eta(z) \tag{29}$$

Table 2 Dispersion and dissipation comparison

Method	Dispersion	Dissipation
SDIRK1s2	$\frac{1}{12}\mu^3 + \mathcal{O}(\mu^5)$	0
SDIRK2s2	$\frac{1}{48}\mu^3 + \mathcal{O}(\mu^5)$	0
SDIRK3s4	$\frac{1}{1440}\left(32 + 25\sqrt[3]{2} + 20\sqrt[3]{4}\right)\mu^5 + \mathcal{O}(\mu^7)$	0
TFSDIRK3s4	$\frac{1}{4320}\left(32 + 25\sqrt[3]{2} + 20\sqrt[3]{4}\right)\left(3r^2 + 4\right)\left(r^2 + 1\right)\mu^5 + \mathcal{O}(\mu^7)$	0
EFSSDIRK1s2	$\frac{1}{12}\left(r^2 + 1\right)\mu^3 + \mathcal{O}(\mu^5)$	0
EFSSDIRK2s2	$\frac{1}{48}\left(r^2 + 1\right)\mu^3 + \mathcal{O}(\mu^5)$	0
EFSSDIRK3s4	$\frac{1}{5760}\left(32 + 25\sqrt[3]{2} + 20\sqrt[3]{4}\right)\left(3r^2 + 4\right)\left(r^2 + 1\right)\mu^5 + \mathcal{O}(\mu^7)$	0

is the *stability function*. The definitions of dispersion and dissipation are given as follows.

Definition 4.1 The quantities

$$P(\mu) = \mu - \arg(R(\mathrm{i}\mu, z)), \quad D(\mu) = 1 - |R(\mathrm{i}\mu, z)|$$

are respectively called the *dispersion (phase-lag)* and the *dissipation (amplification error)*, where $R((\mathrm{i}\mu; z)$ is given by (29).

Definition 4.2 The *dispersion order* is p if

$$P(\mu) = P_{p+1}(r)\mu^{p+1} + \mathcal{O}\left(\mu^{p+3}\right),$$

and the *dissipation order* is q if

$$D(\mu) = D_{q+1}(r)\mu^{q+1} + \mathcal{O}(\mu^{q+3}),$$

where $r = \dfrac{z}{\mu}$. The method is called *zero-dispersive* or *zero-dissipative* if $P(\mu) = 0$ and $D(\mu) = 0$ respectively.

The dispersion and dissipation for the methods derived in Sect. 3 and their limit methods are displayed in Table 2. The table shows that EFSSDIRK3s4 has the lowest phase lag. All the methods have zero dissipation.

5 Numerical experiments

To examine the numerical effectiveness of the newly constructed exponentially fitted symmetric and symplectic diagonally implicit Runge–Kutta methods, we carry out

experiments on four test problems. Some highly efficient codes are selected from the recent literature. The codes used for comparison are listed as follows:

- EFSSDIRK1s2: the one-stage exponentially fitted symmetric and symplectic DIRK method of order two constructed in this paper.
- EFSSDIRK2s2: the two-stage exponentially fitted symmetric and symplectic DIRK method of order two constructed in this paper.
- EFSSDIRK3s4: the three-stage exponentially fitted symmetric and symplectic DIRK method of order four constructed in this paper.
- EFSDIRK2s2: the two-stage exponentially fitted symmetric DIRK method of order two constructed by R. D'Ambrosio and B. Paternoster in [34].
- SSDIRK1s2: the one-stage symmetric and symplectic DIRK method of order two given by Cash [35], which is the limit method of the EFSSDIRK1s2 method as $z \to 0$.
- SSDIRK2s2: the two-stage symmetric and symplectic DIRK method of order two proposed by Cooper [18], which is the limit method of the EFSSDIRK2s2 method as $z \to 0$.
- SSDIRK3s4: the three-stage symmetric and symplectic DIRK method of order four derived by Sanz-Serna and Abia [20], which is the limit method of the EFSSDIRK3s4 method as $z \to 0$.
- SDIRK4s4: the four-stage symplectic DIRK method of order four derived by Feng and Qin [10].
- TFSSDIRK3s4: A three-stage trigonometrically fitted symplectic DIRK method of order four given by Kalogiratou [30].

The effectiveness of the methods is tested by measuring the error in the numerical solution and preservation of Hamiltonian. For each problem, we first integrate the problem on a time interval and give the maximal global error of the solution for different stepsizes of integration. We then integrate the problem on a long time interval with a fixed stepsize and plot the time evolution of the maximal global error of the Hamiltonian.

Problem 1 *The two-body problem* We consider the two-body problem studied in Hairer et al. [3] which involves finding the positions and velocities of two massive bodies that attract each other gravitationally. The first body is located at the origin while the second body moves around the first body in a plane. Denote the position and the velocity of the second body by (q_1, q_2) and (p_1, p_2), respectively. The motion of the second body is governed by the systems of differential equations

$$q_1' = p_1, \quad p_1' = -\frac{q_1}{\sqrt{\left(q_1^2 + q_2^2\right)^3}},$$

$$q_2' = p_2, \quad p_2' = -\frac{q_2}{\sqrt{\left(q_1^2 + q_2^2\right)^3}}.$$
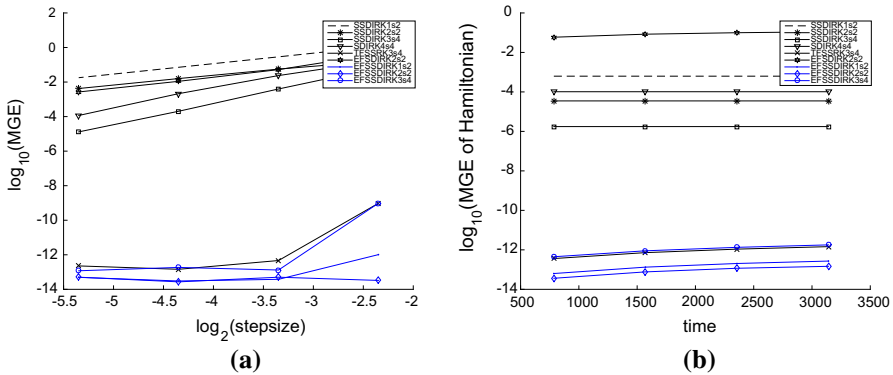
Fig. 1 Problem 1. **a** Accuracy comparison, **b** preservation of Hamiltonian

This is a Hamiltonian system with the Hamiltonian

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

For initial values

$$q_1(0) = 1, \quad p_1(0) = 0, \quad q_2(0) = 0, \quad p_2(0) = 1,$$

the exact solution is $q_1(x) = \cos(x)$, $q_2(x) = \sin(x)$. We integrate the problem on the interval $[0, 10\pi]$ with different stepsizes $h = \pi/2^j$, $j = 3, 4, 5, 6$. Then the problem is integrated with stepsize $h = \pi/15$ on the interval $[0, 1000\pi]$. The numerical results are presented in Fig. 1.

Problem 2 *A nonlinear Hamiltonian system* Consider the Hamiltonian system studied by Franco [36]

$$H(p, q) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{w^2}{2}(q_1^2 + q_2^2) + \frac{\alpha}{6}(q_1^2 + q_2^2)^3,$$

with the initial data

$$q_1(0) = 1, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = w + \epsilon$$

where $\alpha = \epsilon(2w + \epsilon)$. The analytic solution is given by

$$q_1(t) = \cos((w + \epsilon)t), \ q_2(t) = \sin((w + \epsilon)t),$$
$$p_1(t) = -(w + \epsilon)\sin((w + \epsilon)t), \ p_2(t) = (w + \epsilon)\cos((w + \epsilon)t),$$

representing a periodic motion. In this experiment, we have chosen the parameter values $\epsilon = 10^{-2}$, $w = 5$, and the integration carried out on the interval $[0, 10\pi]$ with
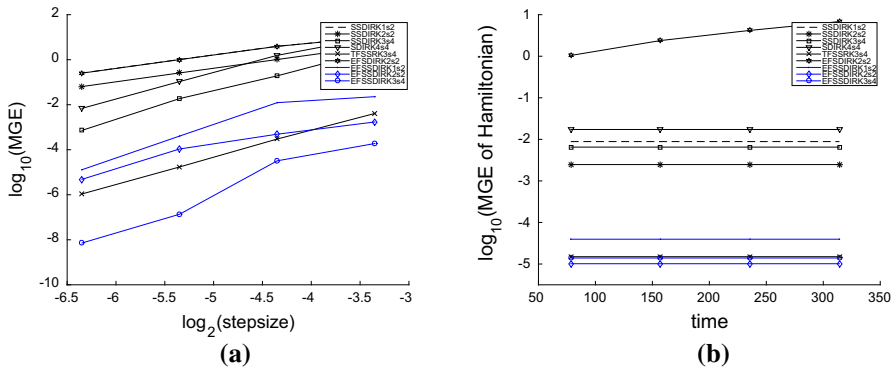
Fig. 2 Problem 2. **a** Accuracy comparison, **b** preservation of Hamiltonian
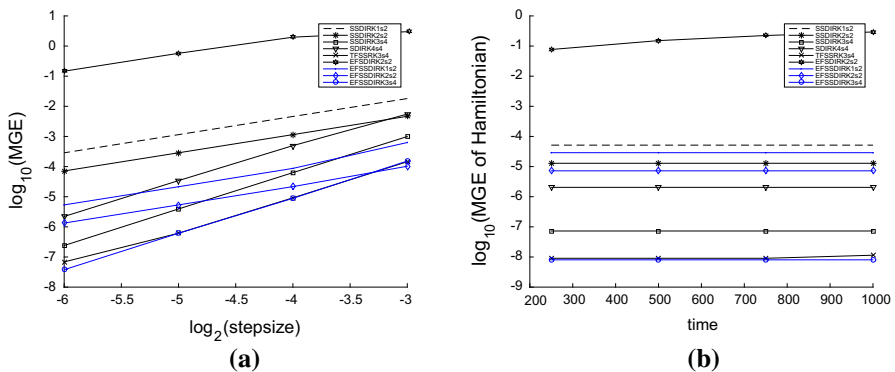

Fig. 3 Problem 3. **a** Accuracy comparison, **b** preservation of Hamiltonian

stepsizes $h = 1/2^i$, $j = 5, 6, 7, 8$. Then we integrate the problem on the interval $[0, 100\pi]$ with stepsize $h = 1/24$. The numerical results are presented in Fig. 2.

Problem 3 *The standard pendulum* Consider the differential equation describing the standard pendulum given by

$$q' = p, \quad p' = -\sin(q), \quad q(0) = 0, \quad p(0) = 1.5.$$

The Hamiltonian of the this problem is

$$H(p, q) = \frac{p^2}{2} - \cos q.$$

We integrate the problem in the interval $[0, 100]$ with stepsizes $h = 1/2^j$, $i = 3, 4, 5, 6$. Then the problem is integrated on the interval $[0, 1000]$ with the stepsize $h = 1/16$. Numerical results obtained are presented in Fig. 3.
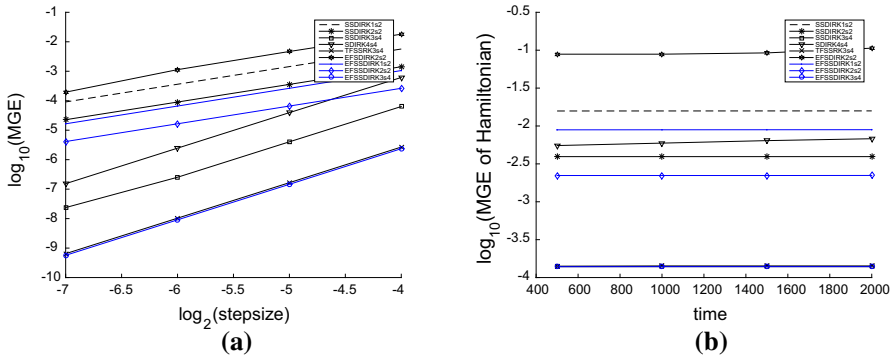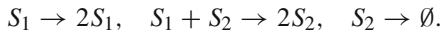
Fig. 4 Problem 4. **a** Accuracy comparison, **b** preservation of Hamiltonian

Problem 4 *The Lotka–Volterra model for chemical oscillators* Consider the chemical reaction system consisting three reactions between two reactants S_1 and S_2 [9,11,37,38]:

$$S_1 \rightarrow 2S_1, \quad S_1 + S_2 \rightarrow 2S_2, \quad S_2 \rightarrow \emptyset.$$

The reaction rates of the three reactions are r, k and d, respectively. Let $u(t)$ and $v(t)$ denote the concentrations of S_1 and S_2 at time t. By the mass-action law, the evolution of the reactants is governed by the following Lotka–Volterra system

$$\dot{u} = (r - kv)u, \quad \dot{v} = (ku - d)v. \tag{30}$$

By the logarithmic transformation $p = \log u$, $q = \log v$, the system (30) becomes a Hamiltonian problem

$$\dot{p} = r - ke^q, \quad \dot{q} = ke^p - d,$$

with the Hamiltonian

$$H(p, q) = ke^p + ke^q - (dp + rq).$$

In this experiment, we take the values for the parameters $k = d = 1$, $r = 2$. The system (5) is integrated with initial values $p(0) = \log 2$, $q(0) = \log 2$ on the interval [0, 100] with fitting frequency $\omega = 1.46$ and stepsizes $h = 1/2^j$, $j = 4, 5, 6, 7$. Then we integrate the problem on the time interval [0, 2000] with initial values $p(0) = \log 0.1$, $q(0) = \log 5$ and stepsize $h = 1/32$. The numerical results are presented in Fig. 4.

It can be observed from Figs. 1, 2, 3 and 4 that in comparison of accuracy and Hamiltonian preservation, the new methods EFSSDIRK1s2, EFSSDIRK2s2, EFSSDIRK3s4 outperform their limit methods SSDIRK1s2, SSDIRK2s2, SSDIRK, respectively. The fourth-order method EFSSDIRK3s4 is comparable to or even more accurate than

Kalogiratou's TFSSDIRK3s4 method. In Problem 1, the second-order method EFSS-DIRK2s2 works as well as the fourth-order method EFSSDIRK3s4 while in Problem 2, EFSSDIRK2s2 even outperforms EFSSDIRK4s4. Among the four fourth-order methods, the four-stage method SDIRK4s4 does the most poorly. It is not surprising since SDIRK4s4 is not a symmetric method.

6 Conclusions and discussions

In this paper, we have adapted the symmetric and symplectic conditions given in [9,13] respectively to the modified DIRK methods for autonomous Hamiltonian systems. Order conditions for modified DIRK methods are obtained through imaginary rooted trees. The exponentially fitting conditions are given following the line of [25]. Three practical symmetric and symplectic methods of algebraic order two and four were constructed respectively using the symmetric, symplectic and exponentially fitted conditions presented in Sect. 2 of this paper. These methods are reduced to classical DIRK methods with constant coefficients which have appeared in the literatures [10,18,20], when the frequency used in the fitting process is set to zero. Phase lags of the methods are analyzed. Although the new three-stage method EFSSDIRK3s4 has the same phase lag order as Kalogiratou's TFSSDIRK3s4 method [30], the leading term of the phase lag is smaller. All these methods are zero-dissipative due to their symplecticity.

Numerical experiments considered in this paper shows that the exponential fitted methods produces more accurate results on Hamiltonian problems than their classical counterparts. We note that in implementation of exponentially fitted or trigonometrically fitted methods, a fitting frequency ω must be prescribed in advance. This fitting frequency is an estimate of the frequency of the solution. If the solution has been given as in Problems 1 and 2, then the frequency of the solution is of course known and the numerical solution is not necessary. However, in most cases, the true solution and its frequency are not available and the choice of a fitting frequency becomes a challenge. More than often, the true frequency, if available, is not suitable for fitting. For instance, in Problem 4 of Sect. 5, the Lotka–Volterra model for chemical oscillators, for the initial value $(p(0), q(0)) = (\log 2, \log 2)$, the exact frequency is known to be $2\pi/4.61487051945103 = 1.361508471515472$, but it can not serve as the fitting frequency for our new EFSSDIRK methods (and for TFSSDIRK3s4). The fact is, as mentioned in Zhang et al. [37], each method has its own best fitting frequency which depend on the differential equation, initial data and the integration interval. In Problems 1 and 2, the fitting frequency is taken as the frequency of the true solution while in Problems 3 and 4 the frequency utilized is obtained with a searching algorithm. For other techniques of determining the fitting frequency, the reader is referred to Ixaru and Vanden Berghe [39], Ramos and Vigo-Aguiar [40] and Vigo-Aguiar and Ramos [41].

Finally, it should be noted that an RK method having more stages does not necessarily lead to higher effectiveness. In Problem 1, for example, the one-stage method EFSSDIRK1s2 and the two-stage method EFSSDIRK2s2 outperform all the other

fourth-order methods with three or four stages. Relative effectiveness of different integrators depends to some extent on the problem they solve.

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