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Explicit symplectic multidimensional exponential fitting modified Runge-Kutta-Nyström methods

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Abstract This paper is concerned with multidimensional exponential fitting modified Runge-Kutta-Nyström (MEFMRKN) methods for the system of oscillatory second-order differential equations $q''(t) + Mq(t) = f(q(t))$, where M is a $d \times d$ symmetric and positive semi-definite matrix and $f(q)$ is the negative gradient of a potential scalar $U(q)$. We formulate MEFMRKN methods and show clearly the relationship between MEFMRKN methods and multidimensional extended Runge-Kutta-Nyström (ERKN) methods proposed by Wu et al. (Comput. Phys. Comm. 181:1955–1962, 2010). Taking into account the fact that the oscillatory system is a separable Hamiltonian system with Hamiltonian $H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T Mq + U(q)$, we derive the symplecticity conditions for the MEFMRKN meth-

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ods. Two explicit symplectic MEFMRKN methods are proposed. Numerical experiments accompanied demonstrate that our explicit symplectic MEFMRKN methods are more efficient than some well-known numerical methods appeared in the scientific literature.

Keywords Exponential fitting · MEFMRKN methods · Symplecticity conditions · ERKN integrators · Oscillatory systems

Mathematics Subject Classification (2000) 65L05 · 65L06 · 65M20

1 Introduction

In the past decade, the study of perturbed oscillators by many researches has been mostly focusing on the one-dimensional case $y''(t) + w^2 y(t) = f(y(t))$, or the multidimensional one where the frequency matrix $M = w^2 I$ is a diagonal matrix. In the more recent years, the research attention has been turned to the system of oscillatory second-order differential equations of the form

$$\begin{cases} q''(t) + Mq(t) = f\big(q(t)\big), \quad t \in [0, T], \\ q(0) = q_0, \quad q'(0) = q'_0, \end{cases} \tag{1}$$

where M is a $d \times d$ symmetric and positive semi-definite matrix implicitly containing the frequencies of the problem, $q : \mathbb{R} \to \mathbb{R}^d$ is the solution of the system and $f(q)$ is the negative gradient of a real-valued function $U(q)$ whose second derivatives are continuous. Problems in the form (1) usually arise in applied mathematics and in physics, astronomy, molecular dynamics, engineering etc. Effective integrators making use of the special structure of M in (1) have been proposed in recent years. For the related work to this topic, we refer the reader to [4, 8, 15, 16, 25–28]. Based on the variation-of-constants formula, some methods for (1) have been proposed and we refer to [9, 11, 15] for some examples. In a more recent paper, Wu et al. [27] formulated a standard form of multidimensional extended Runge-Kutta-Nyström (ERKN) integrators free from matrix decomposition for the general system (1) based on the variation-of-constants formula. On the other hand, it is believed that exponential fitting is also a useful way to construct efficient numerical methods. It is well-known that an approach to constructing an exponential fitting method is to determine the coefficients of the method so that it integrates exactly a set of linearly independent functions which are chosen based on the nature of the solutions of the differential equations to be solved. Much research work has been performed on the problems explicitly containing single-frequency, and some exponential and trigonometrical fitting methods have been proposed. See, e.g., [1, 2, 7, 21, 23, 24, 29] and the references therein. In [23], Tocino and Vio-Aguiar consider the exponential fitting procedure and symplecticity conditions of modified Runge-Kutta-Nyström (RKN) scheme for

$$y''(t) + \omega^2 y(t) = f\big(y(t)\big),$$

where $f(y) = \frac{\partial U}{\partial y}(y)$ is the gradient of a potential scalar. Some other exponential fitting-type methods for multidimensional problems of the form (1) are proposed in [9, 10, 15, 20].

This paper investigates multidimensional exponential fitting modified Runge-Kutta-Nyström (MEFMRKN) methods for the system of oscillatory second order differential equations (1), which adapt to the oscillatory feature of the true flows in both the internal stages and the updates, and make good use of the special structure of (1) brought by Mq. On the other hand, we note that the symplecticity for an oscillatory Hamiltonian system is also very important and much work has been done on this topic. Pioneering work on symplectic integration is due to Vogelaere [5], Ruth [18] and Feng [6]. The symplectic conditions for Runge-Kutta methods are obtained by Sanz-Serna [19] and the symplecticity conditions for RKN methods are derived by Suris [22]. See [3, 14, 17] for more work on this topic. Motivated by these valuable researches, we derive the symplecticity conditions for MEFMRKN methods and present our explicit symplectic MEFMRKN methods.

The rest of this paper is organized as follows. In Sect. 2, for (1) we formulate the MEFMRKN methods and show the relationship between MEFMRKN and ERKN integrators. The analysis of symplecticity conditions for MEFMRKN methods is presented in Sect. 3. We propose two explicit symplectic MEFMRKN methods in Sect. 4. Numerical experiments are given in Sect. 5. Section 6 is devoted to conclusions.

2 MEFMRKN methods

Following [23], we consider multidimensional modified RKN methods for the oscillatory system (1)

$$\begin{cases} Q_i = C_i q_n + D_i\big(hq_n'\big) + h^2 \displaystyle\sum_{j=1}^{s} a_{ij} f(Q_j), \quad i = 1, 2, \ldots, s, \\ q_{n+1} = C q_n + D\big(hq_n'\big) + h^2 \displaystyle\sum_{i=1}^{s} \bar{b}_i f(Q_i), \\ \big(hq_{n+1}'\big) = F q_n + E\big(hq_n'\big) + h^2 \displaystyle\sum_{i=1}^{s} b_i f(Q_i), \end{cases} \tag{2}$$

where $C,\ D,\ C_i,\ D_i,\ E,\ F,\ b_i,\ \bar{b}_i,\ i = 1, 2, \ldots, s$ and $a_{ij},\ i, j = 1, 2, \ldots, s$ are matrix-valued functions of $V = h^2 M$.

Since M is a $d \times d$ symmetric and positive semi-definite matrix in (1), M can be expressed as

$$M = P^T \Omega^2 P = N^2,$$

where P is an orthogonal matrix, Ω is a positive semi-definite diagonal matrix, and $N = P^T \Omega P$. With the usual approach to constructing exponential fitting methods (see [24] for example), we will derive the methods with variable coefficients that are able to integrate exactly the system of second order homogeneous differential equations

$$q'' + N^2 q = \mathbf{0}_{d\times 1}$$

whose solutions belong to the subspace generated by the set of vector-valued functions

$$\big\{\exp(itN)e_k, \exp(-itN)e_k,\ k = 1, 2, \ldots, d\big\},$$

or equivalently, by the basis of vector-valued functions

$$\widetilde{\mathcal{F}} = \big\{\sin(tN)e_k, \cos(tN)e_k,\ k = 1, 2, \ldots, d\big\}.$$

Here e_k, $k = 1, 2, \ldots, d$ are the unit coordinate vectors. Define the following linear vector-valued operators:

$$\begin{aligned}
&\mathcal{L}_i\big[q(t), h, C_i, D_i, (a_{ij})\big]\\
&\quad := q(t + c_i h) - C_i q(t) - h D_i q'(t)\\
&\qquad - h^2 \sum_{j=1}^{s} a_{ij}\big[q''(t + c_j h) + Mq(t + c_j h)\big], \quad i = 1, 2, \ldots, s,\\
&\mathcal{L}\big[q(t), h, C, D, \bar{b}\big]\\
&\quad := q(t + h) - Cq(t) - hDq'(t)\\
&\qquad - h^2 \sum_{i=1}^{s} \bar{b}_i\big[q''(t + c_i h) + Mq(t + c_i h)\big],\\
&\mathcal{DL}\big[q(t), h, E, F, b\big]\\
&\quad := q'(t + h) - Eq'(t) - \frac{1}{h}Fq(t)\\
&\qquad - h \sum_{i=1}^{s} b_i\big[q''(t + c_i h) + Mq(t + c_i h)\big],
\end{aligned} \tag{3}$$

where c_i, $i = 1, 2, \ldots, s$ are real constants in [0, 1], and may be equal. For the set of vector-valued functions $\widetilde{\mathcal{F}}$, with exponential fitting techniques (requiring the above operators to integrate exactly the functions $\widetilde{\mathcal{F}}$ at $t = 0$), the linear operators (3) reduce to

$$\begin{aligned}
\big(\sin(c_i hN) - hD_i N\big)e_k &= \mathbf{0}_{d\times 1}, &\qquad \big(\cos(c_i hN) - C_i\big)e_k &= \mathbf{0}_{d\times 1},\\
\big(\sin(hN) - hDN\big)e_k &= \mathbf{0}_{d\times 1}, &\qquad \big(\cos(hN) - C\big)e_k &= \mathbf{0}_{d\times 1},\\
\big(\cos(hN)N - EN\big)e_k &= \mathbf{0}_{d\times 1}, &\qquad \left(-\sin(hN)N - \frac{1}{h}F\right)e_k &= \mathbf{0}_{d\times 1}.
\end{aligned} \tag{4}$$

Since the formula (4) holds true for $k=1,2,\dots,d$, we have

$$\begin{aligned} \sin(c_i hN) &= hD_i N, \qquad \cos(c_i hN) = C_i,\\ \sin(hN) &= hDN, \qquad \cos(hN) = C,\\ \cos(hN)N &= EN, \qquad -\sin(hN)N = \frac{1}{h}F. \end{aligned} \tag{5}$$

Hence

$$\begin{aligned} &D_i = \sin(c_i hN)(hN)^{-1}, \qquad C_i = \cos(c_i hN), \quad i=1,2,\dots,s,\\ &D = \sin(hN)(hN)^{-1}, \qquad C = \cos(hN),\\ &E = \cos(hN), \qquad F = -hN\sin(hN). \end{aligned} \tag{6}$$

Observe that $\sin(c_i hN)(hN)^{-1}$ and $\sin(hN)(hN)^{-1}$ are well defined also for singular N.

By the definitions of

$$\phi_l(V) := \sum_{k=0}^{\infty} \frac{(-1)^k V^k}{(2k+l)!}, \quad l=0,1,\dots, \tag{7}$$

we obtain

$$\begin{aligned} &D_i = c_i\phi_1\big(c_i^2V\big), \qquad C_i = \phi_0\big(c_i^2V\big), \quad i=1,2,\dots,s,\\ &D = \phi_1(V), \qquad C = \phi_0(V),\\ &E = \phi_0(V), \qquad F = -V\phi_1(V), \end{aligned} \tag{8}$$

where $V = h^2M$.

Therefore, the multidimensional modified RKN methods (2) are formulated as follows:

$$\begin{cases} Q_i = \phi_0\big(c_i^2V\big)q_n + c_i\phi_1\big(c_i^2V\big)\big(hq_n'\big) + h^2\sum_{j=1}^{s} a_{ij} f(Q_j), \quad i=1,2,\dots,s,\\ q_{n+1} = \phi_0(V)q_n + \phi_1(V)\big(hq_n'\big) + h^2\sum_{i=1}^{s} \bar{b}_i f(Q_i),\\ \big(hq_{n+1}'\big) = -V\phi_1(V)q_n + \phi_0(V)\big(hq_n'\big) + h^2\sum_{i=1}^{s} b_i f(Q_i), \end{cases} \tag{9}$$

where b_i, $\bar{b}_i$ and $a_{ij}, i,j=1,2,\dots,s$ are matrix-valued functions of $V=h^2M$. The schemes (9) can be denoted by the Butcher tableau as

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_s \\ \hline & b_1 & \cdots & b_s \end{array}$$

The methods (9) integrate exactly the basis $\widetilde{\mathcal{F}} = \{\sin(tN)e_k, \cos(tN)e_k,\ k = 1, 2, \ldots, d\}$ for both the updates and the internal stages, so they are methods fitted to $\widetilde{\mathcal{F}}$. Namely, we achieve the multidimensional exponential fitting modified RKN or MEFMRKN schemes for the multidimensional oscillatory system (1).

Remark 1 We should note the fact that the coefficients of the MEFMRKN methods (9) only involve the matrix functions of $V = h^2 M$. That is, the MEFMRKN methods do not depend on the matrix decomposition. As for the issue of avoiding matrix decompositions, we refer to [9, 10, 15, 20]. It should be pointed out that the matrix decomposition in actual computation may bring extra error for the accuracy of the decomposition depends on the condition numbers with respect to eigenvalues of matrix M. Moreover, with the variable substitution $z(t) = Pq(t)$, the system (1) becomes the transformed system

$$\begin{cases} z''(t) + \Omega^2 z(t) = Pf\big(P^T z(t)\big), & t \in [0, T], \\ z(0) = z_0 = Pq_0, & z'(0) = z'_0 = Pq'_0, \end{cases} \tag{10}$$

with $f(q) = -\nabla U(q)$. We note the fact that, now the right-hand function in (10) is changed into

$$\tilde{f}(z) = Pf\big(P^T z(t)\big),$$

which is more expensive than $f(q(t))$ to calculate point by point and step by step. Therefore, our MEFMRKN methods avoid matrix decomposition are much more efficient and more practical.

Remark 2 It can be observed that the MEFMRKN methods (9) are consistent with the multidimensional ERKN integrators given in Wu et al. [27], but with different idea and derivation. The ERKN integrators are proposed based on the variation-of-constants formula while the MEFMRKN methods are derived by applying the exponential fitting techniques to the multidimensional modified RKN methods (2). Moreover we will present the symplecticity conditions for MEFMRKN methods and propose two new useful explicit symplectic MEFMRKN methods in the sequel Sections. This work differs from previous research of ERKN integrators and is useful in the field of exponential fitting methods.

3 Symplecticity conditions for MEFMRKN methods

In this section, we present and prove the symplecticity conditions for MEFMRKN methods. We will show the role of symplecticity for oscillatory differential equations (1) by some numerical experiments given in Sect. 5.

It is easy to observe that the system of second order differential equations (1) is equivalent to the following Hamiltonian system:

$$\begin{cases} q' = p, \\ p' = -\nabla U(q) - Mq, \\ q(0) = q_0, \ \ p(0) = p_0, \end{cases} \tag{11}$$

where $q : \mathbb{R} \to \mathbb{R}^d$ represents generalized positions, $p : \mathbb{R} \to \mathbb{R}^d$ represents generalized momenta, and $U(q)$ is a real-valued function with continuous second derivatives. The Hamiltonian of (11) is given by

$$H(p, q) = \frac{1}{2} p^T p + \frac{1}{2} q^T M q + U(q). \tag{12}$$

We will first derive the symplecticity conditions for the multidimensional modified RKN methods (2) then from which we give the symplecticity conditions for the MEFMRKN methods (9).

The next theorem gives the symplecticity conditions for the multidimensional modified RKN methods (2).

Theorem 31 *If the coefficients of an* s*-stage multidimensional modified RKN method* (2) *satisfy the following conditions*:

$$\begin{aligned} EC - FD &= I, \\ Cb_i - F\bar{b}_i &= d_i C_i, \quad d_i \in \mathbb{R}, \ i = 1, 2, \ldots, s, \\ Db_i - E\bar{b}_i &= d_i D_i, \quad i = 1, 2, \ldots, s, \\ \bar{b}_i b_j + d_i a_{ij} &= \bar{b}_j b_i + d_j a_{ji}, \quad i, j = 1, 2, \ldots, s, \end{aligned} \tag{13}$$

then the method is symplectic. Here, d_i *is a real number to be determined in order to ensure the symplecticity conditions.*

Proof First of all, we consider the special case, where M is a diagonal matrix with nonnegative entries

$$M = \text{diag}(m_{11}, m_{22}, \ldots, m_{dd}).$$

Accordingly, $C, \ D, \ E, \ F, \ C_i$ and D_i are all diagonal matrixes. Since b_i, $\bar{b}_i$, and a_{ij} are matrix-valued functions of $V = h^2 M$, they are also diagonal. Define $f_i = f(Q_i)$. Then the modified RKN method (2) becomes

$$\begin{cases} Q_i^J = C_i^J q_n^J + h D_i^J q_n'^J + h^2 \sum\limits_{j=1}^{s} a_{ij}^J f_j^J, \quad i = 1, 2, \ldots, s, \\ q_{n+1}^J = C^J q_n^J + h D^J q_n'^J + h^2 \sum\limits_{i=1}^{s} \bar{b}_i^J f_i^J, \\ q_{n+1}'^J = E^J q_n'^J + \dfrac{1}{h} F^J q_n^J + h \sum\limits_{i=1}^{s} b_i^J f_i^J, \end{cases} \tag{14}$$

where the superscript index $J = 1, 2, \ldots, d$ denotes the Jth component of a vector or the Jth diagonal component of a diagonal matrix. With the notation of external products and from the Hamiltonian system (11), the symplecticity condition of the method is

$$\sum_{J=1}^{d} dq_{n+1}^{J} \wedge dq_{n+1}^{\prime J} = \sum_{J=1}^{d} dq_{n}^{J} \wedge dq_{n}^{\prime J}.$$

By (13) and (14), differentiating q_{n+1}^{J} and $q_{n+1}^{\prime J}$, taking external products, and then summing over all J yield

$$\begin{aligned}\sum_{J=1}^{d} dq_{n+1}^{J} \wedge dq_{n+1}^{\prime J} &= \sum_{J=1}^{d} dq_{n}^{J} \wedge dq_{n}^{\prime J} + h \sum_{J=1}^{d}\sum_{i=1}^{s} d_i dQ_i^J \wedge df_i^J \\ &\quad + h^2 \sum_{J=1}^{d}\sum_{i=1}^{s} \big[\big(D^J b_i^J - E^J \bar{b}_i^J\big) - d_i D_i^J\big] dq_n^{\prime J} \wedge df_i^J \\ &\quad + h^3 \sum_{J=1}^{d}\sum_{i,j=1}^{s} \big[\bar{b}_i^J b_j^J + d_i a_{ij}^J\big] df_i^J \wedge df_j^J. \end{aligned} \tag{15}$$

From (13) and $f(q) = -\nabla U(q)$ where U has continuous second derivatives, we have

$$\begin{aligned}&\sum_{J=1}^{d}\sum_{i=1}^{s} d_i dQ_i^J \wedge df_i^J \\ &= \sum_{i=1}^{s}\sum_{J=1}^{d} d_i dQ_i^J \wedge df_i^J = \sum_{i=1}^{s} d_i \sum_{J,I=1}^{d} dQ_i^J \wedge \left(\frac{\partial f^J}{\partial q^I}(Q_i) dQ_i^I\right) \\ &= \sum_{i=1}^{s} d_i \sum_{J,I=1}^{d} dQ_i^J \wedge \left(-\frac{\partial^2 U(Q_i)}{\partial q^J \partial q^I}\right) dQ_i^I \\ &= -\sum_{i=1}^{s} d_i \sum_{J,I=1}^{d} \left(\frac{\partial^2 U(Q_i)}{\partial q^J \partial q^I}\right) dQ_i^J \wedge dQ_i^I = -\sum_{i=1}^{s} d_i 0 = 0. \end{aligned} \tag{16}$$

According to (13), the last two terms of (15) are equal to 0. Therefore, we obtain

$$\sum_{J=1}^{d} dq_{n+1}^{J} \wedge dq_{n+1}^{\prime J} = \sum_{J=1}^{d} dq_{n}^{J} \wedge dq_{n}^{\prime J}.$$

Keep in mind the fact that M is a $d \times d$ symmetric positive semi-definite matrix. As pointed out in Remark 1, with the variable substitution $z(t) = Pq(t)$, the system (1) is equivalent to a transformed system (10). Thus the symplectic methods for a diagonal matrix with nonnegative entries can be applied to the transformed system. Moreover, the methods are invariant by linear transformations, and therefore, we can write the methods (applied to the transformed system (10)) in terms of $q(t)$ via multiplying by P^T and denoting $Q_i = P^T Z_i,\ q_n = P^T z_n$. This means that the methods with symplecticity conditions (13) can be applied to systems with M symmetric and positive semi-definite. In conclusion, for the system of oscillatory second-order differential equations (1) with symmetric and positive semi-definite M, an s-stage multidimensional modified RKN method (2) satisfying the conditions (13) is a symplectic method. □

Using Theorem 31, we obtain the symplecticity condition of our MEFMRKN methods (9) immediately.

Theorem 32 *An MEFMRKN method* (9) *is symplectic if its coefficients satisfy*

$$\begin{aligned}
&\phi_0(V)b_i + V\phi_1(V)\bar{b}_i = d_i\phi_0\big(c_i^2 V\big), \quad d_i \in \mathbb{R},\ i = 1, 2, \ldots, s,\\
&\phi_1(V)b_i - \phi_0(V)\bar{b}_i = c_i d_i \phi_1\big(c_i^2 V\big), \quad i = 1, 2, \ldots, s,\\
&\bar{b}_i b_j + d_i a_{ij} = \bar{b}_j b_i + d_j a_{ji}, \quad i, j = 1, 2, \ldots, s,
\end{aligned} \tag{17}$$

where $V = h^2 M$.

Proof Inserting (8) into (13) arrives at the results. □

4 Explicit symplectic MEFMRKN methods

An important fact is that symplectic Runge-Kutta schemes for the integration of general Hamiltonian systems are implicit. Therefore, in practice, one has to solve the implicit algebraic equations using some iterative approximation methods, in which case the resulting integration scheme may be no longer symplectic. The advantage of explicit symplectic integrators, when compared with fully implicit or partly implicit methods, is that they do not require the solution of large and complicated systems of nonlinear algebraic or transcendental equations when solving multidimensional problems. Consequently, here, we only consider explicit symplectic MEFMRKN methods.

In this section, using the symplecticity condition (17) in Theorem 32 and exponential fitting, we propose two explicit symplectic MEFMRKN methods.

4.1 Two-stage explicit symplectic MEFMRKN methods

In this subsection, we consider two-stage explicit symplectic MEFMRKN methods. The scheme (9) of a two-stage explicit MEFMRKN method can be denoted by the Butcher tableau

$$\begin{array}{c|cc} c_1 & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} \\ c_2 & a_{21} & \mathbf{0}_{d\times d} \\ \hline & \bar{b}_1 & \bar{b}_2 \\ \hline & b_1 & b_2 \end{array}$$

From Theorem 32, the two-stage MEFMRKN method is symplectic if its coefficients satisfy

$$\begin{aligned} &\phi_0(V)b_1 + V\phi_1(V)\bar{b_1} = d_1\phi_0\big(c_1^2V\big), \\ &\phi_0(V)b_2 + V\phi_1(V)\bar{b_2} = d_2\phi_0\big(c_2^2V\big), \\ &\phi_0(V)\bar{b}_1 + c_1d_1\phi_1\big(c_1^2V\big) = b_1\phi_1(V), \\ &\phi_0(V)\bar{b}_2 + c_2d_2\phi_1\big(c_2^2V\big) = b_2\phi_1(V), \\ &\bar{b}_1b_2 = \bar{b}_2b_1 + d_2a_{21}. \end{aligned} \tag{18}$$

Solving all the equations in (18) with c_1, c_2, d_1, d_2 as parameters gives

$$\begin{aligned} b_1 &= d_1\big(\phi_0(V)\phi_0\big(c_1^2V\big) + c_1V\phi_1(V)\phi_1\big(c_1^2V\big)\big), \\ b_2 &= d_2\big(\phi_0(V)\phi_0\big(c_2^2V\big) + c_2V\phi_1(V)\phi_1\big(c_2^2V\big)\big), \\ \bar{b}_1 &= \big(b_1\phi_1(V) - c_1d_1\phi_1\big(c_1^2V\big)\big)\big(\phi_0(V)\big)^{-1}, \\ \bar{b}_2 &= \big(b_2\phi_1(V) - c_2d_2\phi_1\big(c_2^2V\big)\big)\big(\phi_0(V)\big)^{-1}, \\ a_{21} &= (\bar{b}_1b_2 - \bar{b}_2b_1)(d_2)^{-1}. \end{aligned} \tag{19}$$

Let

$$\begin{aligned} &\mathcal{DL}\big[q(t), h, E, F, b\big] \\ &\quad = q'(t+h) - Eq'(t) - \frac{F}{h}q(t) - h\sum_{i=1}^{2} b_i\big[q''(t+c_ih) + N^2q(t+c_ih)\big] \\ &\quad \text{with } E = \cos(hN),\ F = -hN\sin(hN). \end{aligned}$$

Requiring $\mathcal{DL}[q(t), h, E, F, b]$ to integrate exactly the vector-valued functions

$$\big\{t\sin(Nt)e_k, t\cos(Nt)e_k,\ k = 1, 2, \ldots, d\big\}$$

at $t = 0$ and $h = 0$, we have

$$d_1 = \frac{1-2c_2}{2(c_1-c_2)}, \qquad d_2 = \frac{1-2c_1}{-2(c_1-c_2)}. \tag{20}$$

Take into account the second order conditions of the ERKN integrators given in [27]:

$$b_1 + b_2 = \phi_1(V) + O(h^2),$$
$$b_1c_1 + b_2c_2 = \phi_2(V) + O(h),$$
$$\bar{b}_1 + \bar{b}_2 = \phi_2(V) + O(h).$$

Then we make the choice of $c_1 = \frac{3-\sqrt{3}}{6}$, $c_2 = \frac{3+\sqrt{3}}{6}$.

The choice of c_1 and c_2 together with (19) and (20) gives a two-stage explicit symplectic MEFMRKN method with

$$\begin{aligned} &b_1 = \frac{1}{2}\phi_0(c_2^2V), \qquad b_2 = \frac{1}{2}\phi_0(c_1^2V), \\ &\bar{b}_1 = \frac{1}{2}c_2\phi_1(c_2^2V), \qquad \bar{b}_2 = \frac{1}{2}c_1\phi_1(c_1^2V), \qquad a_{21} = \frac{1}{2\sqrt{3}}\phi_1\left(\frac{V}{3}\right). \end{aligned} \tag{21}$$

Since the coefficients (19) are obtained from the symplecticity conditions (18), they satisfy the symplecticity conditions and this two-stage method is symplectic. We denote the method stated above by SMEFMRKN2s2.

4.2 Three-stage explicit symplectic MEFMRKN methods

We turn to considering three-stage explicit symplectic MEFMRKN methods. The scheme (9) of a three-stage explicit MEFMRKN method can be denoted by the Butcher tableau

$$\begin{array}{c|ccc} c_1 & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} \\ c_2 & a_{21} & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} \\ c_3 & a_{31} & a_{32} & \mathbf{0}_{d\times d} \\ \hline & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 \\ \hline & b_1 & b_2 & b_3 \end{array}$$

From (17), the symplecticity condition for the three-stage MEFMRKN method is

$$\begin{aligned} &\phi_0(V)b_1 + V\phi_1(V)\bar{b}_1 = d_1\phi_0(c_1^2V), \qquad &&\phi_0(V)b_2 + V\phi_1(V)\bar{b}_2 = d_2\phi_0(c_2^2V), \\ &\phi_0(V)b_3 + V\phi_1(V)\bar{b}_3 = d_3\phi_0(c_3^2V), \qquad &&\phi_0(V)\bar{b}_1 + c_1d_1\phi_1(c_1^2V) = b_1\phi_1(V), \\ &\phi_0(V)\bar{b}_2 + c_2d_2\phi_1(c_2^2V) = b_2\phi_1(V), \qquad &&\phi_0(V)\bar{b}_3 + c_3d_3\phi_1(c_3^2V) = b_3\phi_1(V), \\ &\bar{b}_1b_2 = \bar{b}_2b_1 + d_2a_{21}, \qquad &&\bar{b}_1b_3 = \bar{b}_3b_1 + d_3a_{31}, \\ &\bar{b}_2b_3 = \bar{b}_3b_2 + d_3a_{32}. \end{aligned} \tag{22}$$

Choosing $c_1, c_2, c_3, d_1, d_2, d_3$ as parameters and solving all the equations in (22), we get

$$\begin{aligned}
&b_1 = d_1\big(\phi_0(V)\phi_0\big(c_1^2V\big) + c_1V\phi_1(V)\phi_1\big(c_1^2V\big)\big),\\
&b_2 = d_2\big(\phi_0(V)\phi_0\big(c_2^2V\big) + c_2V\phi_1(V)\phi_1\big(c_2^2V\big)\big),\\
&b_3 = d_3\big(\phi_0(V)\phi_0\big(c_3^2V\big) + c_3V\phi_1(V)\phi_1\big(c_3^2V\big)\big),\\
&\bar{b}_1 = \big(b_1\phi_1(V) - c_1d_1\phi_1\big(c_1^2V\big)\big)\big(\phi_0(V)\big)^{-1}, \qquad a_{21} = (\bar{b}_1b_2 - \bar{b}_2b_1)(d_2)^{-1},\\
&\bar{b}_2 = \big(b_2\phi_1(V) - c_2d_2\phi_1\big(c_2^2V\big)\big)\big(\phi_0(V)\big)^{-1}, \qquad a_{31} = (\bar{b}_1b_3 - \bar{b}_3b_1)(d_3)^{-1},\\
&\bar{b}_3 = \big(b_3\phi_1(V) - c_3d_3\phi_1\big(c_3^2V\big)\big)\big(\phi_0(V)\big)^{-1}, \qquad a_{32} = (\bar{b}_2b_3 - \bar{b}_3b_2)(d_3)^{-1}.
\end{aligned} \tag{23}$$

Let

$$\begin{aligned}
&\mathcal{DL}\big[q(t), h, E, F, b\big]\\
&\quad = q'(t+h) - Eq'(t) - \frac{F}{h}q(t) - h\sum_{i=1}^{3} b_i\big[q''(t+c_ih) + N^2q(t+c_ih)\big],\\
&\quad \text{with } E = \cos(hN),\ F = -hN\sin(hN).
\end{aligned}$$

Requiring $\mathcal{DL}[q(t), h, E, F, b]$ to integrate exactly the vector-valued functions

$$\big\{t\sin(Nt)e_k, t\cos(Nt)e_k, t^2\cos(Nt)e_k,\ k = 1, 2, \dots, d\big\}$$

at $t = 0$ and $h = 0$, we have

$$\begin{aligned}
d_1 &= \frac{2 - 3c_3 + c_2(-3 + 6c_3)}{6(c_1 - c_2)(c_1 - c_3)},\\
d_2 &= \frac{-2 + 3c_3 + c_1(3 - 6c_3)}{6(c_1 - c_2)(c_2 - c_3)},\\
d_3 &= \frac{2 - 3c_2 + c_1(-3 + 6c_2)}{6(c_1 - c_3)(c_2 - c_3)}.
\end{aligned} \tag{24}$$

By the third order conditions of the ERKN integrators given in [27], we have

$$\begin{aligned}
&b_1 + b_2 + b_3 = \phi_1(V) + O\big(h^3\big),\\
&b_1c_1 + b_2c_2 + b_3c_3 = \phi_2(V) + O\big(h^2\big),\\
&b_1c_1^2 + b_2(V)c_2^2 + b_3(V)c_3^2 = 2\phi_3(V) + O(h),\\
&b_2a_{21}(\mathbf{0}) + b_3\big(a_{31}(\mathbf{0}) + a_{32}(\mathbf{0})\big) = \phi_3(V) + O(h),\\
&\bar{b}_1 + \bar{b}_2 + \bar{b}_3 = \phi_2(V) + O\big(h^2\big),\\
&\bar{b}_1c_1 + \bar{b}_2c_2 + \bar{b}_3c_3 = \phi_3(V) + O(h),
\end{aligned}$$

where $a_{ij}(\mathbf{0})$ denotes the constant matrix of $a_{ij}(V)$ when $V \to \mathbf{0}_{d\times d}$. Then we obtain

$$c_1 = \frac{1}{5}, \qquad c_2 = \frac{15-\sqrt{85}}{30}, \qquad c_3 = \frac{4}{5}. \tag{25}$$

These parameters determined by (25) together with (23) and (24) lead to an explicit symplectic MEFMRKN method with

$$\begin{aligned}
b_1 &= \frac{15+\sqrt{85}}{12}\phi_0\left(\frac{16}{25}V\right),\\
b_2 &= -\frac{3}{2}\phi_0\left(\frac{(15+\sqrt{85})^2}{900}V\right),\\
b_3 &= \frac{15-\sqrt{85}}{12}\phi_0\left(\frac{1}{25}V\right),\\
\bar{b}_1 &= \frac{4(15+\sqrt{85})}{60}\phi_1\left(\frac{16}{25}V\right),\\
\bar{b}_2 &= -\frac{15+\sqrt{85}}{20}\phi_1\left(\frac{(15+\sqrt{85})^2}{900}V\right),\\
\bar{b}_3 &= -\frac{-15+\sqrt{85}}{60}\phi_1\left(\frac{1}{25}V\right),\\
a_{21} &= -\frac{(15+\sqrt{85})(-9+\sqrt{85})}{360}\phi_1\left(\frac{(-9+\sqrt{85})^2}{900}V\right),\\
a_{31} &= \frac{3(15+\sqrt{85})}{60}\phi_1\left(\frac{9}{25}V\right),\\
a_{32} &= -\frac{9+\sqrt{85}}{20}\phi_1\left(\frac{(9+\sqrt{85})^2}{900}V\right).
\end{aligned} \tag{26}$$

Moreover, it can be verified that the coefficients of this method satisfy the symplecticity conditions and then this method is symplectic. We denote the method described above as SMEFMRKN3s3.

Remark 3 It is observed that $(\phi_0(V))^{-1}$ and d_i in (19) and (23) might cause numerical instability. However, by choosing the values of c_i and d_i and simplifying the coefficients as in (21) and (26), we avoid the possibility of numerical instability.

5 Numerical experiments

In this section, we use two kinds of problems to show the efficiency and robustness of our new methods compared with some existing methods.

5.1 The problems containing explicitly single-frequency

In order to compare our symplectic exponential fitting methods with existing exponential and trigonometrical fitting methods proposed for problems explicitly containing single-frequency, we consider two problems containing single-frequency in this subsection. The methods we select for comparison are:

- SV: The classical Störmer-Verlet formula;
- SEFRKN2s: The two-stage symplectic exponential fitting modified RKN method given in [24];
- E: The symmetric Gautschi's method of order two given in [11];
- EFRKN3s: The three-stage exponential fitting modified RKN method given in [7];
- SRKN3s4: The three-stage symplectic RKN method of order four given in [13];
- SMEFMRKN2s2: The two-stage symplectic MEFMRKN method of order two derived in this paper;
- SMEFMRKN3s3: The three-stage symplectic MEFMRKN method of order three derived in this paper.

For each experiment, we display the efficiency curves (accuracy versus the computational cost measured by the number of function evaluations required by each method) and the energy conservation for different methods.

Problem 1 Consider the two-body problem

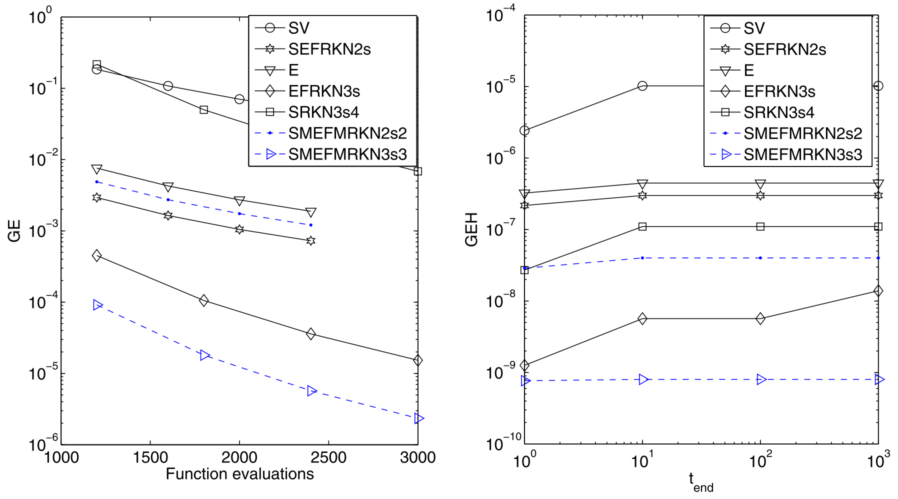
$$q_1'' = -\frac{q_1}{(q_1^2+q_2^2)^{3/2}}, \qquad q_1(0) = 1-e, \qquad q_1'(0) = 0,$$

$$q_2'' = -\frac{q_2}{(q_1^2+q_2^2)^{3/2}}, \qquad q_2(0) = 0, \qquad q_2'(0) = \sqrt{\frac{1+e}{1-e}},$$

where $e \in [0, 1)$ is the (constant) eccentricity of the elliptic orbit. The Hamiltonian function of the system is given by

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

Following [24], the frequency is chosen as 1, namely, $M = I_{2\times 2}$ in this case. In our experiment we use $e = 0.01$ and the different step sizes $h = \frac{1}{4i}$, $i = 3,4,5,6$ for the methods SV, SEFRKN2s and E, $h = \frac{1}{2i}$, $i = 3,4,5,6$ for SMEFMRKN2s2 and $h = \frac{1}{2i}$, $i = 2,3,4,5$ for the three-stage methods on the interval $[0, 100]$. The efficiency curves are presented in Fig. 1(i). Then we solve the problem with step size $h = \frac{1}{16}$ on the intervals $[0, 10^i]$, $i = 0,1,2,3$. Compute the global errors of Hamiltonian $GEH = \max|H_n - H_0|$. The energy conservation (the global errors of Hamiltonian GEH versus the time) are shown in Fig. 1(ii).



(i) (ii)

Fig. 1 Results for Problem 1: (**i**) The global error (*GE*) over the integration interval against the number of function evaluations. (**ii**) The maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against t_{end}

Problem 2 Consider the Hénon-Heiles Model (see Hairer et al. [12])

$$q_1'' + q_1 = -2q_1q_2, \qquad q_1(0) = \sqrt{\frac{11}{96}}, \qquad q_1'(0) = 0,$$

$$q_2'' + q_2 = -q_1^2 + q_2^2, \qquad q_2(0) = 0, \qquad q_2'(0) = \frac{1}{4},$$

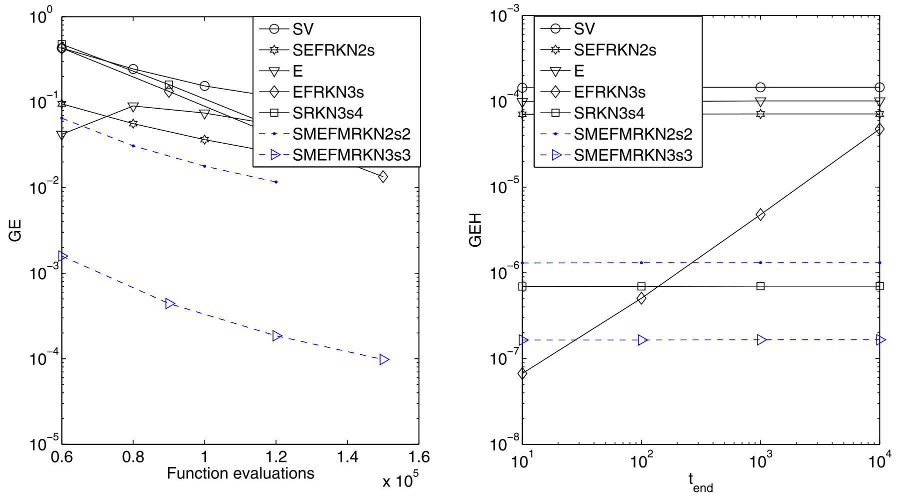
where $M = I_{2\times 2}$. The Hamiltonian function of the system is given by

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

We first solve the problem on the interval $[0, 5000]$ with $h = \frac{1}{4i},\ i = 3, 4, 5, 6$ for the methods SV, SEFRKN2s and E, $h = \frac{1}{2i},\ i = 3, 4, 5, 6$ for SMEFMRKN2s2 and $h = \frac{1}{2i},\ i = 2, 3, 4, 5$ for the three-stage methods. The numerical results are presented in Fig. 2(i). Then we integrate this problem with the step size $h = \frac{1}{10}$ on the interval $[0, 10^i],\ i = 1, 2, 3, 4$. See Fig. 2(ii).

5.2 The systems (1) implicitly containing multiple frequencies of the problems

In this subsection, we pay attention to (1) with a symmetric and positive semi-definite matrix M implicitly containing multiple frequencies of the problem. We should note



(i) (ii)

Fig. 2 Results for Problem 2: (**i**) The global error (*GE*) over the integration interval against the number of function evaluations. (**ii**) The maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against t_{end}

the fact that the existing exponential and trigonometrical fitting methods for the problems containing single-frequency are not applicable to the multidimensional problems (1). Whereas our MEFMRKN methods (9) are formulated adapting to the multidimensional problem (1), therefore our MEFMRKN methods are more practical. In this subsection we use three multidimensional problems to compare our MEFMRKN methods with the existing methods. The methods we select for comparison are some of those shown in Sect. 5.1, but now the methods SEFRKN2s and EFRKN3s are put aside in the following numerical experiments.

Problem 3 Consider a nonlinear wave equation

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial^2 u}{\partial x^2} = -\dfrac{1}{5}u^3 - \dfrac{1}{10}u^2, \quad 0 < x < 1,\ t > 0, \\ u(0,t) = u(1,t) = 0, \qquad u(x,0) = \dfrac{\sin(\pi x)}{2}, \qquad u_t(x,0) = 0. \end{cases}$$

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

$$\begin{cases} \dfrac{\partial^2 u_i}{\partial t^2} - \dfrac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = -\dfrac{1}{5}u_i^3 - \dfrac{1}{10}u_i^2, \quad 0 < t \le t_{end}, \\ u_i(0) = \dfrac{\sin(\pi x_i)}{2}, \quad u_i''(0) = 0, \quad i = 1, \ldots, N-1, \end{cases}$$

where $\Delta x = 1/N$ is the spatial mesh step and $x_i = i\Delta x$. This semi-discrete oscillatory system has the form

$$\begin{cases} \dfrac{\partial^2 U}{\partial t^2} + MU = F(t,U), \quad 0 < t \le t_{end}. \\ U(0) = \left(\dfrac{\sin(\pi x_1)}{2}, \dots, \dfrac{\sin(\pi x_{N-1})}{2}\right)^T, \quad U'(0) = \mathbf{0}, \end{cases} \tag{27}$$

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

$$\begin{aligned} M &= \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}, \\ F(t,U) &= F(t,U) \\ &= \left(-\frac{1}{5}u_1^3 - \frac{1}{10}u_1^2, \dots, -\frac{1}{5}u_{N-1}^3 - \frac{1}{10}u_{N-1}^2\right)^T. \end{aligned} \tag{28}$$

The Hamiltonian of (27) is given by

$$H\big(U',U\big) = \frac{1}{2}U'^T U' + \frac{1}{2}U^T MU + G(U),$$

where

$$G(U) = \frac{1}{20}u_1^4 + \frac{1}{30}u_1^3 + \cdots + \frac{1}{20}u_{N-1}^4 + \frac{1}{30}u_{N-1}^3.$$

The system is integrated on the interval $t \in [0,30]$ with $N = 20$ and integration step sizes $h = \frac{1}{50i},\ i = 1,2,3,4$ for the methods SV and E and $h = \frac{1}{25i},\ i = 1,2,3,4$ for the other methods. The efficiency curves are presented in Fig. 3. Then we integrate this problem with step size $h = \frac{1}{50}$ on the interval $[0, t_{end}]$, $t_{end} = 40 \times 3^i$ with $i = 1,2,3,4$. Table 1 presents the energy conservation for different methods. In addition, Fig. 4 gives the time evolution of the wave at $x = 0.5$ for methods SMEFMRKN2s2 and SMEFMRKN3s3 with $h = \frac{1}{25}$ on the interval [0, 10].

Problem 4 Consider the sine-Gordon equation with periodic boundary conditions (see Franco [8])

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial^2 u}{\partial x^2} - \sin u, \quad -1 < x < 1,\ t > 0, \\ u(-1,t) = u(1,t). \end{cases}$$

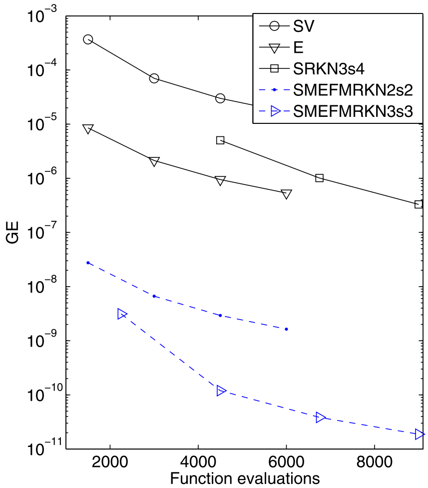


Fig. 3 Results for Problem 3: The global error (GE) over the integration interval against the number of function evaluations

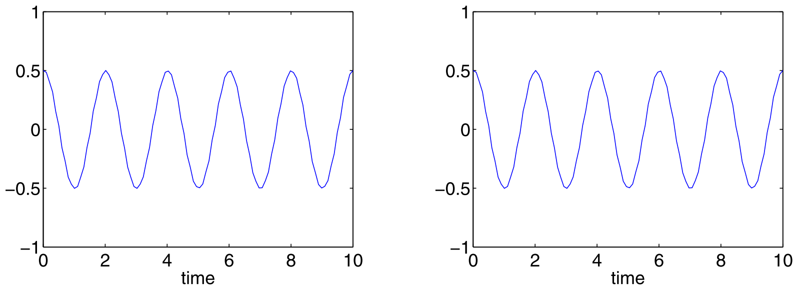


Fig. 4 Results for Problem 3: The time evolution of the wave at $x = 0.5$ for methods SMEFMRKN2s2 (**i**) and SMEFMRKN3s3 (**ii**)

Table 1 Results for Problem 3: The maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ for different t_{end}

Methods	$t_{end} = 120$	$t_{end} = 360$	$t_{end} = 1080$	$t_{end} = 3240$
SV	0.0123	0.0123	0.0123	0.0123
E	0.1452e–003	0.1452e–003	0.1452e–003	0.1452e–003
SRKN3s4	0.1528e–004	0.1528e–004	0.1528e–004	0.1528e–004
SMEFMRKN2s2	0.7285e–007	0.7285e–007	0.7285e–007	0.7285e–007
SMEFMRKN3s3	0.4822e–007	0.4822e–007	0.4823e–007	0.4825e–007

We carry out a semi-discretization on the spatial variable by using second-order symmetric differences and obtain the following system

$$\frac{\partial^2 U}{\partial t^2} + MU = F(t, U), \quad 0 < t \leq t_{end}, \tag{29}$$

where $U(t) = (u_1(t), \dots, u_N(t))^T$ with $u_i(t) \approx u(x_i, t)$, $x_i = -1 + i\Delta x, i = 1, \dots, N$, $\Delta x = 2/N$, and

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

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

The Hamiltonian of (29) is given by

$$H\big(U', U\big) = \frac{1}{2}U'^T U' + \frac{1}{2}U^T MU - \big(\cos(u_1) + \cdots + \cos(u_N)\big).$$

Following the paper [8], we take the initial conditions as

$$U(0) = (\pi)_{i=1}^N, \quad U_t(0) = \sqrt{N}\left(0.01 + \sin\left(\frac{2\pi i}{N}\right)\right)_{i=1}^N \quad \text{with } N = 64.$$

The problem is integrated in the interval [0, 10] with step sizes $h = \frac{0.1}{8i}$, $i = 1, 2, 3, 4$ for the methods SV and E and $h = \frac{0.1}{4i}$, $i = 1, 2, 3, 4$ for the other methods. Figure 5(i) shows the error in the positions at $t_{end} = 10$ versus the computational effort. We integrate this problem with step size $h = \frac{1}{50}$ in the interval $[0, t_{end}]$, $t_{end} = 10 \times 5^i$, $i = 0, 1, 2, 3$. See Fig. 5(ii).

Problem 5 We consider a Fermi-Pasta-Ulam Problem (this problem is considered by Hairer et al. in [11, 12]).

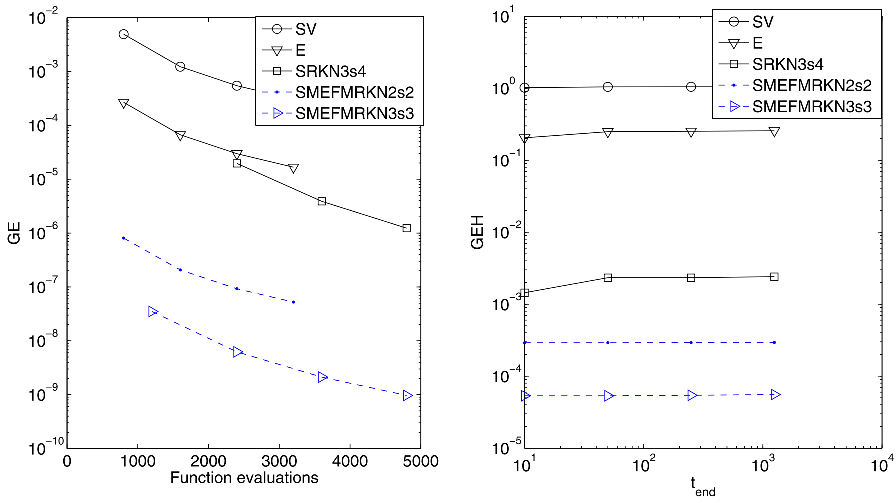
The Hamiltonian is

$$H(y, x) = \frac{1}{2}\sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{m+i}^2 + \frac{1}{4}\Bigg[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m - x_{2m})^4\Bigg],$$

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

The corresponding Hamiltonian system is

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



(i) (ii)

Fig. 5 Results for Problem 4: (**i**) The global error (*GE*) over the integration interval against the number of function evaluations. (**ii**) The maximum global error of Hamiltonian $GEH = \max|H_n - H_0|$ against t_{end}

which is equivalent to $x'' = -H_x(y, x)$. This leads to

$$x''(t) + Mx(t) = -\nabla U(x), \quad t \in [0, t_{end}],$$

where

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

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

Following Hairer et al. [12], we choose $m = 3,\ \omega = 50$,

$$x_1(0) = 1, \qquad y_1(0) = 1, \qquad x_4(0) = \frac{1}{\omega}, \qquad y_4(0) = 1,$$

and choose zero for the remaining initial values.

Figure 6 displays the efficiency curves on the interval $t \in [0, 25]$ with the integration step sizes $h = \frac{0.1}{8i},\ i = 1, 2, 3, 4$ for the methods SV and E and $h = \frac{0.1}{4i},\ i = 1, 2, 3, 4$ for the other methods. Then we integrate this problem with step size $h = 0.0025$ on the interval $[0, t_{end}]$ and $t_{end} = 25 \times 2^i$ with $i = 0, 1, \ldots, 4$. The global errors of Hamiltonian are shown in Table 2.

In this section, we show our MEFMRKN methods are applicable to both single-frequency problems and multi-frequency problems (1) with positive semi–definite

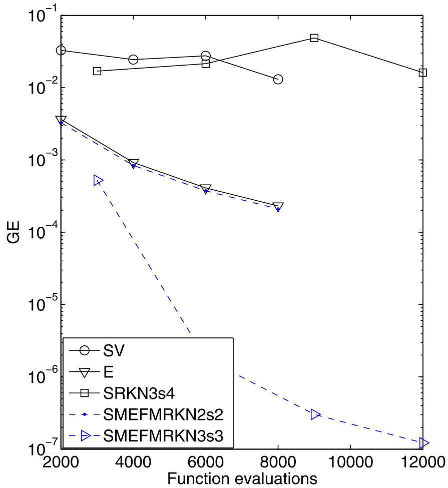


Fig. 6 Results for Problem 5: The global error (GE) over the integration interval against the number of function evaluations

Table 2 Results for Problem 5: The maximum global error of Hamiltonian $GEH = \max|H_n - H_0|$ for different t_{end}

Methods	$t_{end} = 25$	$t_{end} = 50$	$t_{end} = 100$	$t_{end} = 200$	$t_{end} = 400$
SV	0.0020	0.0020	0.0020	0.0020	0.0020
E	0.2532e–003	0.2532e–003	0.2532e–003	0.2641e–003	0.2974e–003
SRKN3s4	0.9480e–005	0.9480e–005	0.9480e–005	0.9480e–005	0.9480e–005
SMEFMRKN2s2	0.1399e–005	0.1469e–005	0.1469e–005	0.1469e–005	0.1469e–005
SMEFMRKN3s3	0.4370e–007	0.4370e–007	0.4370e–007	0.4370e–007	0.4370e–007

matrix containing implicitly the frequencies. In other words, our MEFMRKN methods are widely applicable and much more practical. Furthermore, the results of the numerical experiments confirm that our methods generally have better accuracy for the same numbers of the function evaluations. Meanwhile it can be observed that for the Hamiltonian systems, when t_{end} increases, the global errors GEH of our methods nearly do not increase and are smaller than those of other methods. Namely, our methods preserve better the Hamiltonian essentially.

6 Conclusions

In the present paper, MEFMRKN methods for the system of oscillatory second-order equations (1) are presented and studied. The relationship between MEFMRKN methods and multidimensional ERKN methods is also discussed. Because the oscillatory system (1) with $f(q) = -\nabla U(q)$ is simply a separable Hamiltonian system (11) with Hamiltonian $H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T Mq + U(q)$, we derive the symplecticity conditions for the MEFMRKN methods. Using the exponential fitting and the symplecticity conditions for the MEFMRKN methods, we propose two useful explicit symplectic MEFMRKN methods. Numerical experiments in this paper demonstrate that our explicit symplectic MEFMRKN methods are more effective than some well-known methods in the scientific literature in both energy conservation and computational efficiency.

Lastly, we point out that the discussions in this paper can be extended easily to separable Hamiltonian system with Hamiltonian $H(p,q) = \frac{1}{2}p^T M_0 p + \frac{1}{2}q^T Mq + U(q)$, where M_0 and M are both symmetric and positive semi-definite matrixes with the condition $M_0 M = M M_0$. This system is equivalent to oscillatory second-order equation $q'' + M_0 Mq = -M_0 \nabla U(q)$, which coincides with the form (1).

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