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HIGH-ORDER SYMPLECTIC AND SYMMETRIC COMPOSITION METHODS FOR MULTI-FREQUENCY AND MULTI-DIMENSIONAL OSCILLATORY HAMILTONIAN SYSTEMS*

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Abstract

The multi-frequency and multi-dimensional adapted Runge-Kutta-Nyström (ARKN) integrators, and multi-frequency and multi-dimensional extended Runge-Kutta-Nyström (ERKN) integrators have been developed to efficiently solve multi-frequency oscillatory Hamiltonian systems. The aim of this paper is to analyze and derive high-order symplectic and symmetric composition methods based on the ARKN integrators and ERKN integrators. We first consider the symplecticity conditions for the multi-frequency and multi-dimensional ARKN integrators. We then analyze the symplecticity of the adjoint integrators of the multi-frequency and multi-dimensional symplectic ARKN integrators and ERKN integrators, respectively. On the basis of the theoretical analysis and by using the idea of composition methods, we derive and propose four new high-order symplectic and symmetric methods for the multi-frequency oscillatory Hamiltonian systems. The numerical results accompanied in this paper quantitatively show the advantage and efficiency of the proposed high-order symplectic and symmetric methods.

Mathematics subject classification: 65L05, 65L06, 65M20, 65P10
Key words: Symplectic and symmetric composition methods, Multi-frequency and multi-dimensional ERKN integrators, ARKN integrators, Multi-frequency oscillatory Hamiltonian systems.

1. Introduction

Geometric numerical integration is designed specially for the numerical solution of differential equations which possess some geometric/physical properties (Hamiltonian, divergence-free, symmetry, symplecticity, etc.) that should be preserved by numerical methods as much as possible. We refer the reader to [3, 4, 10, 13, 15, 18, 30] for this topic. Oscillation is also an important physical property. In fact, differential equations having oscillatory solutions are usually encountered in many fields of the applied sciences and engineering, such as celestial mechanics, theoretical physics, quantum chemistry and molecular dynamics. The modeling and simulation of oscillations is of particular interest in applications. A lot of theoretical and numerical analysis has been made on this research [10, 30]. A variety of methods and analytical tools arise in this area such as stroboscopic averaging methods, heterogeneous multiscale methods, the technique of modified Fourier expansions. For these mehtods, we refer the reader to [5–7, 9, 17] and the references therein.

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Among typical topics is the numerical integration of an oscillatory system of the form

$$\begin{cases} q''(t) + Kq(t) = f(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, \quad q'(t_0) = q'_0, \end{cases} \tag{1.1}$$

where K is a $d \times d$ positive semi-definite matrix that implicitly contains the frequencies of the oscillatory problem and $f : \mathbb{R}^d \to \mathbb{R}^d$, $q \in \mathbb{R}^d, q' \in \mathbb{R}^d$. It should be noted that (1.1) is a *multi-frequency and multi-dimensional nonlinear oscillatory problem*. The design and analysis of numerical method for nonlinear oscillators is an important problem that has received a great deal of attention in the last few years.

It has now become a common practice in geometric numerical integration that, numerical algorithms should take advantage of the special structure of the underlying problem. In [28], the authors took account of the special structure of system (1.1) brought by the linear term Kq and proposed the so-called multi-frequency and multi-dimensional ARKN (Adapted Runge-Kutta-Nyström) integrators. An outstanding advantage of multi-frequency and multi-dimensional ARKN integrators for (1.1) is that their updates are incorporated with the special structure of the system (1.1) so that they naturally integrate exactly the multi-frequency oscillatory homogeneous system $y'' + Ky = 0$. Very recently, Wu *et al.* [29] formulated a standard form of the multi-frequency and multi-dimensional ERKN (extended Runge-Kutta-Nyström) methods in which both the internal stages and updates are incorporated with the special structure of the system (1.1). The ERKN methods exactly integrate the multi-frequency oscillatory homogeneous system $y''+Ky = 0$ as well. The ERKN integrators exhibit the correct qualitative behaviour much better than the classical RKN methods. For references on this topic, we refer the reader to [19, 21, 23, 25–28, 31].

On the other hand, the idea of composition methods is quite useful to improve the order of a basic method while preserving some desirable properties. It is well-known that numerical integrators of arbitrarily high order can be achieved by composition of an integrator with low order. Let φ_h be a basic method and $\gamma_1, \ldots, \gamma_s$ real numbers. Then we call its composition

$$\psi_h = \varphi_{\gamma_s h} \circ \cdots \circ \varphi_{\gamma_1 h} \tag{1.2}$$

the corresponding *composition method*.

A more general case is that consider the composition of both the basic integrators and its adjoint integrators with different stepsizes, i.e., replace composition (1.2) by the more general formula

$$\psi_h = \varphi_{\alpha_s h} \circ \varphi^*_{\beta_s h} \circ \cdots \circ \varphi^*_{\beta_2 h} \circ \varphi_{\alpha_1 h} \circ \varphi^*_{\beta_1 h}. \tag{1.3}$$

The adjoint method of a method is defined as follows [11].

Definition 1.1. *The adjoint method Φ^*_h of a method Φ_h is defined as the inverse map of the original method with reversed time step $-h$, i.e., $\Phi^*_h := \Phi^{-1}_{-h}$. A method with $\Phi^*_h = \Phi_h$ is called symmetric.*

With regard to composition methods, we refer the reader to [1, 2, 14, 16, 22, 32]. For a systematic introduction of the idea of composition methods, including the order conditions for composition methods, we refer to [10].

In this paper, we focus ourselves on the compositions of multi-frequency and multi-dimensional symplectic ARKN and ERKN integrators. The remainder of this paper is organized as follows. In Section 2 and Section 3, we derive some properties for ARKN and ERKN integrators. Based on these properties, we derive four novel high-order symplectic and symmetric methods by using the composition of multi-frequency and multi-dimensional symplectic ARKN and ERKN integrators, respectively. In Section 4, numerical experiments are carried out and the advantage and efficiency of the new methods are shown by the numerical results. Section 5 is devoted to conclusions.

2. Composition of ARKN Integrators for System (1.1)

To begin with, we consider the matrix-valued functions which have been first defined in [31]

$$\phi_l(M) := \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+l)!}, \qquad l = 0, 1. \tag{2.1}$$

Some properties of the matrix-valued functions (2.1) are given in the following proposition, which can be proved in a straightforward way.

Proposition 2.1. *For symmetric and positive semi-definite matrix M, the ϕ-functions $\phi_l(M)$ for $l = 0, 1,$ defined by* (2.1) *satisfy:*

(i)

$$\phi_0^2(M) + M\phi_1^2(M) = I, \tag{2.2}$$

where I is the identity matrix with the same dimension as M;

(ii)

$$\phi_0(a^2M)\phi_0(b^2M) \pm abM\phi_1(a^2M)\phi_1(b^2M) = \phi_0((a \mp b)^2M) \tag{2.3a}$$

$$b\phi_1(b^2M)\phi_0(a^2M) \pm a\phi_1(a^2M)\phi_0(b^2M) = (b \pm a)\phi_1((b \pm a)^2M), \forall a, b \in \mathbb{R}. \tag{2.3b}$$

In the recent paper [31], the authors presented the following variation-of-constants formula for the exact solution and its derivative for the multi-frequency oscillatory system (1.1):

Theorem 2.1. *If $K \in \mathbb{R}^{d\times d}$ is a positive semi-definite matrix and $f : \mathbb{R}^d \to \mathbb{R}^d$ is continuous in* (1.1)*, then the solution of* (1.1) *and its derivative satisfy*

$$q(t) = \phi_0((t-t_0)^2K)q_0 + (t-t_0)\phi_1((t-t_0)^2K)q_0' + \int_{t_0}^{t} (t-\xi)\phi_1((t-\xi)^2K)\hat{f}(\xi)d\xi, \tag{2.4a}$$

$$q'(t) = -(t-t_0)K\phi_1((t-t_0)^2K)q_0 + \phi_0((t-t_0)^2K)q_0' + \int_{t_0}^{t} \phi_0((t-\xi)^2K)\hat{f}(\xi)d\xi, \tag{2.4b}$$

for any real number t_0, t, where $\hat{f}(\xi) = f(q(\xi))$.

We note that if K is a symmetric and positive semi-definite matrix, K has the decomposition: $K = P^T\Omega^2P = W^2$ with $W = P^T\Omega P$. However, (2.4b) does not involve the decomposition of matrix K. This point is important, especially for the computational issues of an integrator based on (2.4b), since K is not necessarily diagonal nor symmetric in (1.1) and the decomposition $K = W^2$ is not always feasible.

It follows immediately from (2.4b) that

$$\begin{aligned} q(t_n + \nu h) =& \phi_0\big(\nu^2h^2K\big)q_n + h\phi_1\big(\nu^2h^2K\big)q_n' \\ &+ h^2\int_0^{\nu} (\nu-\gamma)\phi_1\big((\nu-\gamma)^2h^2K\big)\hat{f}(t_n + h\gamma)d\gamma, \end{aligned} \tag{2.5a}$$

$$\begin{aligned} q'(t_n + \nu h) =& -\nu hK\phi_1\big(\nu^2h^2K\big)q_n + \phi_0\big(\nu^2h^2K\big)q_n' \\ &+ \nu h\int_0^{\nu} \phi_0\big((\nu-\gamma)^2h^2K\big)\hat{f}(t_n + h\gamma)d\gamma, \end{aligned} \tag{2.5b}$$

for $0 < \nu < 1$, and

$$q(t_n + h) = \phi_0\big(h^2K\big)q_n + h\phi_1\big(h^2K\big)q'_n + h^2\int_0^1 (1-\gamma)\phi_1\big((1-\gamma)^2h^2K\big)\hat{f}(t_n + h\gamma)d\gamma, \tag{2.6a}$$

$$q'(t_n + h) = -hK\phi_1\big(h^2K\big)q_n + \phi_0\big(h^2K\big)q'_n + h\int_0^1 \phi_0\big((1-\gamma)^2h^2K\big)\hat{f}(t_n + h\gamma)d\gamma. \tag{2.6b}$$

From (2.6a), revising the updates of classical RKN methods obtains the following s-stage multi-frequency and multi-dimensional ARKN integrators proposed in [31]:

$$Q_i = q_n + c_ihq'_n + h^2\sum_{j=1}^{s}\bar{a}_{ij}\big(f(Q_j) - KQ_j\big), \qquad i = 1, \cdots, s, \tag{2.7a}$$

$$q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q'_n + h^2\sum_{i=1}^{s}\bar{b}_i(V)f(Q_i), \tag{2.7b}$$

$$q'_{n+1} = \phi_0(V)q'_n - hK\phi_1(V)q_n + h\sum_{i=1}^{s}b_i(V)f(Q_i), \tag{2.7c}$$

where, $\bar{a}_{ij} \in \mathbb{R}, i, j = 1, \cdots, s$, the weights $b_i, \bar{b}_i : \mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}, i = 1, \cdots, s$ are matrix-valued functions of $V = h^2K$.

A numerical method has *order* p, if for a sufficiently smooth problem (1.1) the conditions

$$e_{n+1} := q_{n+1} - q(t_n + h) = \mathcal{O}(h^{p+1}), \tag{2.8a}$$

$$e'_{n+1} := q'_{n+1} - q'(t_n + h) = \mathcal{O}(h^{p+1}) \tag{2.8b}$$

are satisfied, where $q(t_n + h)$ and $q'(t_n + h)$ are the exact solution of (1.1) and its derivative at $t_n + h$, respectively, q_{n+1} and q'_{n+1} are the one step numerical results obtained by the method from the exact starting values $q_n = q(t_n)$ and $q'_n = q'(t_n)$ (the local assumptions). The order conditions of the multi-frequency and multi-dimensional ARKN integrators (2.7c) have been investigated in [31].

The following theorem gives the adjoint integrator of a multi-frequency and multi-dimensional ARKN integrator.

Theorem 2.2. *The adjoint integrator of an s-stage multi-frequency and multi-dimensional ARKN integrator* (2.7c) *with stepsize h has the following form*

$$Q_i = \Big(\phi_0(V) + c_{s+1-i}V\phi_1(V)\Big)q_n + \Big(\phi_1(V) - c_{s+1-i}\phi_0(V)\Big)hq'_n + h^2\sum_{j=1}^{s}\bar{a}_{s+1-i,s+1-j}\Big(f(Q_j) - KQ_j\Big) + h^2\sum_{j=1}^{s}\Big(\bar{b}^*_j(V) - c_{s+1-i}b^*_j(V)\Big)f(Q_j), \tag{2.9a}$$

$$q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q'_n + h^2\sum_{i=1}^{s}\bar{b}^*_i(V)f(Q_i), \tag{2.9b}$$

$$q'_{n+1} = -hK\phi_1(V)q_n + \phi_0(V)q'_n + h\sum_{i=1}^{s}b^*_i(V)f(Q_i), \tag{2.9c}$$

where

$$\bar{b}^*_i(V) = \phi_1(V)b_{s+1-i}(V) - \phi_0(V)\bar{b}_{s+1-i}(V), \tag{2.10a}$$

$$b^*_i(V) = V\phi_1(V)\bar{b}_{s+1-i}(V) + \phi_0(V)b_{s+1-i}(V), \quad i = 1, 2, \ldots, s. \tag{2.10b}$$

Proof. Exchanging $q_{n+1} \leftrightarrow q_n,\ q'_{n+1} \leftrightarrow q'_n$ and replacing h by $-h$ in the ARKN integrator (2.7c) yields

$$Q_i = q_{n+1} - c_i h q'_{n+1} + h^2 \sum_{j=1}^{s} \bar{a}_{ij}\Big(f(Q_j) - KQ_j\Big), \qquad i = 1, 2, \cdots, s, \tag{2.11a}$$

$$q_n = \phi_0(V) q_{n+1} - h\phi_1(V) q'_{n+1} + h^2 \sum_{i=1}^{s} \bar{b}_i(V) f(Q_i), \tag{2.11b}$$

$$q'_n = hK\phi_1(V) q_{n+1} + \phi_0(V) q'_{n+1} - h \sum_{i=1}^{s} b_i(V) f(Q_i). \tag{2.11c}$$

It follows from (2.11a) that

$$\begin{aligned} Q_i = {} & \big(\phi_0(V) + c_i V\phi_1(V)\big) q_n + \big(\phi_1(V) - c_i\phi_0(V)\big) h q'_n - h^2 \sum_{j=1}^{s} \bar{a}_{ij} K Q_j + h^2 \sum_{j=1}^{s} \Big(\bar{a}_{ij} \\ & - c_i\big(\phi_0(V) b_j(V) + V\phi_1(V)\bar{b}_j(V)\big) + \big(\phi_1(V) b_j(V) - \phi_0(V)\bar{b}_j(V)\big)\Big) f(Q_j), \\ q_{n+1} = {} & \phi_0(V) q_n + h\phi_1(V) q'_n + h^2 \sum_{i=1}^{s} \Big(\phi_1(V) b_i(V) - \phi_0(V)\bar{b}_i(V)\Big) f(Q_i), \\ q'_{n+1} = {} & -hK\phi_1(V) q_n + \phi_0(V) q'_n + h \sum_{i=1}^{s} \Big(\phi_0(V) b_i(V) + V\phi_1(V)\bar{b}_i(V)\Big) f(Q_i). \end{aligned}$$

Replacing all indices i and j by $s+1-i$ and $s+1-j$, respectively, we obtain the result of the theorem. □

From Theorem 2.2, it is easy to see that the adjoint integrator of an ARKN integrator is not again an ARKN integrator.

If $f(q)$ in (1.1) is the negative gradient of a real-valued function $U(q)$ and K is a symmetric and positive semi-definite matrix, let $p = q'$, then (1.1) is in fact identical to the following *multi-frequency and multi-dimensional Hamiltonian system*

$$\begin{cases} q' = H_p(p, q), \\ p' = -H_q(p, q), \\ q(t_0) = q_0,\ p(t_0) = p_0 \end{cases} \tag{2.12}$$

with the Hamiltonian

$$H(p, q) = \frac{1}{2} p^T p + \frac{1}{2} q^T K q + U(q). \tag{2.13}$$

The following theorem gives the symplecticity conditions of a multi-frequency and multi-dimensional ARKN integrator.

Theorem 2.3. *If the coefficients of an s-stage multi-frequency and multi-dimensional ARKN integrator* (2.7c) *satisfy the following conditions*

$$\begin{aligned} & b_i(V)\phi_0(V) + \bar{b}_i(V) V\phi_1(V) = d_i I, \quad d_i \in \mathbb{R}, && i = 1, \cdots, s, && (2.14\text{a}) \\ & b_i(V)\phi_1(V) - \bar{b}_i(V)\phi_0(V) = c_i d_i I, && i = 1, \cdots, s, && (2.14\text{b}) \\ & d_i \bar{a}_{ij} = 0, \quad b_i(V)\bar{b}_j(V) = b_j(V)\bar{b}_i(V), && i, j = 1, \cdots, s, && \\ & && i, j = 1, \cdots, s, && (2.14\text{c}) \end{aligned}$$

then the integrator is symplectic.

Proof. With the notation of differential 2-form used in [18], symplecticity of the methods (2.7c) for system (1.1) is identical to

$$\sum_{J=1}^{d} dq_{n+1}^J \wedge dq'^J_{n+1} = \sum_{J=1}^{d} dq_n^J \wedge dq'^J_n. \tag{2.15}$$

We first consider the special case, where K is a diagonal matrix with nonnegative entries, i.e., $K = \mathrm{diag}(k_{11}, k_{22}, \cdots, k_{dd})$, then $V = \mathrm{diag}(v_{11}, v_{22}, \cdots, v_{dd})$ with $v_{jj} = h^2 k_{jj}, j = 1, \cdots, d$. Accordingly, $\phi_0(V)$, $\phi_1(V)$, $b_i(V)$ and $\bar{b}_i(V)$ are all diagonal matrices. Denote $f_i = f(Q_i)$, then the ARKN integrator (2.7c) becomes

$$Q_i^J = q_n^J + c_i h q_n^{'J} + h^2 \sum_{j=1}^{s} a_{ij}(f_j^J - k_{JJ}Q_j^J), \quad i = 1, \ldots, s, \tag{2.16a}$$

$$q_{n+1}^J = \phi_0(v_{JJ}) q_n^J + \phi_1(v_{JJ}) h q_n^{'J} + h^2 \sum_{i=1}^{s} \bar{b}_i(v_{JJ}) f_i^J, \tag{2.16b}$$

$$q_{n+1}^{'J} = -h k_{JJ} \phi_1(v_{JJ}) q_n^J + \phi_0(v_{JJ}) q_n^{'J} + h \sum_{i=1}^{s} b_i(v_{JJ}) f_i^J, \tag{2.16c}$$

where the superscript indices $J = 1, 2, \ldots, d$ denote the Jth component of a vector. Differentiating q_{n+1}^J and $q_{n+1}^{'J}$ and taking external products arrives at

$$\begin{aligned} dq_{n+1}^J \wedge dq_{n+1}^{'J} = {} & \Big(\phi_0^2(v_{JJ}) + v_{JJ}\phi_1^2(v_{JJ})\Big) dq_n^J \wedge dq_n^{'J} \\ & + h \sum_{i=1}^{s} \Big(b_i(v_{JJ})\phi_0(v_{JJ}) + \bar{b}_i(v_{JJ}) v_{JJ} \phi_1(v_{JJ})\Big) dq_n^J \wedge df_i^J \\ & + h^2 \sum_{i=1}^{s} \Big(b_i(v_{JJ})\phi_1(v_{JJ}) - \bar{b}_i(v_{JJ})\phi_0(v_{JJ})\Big) dq_n^{'J} \wedge df_i^J \\ & + h^3 \sum_{i,j=1}^{s} \bar{b}_i(v_{JJ}) b_j(v_{JJ}) df_i^J \wedge df_j^J. \end{aligned}$$

It follows from the identity $\phi_0^2(v_{JJ}) + v_{JJ}\phi_1^2(v_{JJ}) = 1$ that

$$\begin{aligned} dq_{n+1}^J \wedge dq_{n+1}^{'J} = {} & dq_n^J \wedge dq_n^{'J} + h \sum_{i=1}^{s} \Big(b_i(v_{JJ})\phi_0(v_{JJ}) + \bar{b}_i(v_{JJ}) v_{JJ}\phi_1(v_{JJ})\Big) dq_n^J \wedge df_i^J \\ & + h^2 \sum_{i=1}^{s} \Big(b_i(v_{JJ})\phi_1(v_{JJ}) - \bar{b}_i(v_{JJ})\phi_0(v_{JJ})\Big) dq_n^{'J} \wedge df_i^J \\ & + h^3 \sum_{i,j=1}^{s} \bar{b}_i(v_{JJ}) b_j(v_{JJ}) df_i^J \wedge df_j^J. \end{aligned} \tag{2.17}$$

Differentiating the first formula of (2.16) yields

$$dq_n^J = dQ_i^J - c_i h dq'^J_n - h^2 \sum_{j=1}^{s} \bar{a}_{ij}\Big(df_j^J - k_{JJ} dQ_j^J\Big), \qquad i = 1, \cdots, s.$$

Thus

$$dq_n^J \wedge df_i^J = dQ_i^J \wedge df_i^J - c_i h dq'^J_n \wedge df_i^J - h^2 \sum_{j=1}^{s} \bar{a}_{ij}\Big(df_j^J - k_{JJ} dQ_j^J\Big) \wedge df_i^J. \tag{2.18}$$

Substituting (2.18) into (2.17) gives

$$
\begin{aligned}
&dq^J_{n+1} \wedge dq'^J_{n+1} \\
&= dq^J_n \wedge dq'^J_n + h\sum_{i=1}^{s}\Big((b_i(v_{JJ})\phi_0(v_{JJ}) + \bar{b}_i(v_{JJ})v_{JJ}\phi_1(v_{JJ}))\Big)dQ^J_i \wedge df^J_i \\
&\quad + h\sum_{i,j=1}^{s}\Big(v_{JJ}b_i(v_{JJ})\bar{a}_{ij}\phi_0(v_{JJ}) + v^2_{JJ}\bar{b}_i(v_{JJ})\bar{a}_{ij}\phi_1(v_{JJ})\Big)dQ^J_j \wedge df^J_i \\
&\quad + h^2\sum_{i=1}^{s}\Big(b_i(v_{JJ})\phi_1(v_{JJ}) - \bar{b}_i(v_{JJ})c_i v_{JJ}\phi_1(v_{JJ}) - b_i(v_{JJ})c_i\phi_0(v_{JJ}) - \bar{b}_i(v_{JJ})\phi_0(v_{JJ})\Big) \\
&\quad dq'^J_n \wedge df^J_i + h^3\sum_{i,j=1}^{s}[b_i(v_{JJ})\bar{a}_{ij}\phi_0(v_{JJ}) + \bar{b}_i(v_{JJ})\bar{a}_{ij}v_{JJ}\phi_1(v_{JJ}) + \bar{b}_i(v_{JJ})b_j(v_{JJ})]df^J_i \wedge df^J_j
\end{aligned}
\tag{2.19}
$$

for each $J = 1, \cdots, d$. Summing over all J obtains

$$
\begin{aligned}
&\sum_{J=1}^{d} dq^J_{n+1} \wedge dq'^J_{n+1} \\
&= \sum_{J=1}^{d} dq^J_n \wedge dq'^J_n + h\sum_{i=1}^{s}\sum_{J=1}^{d}\Big((b_i(v_{JJ})\phi_0(v_{JJ}) + \bar{b}_i(v_{JJ})v_{JJ}\phi_1(v_{JJ}))\Big)dQ^J_i \wedge df^J_i \\
&\quad + h\sum_{i,j=1}^{s}\sum_{J=1}^{d}\Big(v_{JJ}b_i(v_{JJ})\bar{a}_{ij}\phi_0(v_{JJ}) + v^2_{JJ}\bar{b}_i(v_{JJ})\bar{a}_{ij}\phi_1(v_{JJ})\Big)dQ^J_j \wedge df^J_i \\
&\quad + h^2\sum_{i=1}^{s}\sum_{J=1}^{d}\Big(b_i(v_{JJ})\phi_1(v_{JJ}) - \bar{b}_i(v_{JJ})c_i v_{JJ}\phi_1(v_{JJ}) - b_i(v_{JJ})c_i\phi_0(v_{JJ}) - \bar{b}_i(v_{JJ})\phi_0(v_{JJ})\Big) \\
&\quad dq'^J_n \wedge df^J_i + h^3\sum_{i,j=1}^{s}\sum_{J=1}^{d}\Big(b_i(v_{JJ})\bar{a}_{ij}\phi_0(v_{JJ}) \\
&\quad + \bar{b}_i(v_{JJ})\bar{a}_{ij}v_{JJ}\phi_1(v_{JJ}) + \bar{b}_i(v_{JJ})b_j(v_{JJ})\Big)df^J_i \wedge df^J_j.
\end{aligned}
\tag{2.20}
$$

By first and second equations in (2.14a) , h^2 term in the right-hand side vanishes and (2.20) can be rewritten as

$$
\begin{aligned}
&\sum_{J=1}^{d} dq^J_{n+1} \wedge dq'^J_{n+1} \\
&= \sum_{J=1}^{d} dq^J_n \wedge dq'^J_n + h\sum_{i=1}^{s} d_i \sum_{J=1}^{d} dQ^J_i \wedge df^J_i + h\sum_{i,j=1}^{s} d_i\bar{a}_{ij}\sum_{J=1}^{d} v_{JJ}dQ^J_j \wedge df^J_i \\
&\quad + h^3\sum_{i,j=1}^{s}\sum_{J=1}^{d}\Big(\bar{a}_{ij}d_i + \bar{b}_i(v_{JJ})b_j(v_{JJ})\Big)df^J_i \wedge df^J_j.
\end{aligned}
\tag{2.21}
$$

Since

$$
df^J_i \wedge dQ^J_i = \Big(\sum_{I=1}^{d}\frac{\partial f^J}{\partial q^I}(Q_i)dQ^I_i\Big) \wedge dQ^J_i = \sum_{I=1}^{d}\frac{\partial f^J}{\partial q^I}(Q_i)dQ^I_i \wedge dQ^J_i,
$$

it follows from $f = -\nabla U$ that

$$
\begin{aligned}
\sum_{J=1}^{d} df^J_i \wedge dQ^J_i &= \sum_{I,J=1}^{d}\Big(\frac{\partial f^J}{\partial q^I}(Q_i)dQ^I_i\Big) \wedge dQ^J_i \\
&= \sum_{I<J}\big(\frac{\partial f^J}{\partial q^I}(Q_i) - \frac{\partial f^I}{\partial q^J}(Q_i)\big)dQ^I_i \wedge dQ^J_i \\
&= \sum_{I<J}\big[-\frac{\partial^2 U}{\partial q^J\partial q^I}(Q_i) + \frac{\partial^2 U}{\partial q^I\partial q^J}(Q_i)\big]dQ^I_i \wedge dQ^J_i = 0,
\end{aligned}
\tag{2.22}
$$

where the last term vanishes by symmetry of the partial derivatives. Therefore, by (2.22) and the assumptions (2.14a), we have

$$\sum_{J=1}^{d} dq_{n+1}^J \wedge dq'^J_{n+1} = \sum_{J=1}^{d} dq_n^J \wedge dq'^J_n.$$

For general case, since K is a symmetric and positive semi-definite matrix, K has the following decomposition:

$$K = P^T \Omega^2 P = W^2 \text{ with } W = P^T \Omega P, \tag{2.23}$$

where P is an orthogonal matrix and Ω is a diagonal matrix with nonnegative diagonal entries which are the square roots of the eigenvalues of K. Accordingly, by using the variable substitution $z(t) = Pq(t)$, the system (1.1) is identical to the system

$$\begin{cases} z''(t) + \Omega^2 z(t) = Pf(P^T z(t)), & t \in [t_0, T], \\ z(t_0) = z_0 = Py_0, \quad q'(t_0) = q'_0 = Pq'_0, \end{cases} \tag{2.24}$$

where $f(q) = -\nabla_q U(q),\ Pf\big(P^{\mathrm{T}} z(t)\big) = -P\nabla_q U\big(P^{\mathrm{T}} z(t)\big) = -\nabla_z U\big(P^{\mathrm{T}} z(t)\big)$.

Then the symplectic multi-frequency and multi-dimensional ARKN integrator for the case where K is diagonal with nonnegative entries can be applied to the transformed system. Furthermore, the methods are invariant by linear transformations and therefore, the methods applied to the system (1.1) can be expressed in terms of $z(t)$ via the multiplication by P and with the notation $Z_i = PQ_i,\ z_n = Pq_n$. Then we have

$$\begin{aligned} &\sum_{J=1}^{d} dz_{n+1}^J \wedge dz'^J_{n+1} = \sum_{J=1}^{d} \mathrm{d} \sum_{i=1}^{d} (p_{Ji} q_{n+1}^i) \wedge \sum_{J=1}^{d} \mathrm{d} \sum_{k=1}^{d} (p_{Jk} q'^k_{n+1}) \\ &= \sum_{J=1}^{d} \sum_{i=1}^{d} (p_{Ji} \mathrm{d} q_{n+1}^i) \wedge \sum_{J=1}^{d} \sum_{k=1}^{d} (p_{Jk} \mathrm{d} q'^k_{n+1}) \\ &= \sum_{J=1}^{d} \sum_{i=1}^{d} \sum_{k=1}^{d} p_{Ji} p_{Jk} (\mathrm{d} q_{n+1}^i \wedge \mathrm{d} q'^k_{n+1}) = \sum_{J=1}^{d} \mathrm{d} q_{n+1}^J \wedge \mathrm{d} q'^J_{n+1}. \end{aligned} \tag{2.25}$$

Likewise,

$$\sum_{J=1}^{d} \mathrm{d} z_n \wedge \mathrm{d} z'^J_n = \sum_{J=1}^{d} \mathrm{d} q_n^J \wedge \mathrm{d} q'^J_n. \tag{2.26}$$

Therefore, it follows from (2.25) and (2.26) that

$$\sum_{J=1}^{d} dq_{n+1}^J \wedge dq'^J_{n+1} = \sum_{J=1}^{d} dq_n^J \wedge dq'^J_n.$$

The orthogonality of the matrix $P = (p_{Ji})_{d\times d}$ is used in the proof of (2.25). The proof is complete. $\square$

Remark 2.1. It is clear from Theorem 2.3 that a symplectic ARKN method for a single-frequency oscillatory Hamiltonian system cannot ensure itself to be again a symplectic method when applied to multi-frequency and multi-dimensional oscillatory Hamiltonian system since a symplectic multi-frequency and multi-dimensional ARKN method requires additional conditions in comparison with a symplectic single-frequency ARKN method as shown in (2.14a). With regard to symplecticity conditions for single-frequency ARKN methods, we refer to [19, 20]. For exactly the same reason, a symplectic ERKN method for a single-frequency oscillatory Hamiltonian system cannot ensure itself to be again a symplectic method when applied to multi-frequency and multi-dimensional oscillatory Hamiltonian systems.

Remark 2.2. From the first two equations in symplecticity conditions (2.14a), we can solve $b_i(V), \bar{b}_i(V)$ explicitly:

$$b_i(V) = d_i\Big(\phi_0(V) + c_i V\phi_1(V)\Big), \tag{2.27a}$$

$$\bar{b}_i(V) = d_i\Big(\phi_1(V) - c_i\phi_0(V)\Big), \quad i = 1, \ldots, s. \tag{2.27b}$$

Thus, if $d_i \neq 0$ for some i, then $b_i(V), \bar{b}_i(V) \neq 0$, and the third equation of conditions (2.14a) indicates $\bar{a}_{ij} = 0, j = 1, \ldots, s$. Therefore, the i-stage with nonzero $b_i(V)$ and $\bar{b}_i(V)$, is independent of internal stages. On the other hand, if $d_i = 0$ for some i, then $b_i(V) = \bar{b}_i(V) = 0$ and the i-stage, can neither contribute to the updates of ARKN integrators, nor to any other internal stages with nonzero $b_i(V)$ and $\bar{b}_i(V)$. Hence, in the rest of this section, we always assume that $d_i \neq 0, i = 1, \ldots, s$.

Before going on to give the analysis of symplecticiy of the adjoint integrator of a multi-frequency and multi-dimensional ARKN integrator, we present the following theorem.

Theorem 2.4. *If the coefficients of an s-stage multi-frequency and multi-dimensional ARKN integrator satisfy conditions* (2.14a)*, i.e., the integrator is symplectic, then,* $c_1 = c_2 = \cdots = c_s$.

Proof. From (2.27a), choosing arbitrary i and j, we have

$$b_i(V)\bar{b}_j(V) = d_i d_j\Big(\phi_0(V) + c_i V\phi_1(V)\big)\big(\phi_1(V) - c_j\phi_0(V)\Big),$$
$$b_j(V)\bar{b}_i(V) = d_i d_j\Big(\phi_0(V) + c_j V\phi_1(V)\big)\big(\phi_1(V) - c_i\phi_0(V)\Big).$$

By the fourth equation of conditions (2.14a), we obtain

$$\begin{aligned}&\big(\phi_0(V) + c_i V\phi_1(V)\big)\big(\phi_1(V) - c_j\phi_0(V)\big)\\ =&\big(\phi_0(V) + c_j V\phi_1(V)\big)\big(\phi_1(V) - c_i\phi_0(V)\big),\end{aligned}$$

or

$$(c_i - c_j)\big(\phi_0^2(V) + V\phi_1^2(V)\big) = 0.$$

Using (2.2), we have $c_i = c_j$ for arbitrary i and j. □

By Remark 2.2 and Theorem 2.4, we present the following conclusion.

Theorem 2.5. *The multi-frequency and multi-dimensional symplectic ARKN integrator has only one stage.*

Proof. From Remark 2.2 we have $\bar{a}_{ij} = 0, i, j = 1, \ldots, s$, and from Theorem 2.4 we have $c_1 = c_2 = \cdots = c_s$. □

By Theorem 2.5, it can be verified that the order of a multi-frequency and multi-dimensional symplectic ARKN cannot exceed two (see [19]).

We now present the analysis on the symplecticiy of the adjoint integrator for a multi-frequency and multi-dimensional ARKN integrator. It follows from Theorem 2.3 and Theorem 2.5 that a multi-frequency and multi-dimensional symplectic ARKN integrator has the following form

$$Q_1 = q_n + c_1 h q_n', \tag{2.28a}$$

$$q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q_n' + h^2\bar{b}_1(V)f(Q_1), \tag{2.28b}$$

$$q_{n+1}' = \phi_0(V)q_n' - hK\phi_1(V)q_n + hb_1(V)f(Q_1), \tag{2.28c}$$

where

$$b_1(V) = d_1\big(\phi_0(V) + c_1 V\phi_1(V)\big), \quad \bar{b}_1(V) = d_1\big(\phi_1(V) - c_1\phi_0(V)\big),$$

and the corresponding adjoint integrator is given by

$$Q_1 = \big(\phi_0(V) + c_1 V\phi_1(V)\big)q_n + \big(\phi_1(V) - c_1\phi_0(V)\big)hq_n' \tag{2.29a}$$

$$q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q_n' + h^2\bar{b}_1^*(V)f(Q_1), \tag{2.29b}$$

$$q_{n+1}' = -hK\phi_1(V)q_n + \phi_0(V)q_n' + hb_1^*(V)f(Q_1), \tag{2.29c}$$

where

$$\bar{b}_1^*(V) = \phi_1(V)b_1(V) - \phi_0(V)\bar{b}_1(V) = c_1 d_1 I,$$
$$b_1^*(V) = V\phi_1(V)\bar{b}_1(V) + \phi_0(V)b_1(V) = d_1 I.$$

By (2.29a), we have the following result on the symplecticiy of the adjoint integrator for a multi-frequency and multi-dimensional ARKN integrator.

Theorem 2.6. *The adjoint integrator* (2.29a) *of a multi-frequency and multi-dimensional symplectic ARKN integrator* (2.28) *is symplectic.*

Proof. By Theorem 2.5, symplectic ARKN integrator has only one stage. Thus it is easy to verify that its adjoint method is symplectic and we skip the details. □

From the analysis described above, it is clear that high-order symplectic ARKN integrators do not exist. Furthermore, since the adjoint integrator of an ARKN integrator is not again an ARKN integrator, an ARKN integrator cannot be symmetric. To get through this barrier, we can resort to the composition of ARKN integrators to obtain high-order symplectic and symmetric methods, although they are not ARKN integrators any more.

Consider the following one-stage ARKN method of order two, which can be viewed as an extended version of Störmer-Verlet method [24]

$$Q_1 = q_n + \frac{1}{2}hq_n', \tag{2.30a}$$

$$q_{n+1} = \phi_0(V)q_n + \phi_1(V)(hq_n') + h^2\big(\phi_1(V) - \frac{1}{2}\phi_0(V)\big)f(Q_1), \tag{2.30b}$$

$$q_{n+1}' = -hK\phi_1(V)q_n + \phi_0(V)q_n' + h\big(\phi_0(V) + \frac{1}{2}V\phi_1(V)\big)f(Q_1). \tag{2.30c}$$

It can be observed that (2.30) is a symplectic method and its adjoint integrator is also symplectic by Theorem 2.6. If we let $V \to \mathbf{0}$ in (2.30), then (2.30) reduces to the Störmer-Verlet formula for (1.1) or (2.12):

$$Q_1 = q_n + \frac{h}{2}q_n', \tag{2.31a}$$

$$q_{n+1} = q_n + hq_n' + \frac{h^2}{2}g(Q_1), \tag{2.31b}$$

$$q_{n+1}' = q_n' + hg(Q_1), \tag{2.31c}$$

where $g(q) = f(q) - Kq$.

Using (2.30) as the basic method, consider the fourth order symmetric composition of the form (1.3) with coefficients [10]

$$\alpha_1 = \beta_3 = \frac{1}{2(2-2^{1/3})}, \quad \alpha_2 = \beta_2 = -\frac{2^{1/3}}{2(2-2^{1/3})}, \quad \alpha_3 = \beta_1 = \frac{1}{2(2-2^{1/3})}. \tag{2.32}$$

We denote the composition of (2.30) with coefficients (2.32) by CARKNp4s6.

As pointed out in [10], for achieving a composition method of high order, the solutions with the minimal number of stages do not give the best methods. Thus, we consider the following fourth order symmetric composition coefficients given in [2]:

$$\begin{aligned} &\alpha_1 = \beta_6 = 0.16231455076687, && \alpha_2 = \beta_5 = 0.37087741497958,\\ &\alpha_3 = \beta_4 = 0.059762097006575, && \alpha_4 = \beta_3 = -0.40993371990193,\\ &\alpha_5 = \beta_2 = 0.23399525073150, && \alpha_6 = \beta_1 = 0.082984406417405. \end{aligned} \tag{2.33}$$

We denote the composition of (2.30) with the coefficients (2.33) by CARKNp4s12. Both CARKNp4s6 and CARKNp4s12 methods are symplectic and symmetric and of order four.

3. Composition of ERKN Integrators for (1.1)

Another effecient method for the oscillatory system (1.1) is so-called multi-frequency and multi-dimensional ERKN integrators [29]. ERKN integrators are designed by taking advantage of the special structure brought by Kq in both the updates and the internal stages. In light of the variation-of constants formula (2.5a)-(2.6a) for (1.1), reforming both the internal stages and updates of a classical RKN method leads to the definition of ERKN methods.

Definition 3.1. *An s-stage multi-frequency and multi-dimensional ERKN integrator with stepsize h for oscillatory system* (1.1) *is defined to be*

$$Q_i = \phi_0(c_i^2V)q_n + hc_i\phi_1(c_i^2V)q_n' + h^2\sum_{j=1}^{s} a_{ij}(V)f(Q_j), \quad i = 1,\dots,s, \tag{3.1a}$$

$$q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q_n' + h^2\sum_{i=1}^{s}\bar{b}_i(V)f(Q_i), \tag{3.1b}$$

$$q_{n+1}' = -hK\phi_1(V)q_n + \phi_0(V)q_n' + h\sum_{i=1}^{s} b_i(V)f(Q_i), \tag{3.1c}$$

where $b_i,\ \bar{b}_i,\ i = 1,\dots,s,$ and $a_{ij},\ i,j = 1,\dots,s$ are matrix-valued functions of $V = h^2K$.

The order conditions for multi-frequency and multi-dimensional ERKN integrator can be found in [25]. We are now concerned with the adjoint integrators of ERKN integrators.

Theorem 3.1. *The adjoint integrator of an s-stage multi-frequency and multi-dimensional ERKN integrator* (3.1) *with stepsize h has the following form:*

$$Q_i = \phi_0(c_i^{*2}V)q_n + c_i^*\phi_1(c_i^{*2}V)hq_n' + h^2\sum_{j=1}^{s} a_{ij}^*(V)f(Q_j), \quad i = 1,2,\dots,s, \tag{3.2a}$$

$$q_{n+1} = \phi_0(V)q_n + h\phi_1(V)q_n' + h^2\sum_{i=1}^{s}\bar{b}_i^*(V)f(Q_i), \tag{3.2b}$$

$$q_{n+1}' = -hM\phi_1(V)q_n + \phi_0(V)q_n' + h\sum_{i=1}^{s} b_i^*(V)f(Q_i), \tag{3.2c}$$

where, for $1 \le i,\ j \le s$,

$$c_i^* = 1 - c_{s+1-i}, \quad \bar{b}_i^*(V) = \phi_1(V)b_{s+1-i}(V) - \phi_0(V)\bar{b}_{s+1-i}(V), \tag{3.3a}$$

$$b_i^*(V) = V\phi_1(V)\bar{b}_{s+1-i}(V) + \phi_0(V)b_{s+1-i}(V), \tag{3.3b}$$

$$a_{ij}^*(V) = \phi_0(c_{s+1-i}^2V)\bar{b}_j^*(V) - c_{s+1-i}\phi_1(c_{s+1-i}^2V)b_j^*(V) + a_{s+1-i,s+1-j}(V). \tag{3.3c}$$

Proof. The proof is similar to the theorem 2.2 and we skip the details. □

From Theorem 3.1, we can see that the adjoint integrator of a multi-frequency and multi-dimensional ERKN integrator is again an ERKN integrator.

With regard to the symplecticity conditions of ERKN integrator, we have the following theorem [27].

Theorem 3.2. *An s-stage multi-frequency and multi-dimensional ERKN integrator* (3.1) *is symplectic if its coefficients satisfy the following conditions:*

$$\phi_0(V)b_i(V)+V\phi_1(V)\bar{b}_i(V)=d_i\phi_0(c_i^2V),\ d_i\ \in\ \mathbb{R},\quad i=1,\ldots,s, \tag{3.4a}$$
$$\phi_1(V)b_i(V)-\phi_0(V)\bar{b}_i(V)=c_id_i\phi_1(c_i^2V),\quad i=1,\ldots,s, \tag{3.4b}$$
$$\bar{b}_i(V)b_j(V)+d_ia_{ij}(V)=\bar{b}_j(V)b_i(V)+d_ja_{ji}(V),\quad i,\ j=1,\ldots,s, \tag{3.4c}$$

where $V=h^2K$.

Remark 3.1. *From the first two equations in symplecticity conditions* (3.4)*, we can solve* $b_i(V),\bar{b}_i(V)$ *explicitly:*

$$\begin{aligned}b_i(V)&=d_i\big(\phi_0(V)\phi_0(c_i^2V)+c_iV\phi_1(V)\phi_1(c_i^2V)\big),\\ \bar{b}_i(V)&=d_i\big(\phi_1(V)\phi_0(c_i^2V)-c_i\phi_0(V)\phi_1(c_i^2V)\big),\quad i=1,\ldots,s.\end{aligned}$$

Thus, by (2.3)*, we have*

$$b_i(V)=d_i\phi_0((1-c_i)^2V),\quad \bar{b}_i(V)=d_i(1-c_i)\phi_1((1-c_i)^2V),\quad i=1,\ldots,s. \tag{3.5}$$

In what follows we give the analysis on the symplecticiy of the adjoint integrator of a multi-frequency and multi-dimensional ERKN integrator.

Theorem 3.3. *If the coefficients of an s-stage multi-frequency and multi-dimensional ERKN integrator satisfy conditions* (3.4)*, i.e., the integrator is symplectic, then its adjoint integrator* (3.2) *is also symplectic.*

Proof. It is sufficient to prove that the coefficients of (3.2) satisfy symplecticity conditions (3.4). In fact, by (3.3) and (3.4), the coefficients of the adjoint integrator of a symplectic ERKN integrator satisfy, for $1\le i,\ j\le s$,

$$\begin{aligned}&c_i^*=1-c_{s+1-i},\\ &\bar{b}_i^*(V)=c_{s+1-i}d_{s+1-i}\phi_1(c_{s+1-i}^2V),\quad b_i^*(V)=d_{s+1-i}\phi_0(c_{s+1-i}^2V),\\ &a_{ij}^*(V)=c_{s+1-j}d_{s+1-j}\phi_0(c_{s+1-i}^2V)\phi_1(c_{s+1-j}^2V)\\ &\qquad\qquad -c_{s+1-i}d_{s+1-j}\phi_1(c_{s+1-i}^2V)\phi_0(c_{s+1-j}^2V)+a_{s+1-i,s+1-j}(V).\end{aligned}$$

We then have, for $1\le i,\ j\le s$,

$$\begin{aligned}&\phi_0(V)b_i^*(V)+V\phi_1(V)\bar{b}_i{}^*(V)\\ &\quad=\phi_0(V)d_{s+1-i}\phi_0(c_{s+1-i}^2V)+V\phi_1(V)c_{s+1-i}d_{s+1-i}\phi_1(c_{s+1-i}^2V)\\ &\quad=d_{s+1-i}\phi_0((1-c_{s+1-i})^2V)=d_{s+1-i}\phi_0(c_i^{*2}V),\end{aligned} \tag{3.6a}$$

$$\begin{aligned}&\phi_1(V)b_i^*(V)-\phi_0(V)\bar{b}_i^*(V)\\ &\quad=\phi_1(V)d_{s+1-i}\phi_0(c_{s+1-i}^2V)-\phi_0(V)c_{s+1-i}d_{s+1-i}\phi_1(c_{s+1-i}^2V)\\ &\quad=d_{s+1-i}(1-c_{s+1-i})\phi_1((1-c_{s+1-i})^2V)=d_{s+1-i}c_i^*\phi_1(c_i^{*2}V).\end{aligned} \tag{3.6b}$$

Let $d_i^* = d_{s+1-i}$, then the first two conditions are satisfied in (3.4). Concerning the third condition (3.4), we have

$$\begin{aligned}
&\bar{b}_i^*(V)b_j^*(V) + d_i^* a_{ij}^*(V) - (\bar{b}_j^*(V)b_i^*(V) + d_j^* a_{ji}^*(V))\\
=&c_{s+1-i}d_{s+1-i}\phi_1(c_{s+1-i}^2 V)d_{s+1-j}\phi_0(c_{s+1-j}^2 V)\\
&- c_{s+1-j}d_{s+1-j}\phi_1(c_{s+1-j}^2 V)d_{s+1-i}\phi_0(c_{s+1-i}^2 V)\\
&+ d_{s+1-i}\Big(c_{s+1-j}d_{s+1-j}\phi_0(c_{s+1-i}^2 V)\phi_1(c_{s+1-j}^2 V)\\
&- c_{s+1-i}d_{s+1-j}\phi_1(c_{s+1-i}^2 V)\phi_0(c_{s+1-j}^2 V) + a_{s+1-i,s+1-j}(V)\Big)\\
&- d_{s+1-j}\Big(c_{s+1-i}d_{s+1-i}\phi_0(c_{s+1-j}^2 V)\phi_1(c_{s+1-i}^2 V)\\
&- c_{s+1-j}d_{s+1-i}\phi_1(c_{s+1-j}^2 V)\phi_0(c_{s+1-i}^2 V) + a_{s+1-j,s+1-i}(V)\Big)\\
=&d_{s+1-i}\Big(c_{s+1-j}d_{s+1-j}\phi_0(c_{s+1-i}^2 V)\phi_1(c_{s+1-j}^2 V) + a_{s+1-i,s+1-j}(V)\Big)\\
&- d_{s+1-j}\Big(c_{s+1-i}d_{s+1-i}\phi_0(c_{s+1-j}^2 V)\phi_1(c_{s+1-i}^2 V) + a_{s+1-j,s+1-i}(V)\Big)\\
=&d_{s+1-i}d_{s+1-j}(c_{s+1-j} - c_{s+1-i})\phi_1((c_{s+1-j} - c_{s+1-i})^2 V)\\
&+ d_{s+1-i}a_{s+1-i,s+1-j}(V) - d_{s+1-j}a_{s+1-j,s+1-i}(V).
\end{aligned} \tag{3.7}$$

By (3.5) and the third equation of (3.4), we obtain

$$\begin{aligned}
&d_{s+1-i}a_{s+1-i,s+1-j}(V) - d_{s+1-j}a_{s+1-j,s+1-i}(V)\\
=&\bar{b}_{s+1-j}(V)b_{s+1-i}(V) - \bar{b}_{s+1-i}(V)b_{s+1-j}(V)\\
=&d_{s+1-i}d_{s+1-j}(1 - c_{s+1-j})\phi_1\Big((1 - c_{s+1-j})^2 V\Big)\phi_0\Big((1 - c_{s+1-i})^2 V\Big)\\
&- d_{s+1-i}d_{s+1-j}(1 - c_{s+1-i})\phi_1\Big((1 - c_{s+1-i})^2 V\Big)\phi_0\Big((1 - c_{s+1-j})^2 V\Big)\\
=&d_{s+1-i}d_{s+1-j}(c_{s+1-i} - c_{s+1-j})\phi_1\Big((c_{s+1-i} - c_{s+1-j})^2 V\Big).
\end{aligned} \tag{3.8}$$

Substituting (3.8) into (3.7) yields

$$\bar{b}_i^*(V)b_j^*(V) + d_i^* a_{ij}^*(V) - (\bar{b}_j^*(V)b_i^*(V) + d_j^* a_{ji}^*(V)) = 0.$$

The proof is complete. □

Section 2 points out that the composition of an ARKN integrator is not again an ARKN integrator. However, the composition of an ERKN integrator is still an ERKN integrator as shown in the next theorem.

Theorem 3.4. *The composition of an s_1-stage ERKN integrator with stepsize αh and an s_2-stage ERKN integrator with stepsize βh is a new ERKN integrator with $s = s_1 + s_2$ stages and stepsize $(\alpha+\beta)h$.*

Proof. Let the two ERKN integrators with stepsizes αh and βh be

$$Q_i = \phi_0(c_i^2\alpha^2h^2K)q_n + \alpha h c_i\phi_1(c_i^2\alpha^2h^2K)q_n' + \alpha^2h^2\sum_{j=1}^{s_1} a_{ij}(\alpha^2h^2K)f(Q_j), \quad i = 1,\dots,s_1, \tag{3.9a}$$

$$q_{n+1} = \phi_0(\alpha^2h^2K)q_n + \alpha h\phi_1(\alpha^2h^2K)q_n' + \alpha^2h^2\sum_{i=1}^{s_1}\bar{b}_i(\alpha^2h^2K)f(Q_i), \tag{3.9b}$$

$$q_{n+1}' = -\alpha hK\phi_1(\alpha^2h^2K)q_n + \phi_0(\alpha^2h^2K)q_n' + \alpha h\sum_{i=1}^{s_1} b_i(\alpha^2h^2K)f(Q_i), \tag{3.9c}$$

and

$$Q_i^* = \phi_0(c_i^{*2}\beta^2h^2K)q_n + \beta hc_i^*\phi_1(c_i^{*2}\beta^2h^2K)q_n' + \beta^2h^2\sum_{j=1}^{s_2} a_{ij}^*(\beta^2h^2K)f(Q_j^*),$$
$$i = 1,\ldots,s_2, \tag{3.10a}$$

$$q_{n+1} = \phi_0(\beta^2h^2K)q_n + \beta h\phi_1(\beta^2h^2K)q_n' + \beta^2h^2\sum_{i=1}^{s_2}\bar{b}_i^*(\beta^2h^2K)f(Q_i^*), \tag{3.10b}$$

$$q_{n+1}' = -\beta hK\phi_1(\beta^2h^2K)q_n + \phi_0(\beta^2h^2K)q_n' + \beta h\sum_{i=1}^{s_2} b_i^*(\beta^2h^2K)f(Q_i^*). \tag{3.10c}$$

Denote them by $\varphi_{h_1}^1$ and $\varphi_{h_2}^2$, respectively. Then $\varphi_{h_2}^2\circ\varphi_{h_1}^1$ has the following form

$$Q_i = \phi_0(c_i^2\alpha^2h^2K)q_n + \alpha hc_i\phi_1(c_i^2\alpha^2h^2K)q_n' + \alpha^2h^2\sum_{j=1}^{s_1} a_{ij}(\alpha^2h^2K)f(Q_j),$$
$$i = 1,\ldots,s_1, \tag{3.11a}$$

$$\tilde{q}_{n+1} = \phi_0(\alpha^2h^2K)q_n + \alpha h\phi_1(\alpha^2h^2K)q_n' + \alpha^2h^2\sum_{i=1}^{s_1}\bar{b}_i(\alpha^2h^2K)f(Q_i), \tag{3.11b}$$

$$\tilde{q}_{n+1}' = -\alpha hK\phi_1(\alpha^2h^2K)q_n + \phi_0(\alpha^2h^2K)q_n' + \alpha h\sum_{i=1}^{s_1} b_i(\alpha^2h^2K)f(Q_i), \tag{3.11c}$$

$$Q_i^* = \phi_0(c_i^{*2}\beta^2h^2K)\tilde{q}_{n+1} + \beta hc_i^*\phi_1(c_i^{*2}\beta^2h^2K)\tilde{q}_{n+1}' + \beta^2h^2\sum_{j=1}^{s_2} a_{ij}^*(\beta^2h^2K)f(Q_j^*),$$
$$i = 1,\ldots,s_2, \tag{3.11d}$$

$$q_{n+1} = \phi_0(\beta^2h^2K)\tilde{q}_{n+1} + \beta h\phi_1(\beta^2h^2K)\tilde{q}_{n+1}' + \beta^2h^2\sum_{i=1}^{s_2}\bar{b}_i^*(\beta^2h^2K)f(Q_i^*), \tag{3.11e}$$

$$q_{n+1}' = -\beta hK\phi_1(\beta^2h^2K)\tilde{q}_{n+1} + \phi_0(\beta^2h^2K)\tilde{q}_{n+1}' + \beta h\sum_{i=1}^{s_2} b_i^*(\beta^2h^2K)f(Q_i^*). \tag{3.11f}$$

Let $Q_{s_1+i} = Q_i^*, i = 1,\cdots,s_2$ and $s = s_1 + s_2$. Substituting the second and third terms into the last three terms of (3.11) with some tedious computations and manipulations, we obtain

$$Q_i = \phi_0(c_i^2\alpha^2h^2K)q_n + \alpha hc_i\phi_1(c_i^2\alpha^2h^2K)q_n' + \alpha^2h^2\sum_{j=1}^{s_1} a_{ij}(\alpha^2h^2K)f(Q_j),$$
$$i = 1,\ldots,s_1, \tag{3.12a}$$

$$Q_i = \phi_0((\alpha + c_i^*\beta)^2h^2K)q_n + (\alpha + c_i^*\beta)h\phi_1((\alpha + c_i^*\beta)^2h^2K)q_n' + h^2\sum_{j=1}^{s}\tilde{a}_{ij}f(Q_j),$$
$$i = s_1 + 1,\ldots,s, \tag{3.12b}$$

and

$$q_{n+1} = \phi_0((\alpha+\beta)^2h^2K)q_n + (\alpha+\beta)h\phi_1\Big((\alpha+\beta)^2h^2K\Big)q_n' + (\alpha+\beta)^2h^2\sum_{i=1}^{s}\tilde{\bar{b}}_i f(Q_i),$$

$$q_{n+1}' = -(\alpha+\beta)hK\phi_1((\alpha+\beta)^2h^2K)q_n + \phi_0((\alpha+\beta)^2h^2K)q_n' + (\alpha+\beta)h\sum_{i=1}^{s}\tilde{b}_i f(Q_i),$$

where $\tilde{a}_{ij}, \tilde{\bar{b}}_i, \tilde{b}_i, i, j = 1,\cdots,s$ are the algebraic compositions of the coefficients of the two ERKN integrators, that makes them the matrix-valued functions of $V = h^2K$.

It is noted here that although there exist high-order symplectic and symmetric ERKN integrators, the order conditions together with symmetry and symplecticity conditions are huge for achieving a high-order symplectic and symmetric ERKN integrator. Table 3.1 shows the number of equations that need to be solved from order conditions. It can be observed that as the order of the method grows, the number of equations from order conditions increases rapidly, not to mention the equations from symmetry and symplecticity conditions (the number of equations depends on how many stages of the integrator uses. The equations may be reduced but the number is still very large). Therefore, in practice, the derivation of a high-order symplectic and symmetric ERKN integrator based on order conditions, symmetry conditions and symplecticity conditions is very difficult. However, it will be useful to get high-order symplectic and symmetric ERKN integrators by using a procedure of composition.

Table 3.1: The number of equations from order conditions for order $p = 1, \ldots, 8$.

order p	1	2	3	4	5	6	7	8
number of equations	1	3	6	11	21	40	79	157

Consider the following one-stage ERKN method of order two, which is another extended version of Störmer-Verlet method [24]

$$Q_1 = \phi_0(V/4)q_n + \frac{1}{2}h\phi_1(V/4)q_n', \tag{3.13a}$$

$$q_{n+1} = \phi_0(V)q_n + \phi_1(V)(hq_n') + \frac{h^2}{2}\phi_1(V/4)f(Q_1), \tag{3.13b}$$

$$q_{n+1}' = -hK\phi_1(V)q_n + \phi_0(V)q_n' + h\phi_0(V/4)f(Q_1), \tag{3.13c}$$

It can be verified that (3.13) is symplectic and symmetric. We note that letting $V \to \mathbf{0}$ in (3.13) also gives the Störmer-Verlet formula (2.31).

Using (3.13) as the basic method, since it is symmetric, we consider the sixth order symmetric composition of the form (1.2) with coefficients given in [32]

$$\begin{aligned} &\gamma_1 = \gamma_7 = 0.78451361047755726381949763, &&\gamma_2 = \gamma_6 = 0.23557321335935813368479318,\\ &\gamma_3 = \gamma_5 = -1.17767998417887100694641568, &&\gamma_4 = 1.31518632068391121888424973. \end{aligned} \tag{3.14}$$

We denote the composition of (3.13) with the coefficients (3.14) by CERKNp6s7. The method CERKNp6s7 is symplectic and symmetric of order six. Moreover, it can be seen from Theorem 3.4 that CERKNp6s7 is a seven-stage multi-frequency and multi-dimensional ERKN method of order six.

We also consider the following eighth order symmetric composition coefficients [10]:

$$\begin{aligned} &\gamma_1 = \gamma_{15} = 0.74167036435061295344822780, &&\gamma_2 = \gamma_{14} = -0.40910082580003159399730010,\\ &\gamma_3 = \gamma_{13} = 0.19075471029623837995387626, &&\gamma_4 = \gamma_{12} = -0.57386247111608226665638773,\\ &\gamma_5 = \gamma_{11} = 0.29906418130365592384446354, &&\gamma_6 = \gamma_{10} = 0.33462491824529818378495798,\\ &\gamma_7 = \gamma_9 = 0.31529309239676659663205666, &&\gamma_8 = -0.79688793935291635401978884. \end{aligned} \tag{3.15}$$

We denote the composition of (3.13) with the coefficients (3.15) by CERKNp8s15 which is a symplectic and symmetric ERKN method of order eight.

Remark 3.2. The second-order symmetric Gautschi-type method is also an alternative basic method for oscillatory problem. Take Deuflhard's Trigonometric Method ([8]) for example, let

$\Omega = K^{1/2}$, the one-step form of Deuflhard's method for (1.1) reads

$$q_{n+1} = \cos(h\Omega)q_n + \Omega^{-1}\sin(h\Omega)q'_n + \frac{h^2}{2}(h\Omega)^{-1}\sin(h\Omega)f(q_n), \tag{3.16a}$$

$$q'_{n+1} = -\Omega\sin(h\Omega)q_n + \cos(h\Omega)q'_n + \frac{1}{2}h\Big(\cos(h\Omega)f(q_n) + f(q_{n+1})\Big), \tag{3.16b}$$

The method is also symmetric and symplectic, which makes it a good option as the basic method. It is noted from the definition of the ϕ-functions that the Deuflhard's method can be reformulated as

$$Q_1 = q_n, \tag{3.17a}$$

$$Q_2 = \phi_0(V)q_n + \phi_1(V)(hq'_n) + \frac{h^2}{2}\phi_1(V)f(Q_1), \tag{3.17b}$$

$$q_{n+1} = \phi_0(V)q_n + \phi_1(V)(hq'_n) + \frac{h^2}{2}\phi_1(V)f(Q_1), \tag{3.17c}$$

$$q'_{n+1} = -hK\phi_1(V)q_n + \phi_0(V)q'_n + \frac{h}{2}\Big(\phi_0(V)f(Q_1) + f(Q_2)\Big). \tag{3.17d}$$

In other words, the Deuflhard's method can be viewed as a two-stage ERKN method of order two with FSAL property (the last evaluation at any step is the same as the first evaluation at the next step). Thus it only needs one function evaluation per step.

4. Numerical Experiments

In order to show the robustness and efficiency of the novel symplectic and symmetric methods proposed in this paper in comparison with the existing methods in the scientific literature, we use four problems in numerical experiments. The methods used for comparisons are:

- CRKNp6s7: the composition of Störmer-Verlet method with coefficients (3.14);
- CRKNp8s15: the composition of Störmer-Verlet method with coefficients (3.15);
- CDeuflhardp6s7: the composition of Deuflhard's method with coefficients (3.14);
- CDeuflhardp8s15: the composition of Deuflhard's method with coefficients (3.15);
- SRKNp4s3: the three-stage symplectic Runge-Kutta-Nyström method of order four given in [11];

For each experiment, we will display the efficiency curves: accuracy versus the computational cost measured by the number of function evaluations required by each method and the energy error of each method. If the error is very large, we do not plot the points in the figure of the numerical results.

Example 4.1. Consider the orbital problem with perturbation

$$\begin{aligned} q''_1 + q_1 &= -\frac{2\epsilon + \epsilon^2}{r^5}q_1, \quad q_1(0) = 1,\ q'_1(0) = 0, \\ q''_2 + q_2 &= -\frac{2\epsilon + \epsilon^2}{r^5}q_2, \quad q_2(0) = 0,\ q'_2(0) = 1 + \epsilon, \end{aligned}$$

where $r = \sqrt{q_1^2 + q_2^2}$. This is a Hamiltonian system with the Hamiltonian

$$H = \frac{1}{2}p^T p + \frac{1}{2}q^T K q + U(q),$$

where

$$U(q) = -\frac{2\epsilon + \epsilon^2}{3(q_1^2 + q_2^2)^{\frac{3}{2}}}, \quad K = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The analytic solution is given by

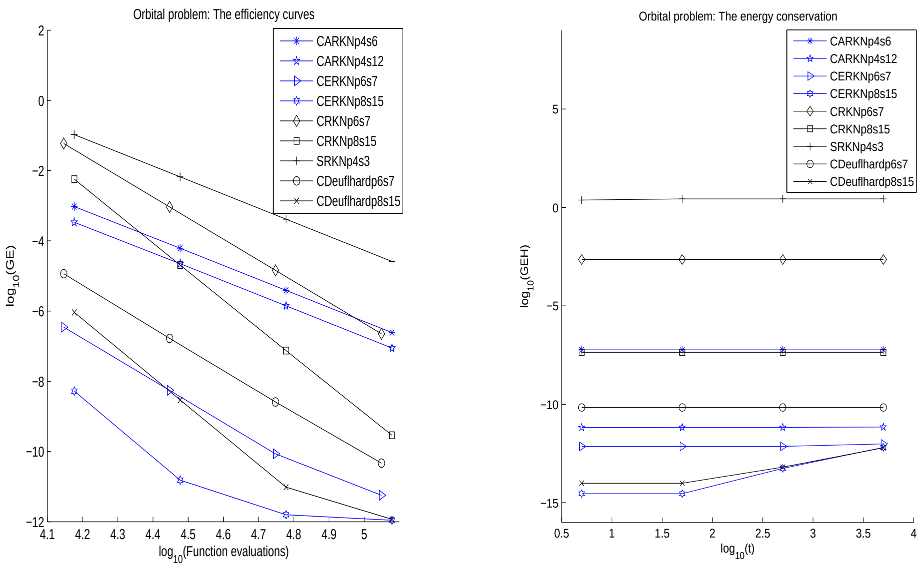
$$q_1(t) = \cos(t + \epsilon t), \quad q_2(t) = \sin(t + \epsilon t).$$

Example 4.1 is solved numerically on the interval [0, 1000] with $\epsilon = 10^{-3}$. We take stepsizes $h = 1/2^j$ for the methods CERKNp8s15, CRKNp8s15, CDeuflhardp8s15, $h = 1/2^{j+1}$ for CERKNp6s7, CRKNp6s7, CDeuflhardp6s7, $h = 6/(15 \times 2^j)$ for CARKNp4s6, $h = 12/(15 \times 2^j)$ for CARKNp4s12, and $h = 3/(15 \times 2^j)$ for SRKNp4s3, where $j = 0, 1, 2, 3$.

Fig. 4.1(a) shows the error of the position q at $t_{end} = 1000$ versus the computational effort. We integrate this problem with stepsize $h = 1.5$ in the interval $[0, t_{end}]$, $t_{end} = 5 \times 10^i$, $i = 0, 1, 2, 3$. Fig. 4.1(b) shows the energy errors of different methods.

Example 4.2. Consider the Fermi-Pasta-Ulam problem, which can be expressed by a Hamiltonian system with the Hamiltonian

$$H(p, q) = \frac{1}{2}p^T p + \frac{1}{2}q^T K q + U(q),$$



(a) (b)

Fig. 4.1. Results for Example 4.1. (a): The logarithm of the global error (GE) over the integration interval against the logarithm of the number of function evaluations. (b): The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{end})$.

where

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

$$U(q) = \frac{1}{4}\left((q_1 - q_{m+1})^4 + \sum_{i=1}^{m-1} (q_{i+1} - q_{m+i+1} - q_i - q_{m+i})^4 + (q_m + q_{2m})^4 \right).$$

Following [10], we choose $\omega = 100$ and

$$m = 3, \quad q_1(0) = 1, \quad p_1(0) = 1, \quad q_4(0) = \frac{1}{\omega}, \quad p_4(0) = 1, \tag{4.1}$$

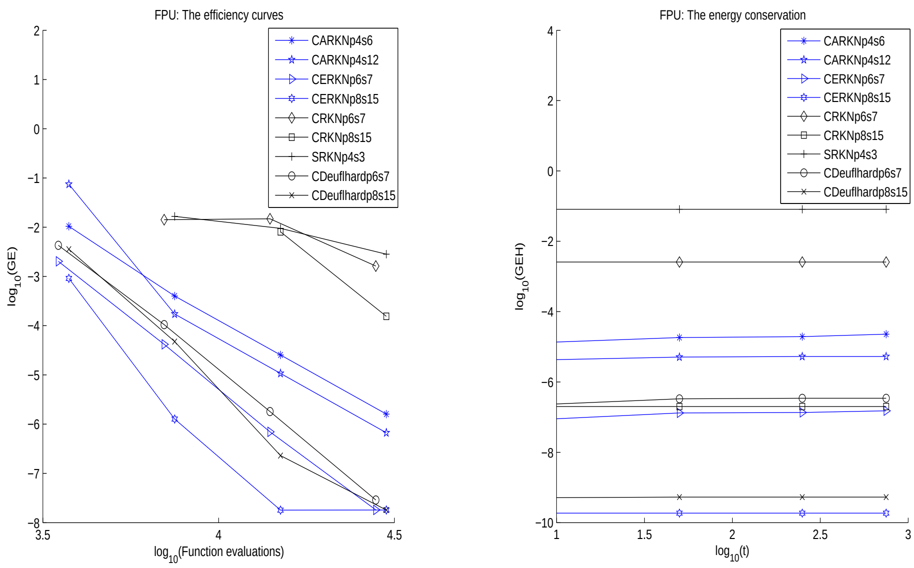
and choose zero for the remaining initial values.

Example 4.2 is integrated in the interval $[0, 20]$ with stepsizes $h = 0.08/2^j$ for the methods CERKNp8s15, CRKNp8s15, CDeuflhardp8s15, $h = 0.08/2^{j+1}$ for CERKNp6s7, CRKNp6s7, CDeuflhardp6s7, $h = 0.08\times 6/(15 \times 2^j)$ for CARKNp4s6, $h = 0.08\times 12/(15 \times 2^j)$ for CARKNp4 -s12, and $h = 0.08 \times 3/(15 \times 2^j)$ for SRKNp4s3, where $j = 0, 1, 2, 3$.

Fig. 4.2(a) shows the error of the position q at $t_{end} = 20$ versus the computational effort. We integrate this problem with stepsize $h = 0.01$ in the interval $[0, t_{end}]$, $t_{end} = 10\times 5^i$, $i = 0, 1, 2, 3$. Fig. 4.2(b) shows the energy errors of different methods.

Example 4.3. Consider the sine-Gordon equation with periodic boundary conditions

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



(a) (b)

Fig. 4.2. Results for Example 4.2. (a): The logarithm of the global error (GE) over the integration interval against the logarithm of the number of function evaluations. (b): The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{end})$.

By semi-discretization on the spatial variable with second-order symmetric differences, and introducing generalized momenta $p = q'$, we obtain a Hamiltonian system with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T K q + U(q),$$

where $q(t) = (u_1(t), \ldots, u_d(t))^T$ and $U(q) = -(\cos(u_1)+\ldots+\cos(u_d))$ with $u_i(t) \approx u(x_i, t)$, $x_i = -1 + i\Delta x, i = 1, \ldots, d$, $\Delta x = 2/d$, and

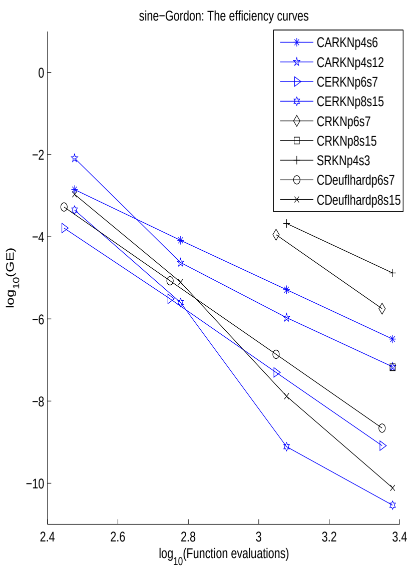
$$K = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}. \tag{4.2}$$

We take $d = 32$ and the initial conditions as

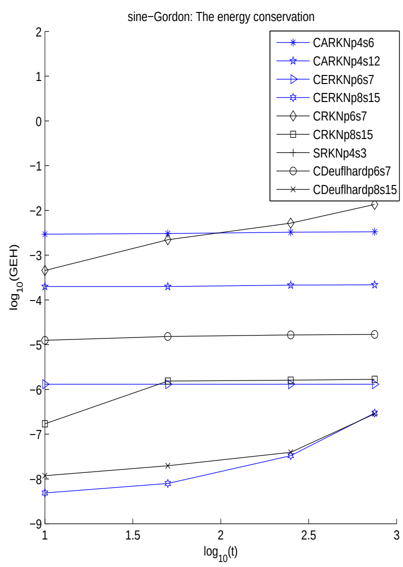
$$q(0) = (\pi)_{i=1}^d, \quad p(0) = \sqrt{d}\left(0.01 + \sin(\frac{2\pi i}{d})\right)_{i=1}^d.$$

The problem is integrated in the interval $[0, 10]$ with stepsizes $h = 1/2^j$ for the methods CERKNp8s15, CRKNp8s15, CDeuflhardp8s15, $h = 1/2^{j+1}$ for CERKNp6s7, CRKNp6s7, CDeuflhardp6s7, $h = 6/(15 \times 2^j)$ for CARKNp4s6, $h = 12/(15 \times 2^j)$ for CARKNp4s12, and $h = 3/(15 \times 2^j)$ for SRKNp4s3, where $j = 1, 2, 3, 4$.

Fig. 4.3(a) shows the error of the position q at $t_{end} = 10$ versus the computational effort. We integrate this problem with stepsize $h = 0.08$ in the interval $[0, t_{end}]$, $t_{end} = 10\times5^i$, $i = 0, 1, 2, 3$. Fig. 4.3(b) shows the energy errors of different methods.



(a)



(b)

Fig. 4.3. Results for Example 4.3. (a): The logarithm of the global error (GE) over the integration interval against the logarithm of the number of function evaluations. (b): The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{end})$.

Example 4.4. Consider the nonlinear Klein-Gordon equation [12]

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial^2 u}{\partial x^2} + u + u^3 = 0, \quad 0 < x < L, \quad t > 0, \\ u(x,0) = A\big(1 + \cos(\frac{2\pi}{L}x)\big), \\ u_t(x,0) = 0, \quad u(0,t) = u(L,t), \end{cases}$$

where $L = 1.28$, $A = 0.9$.

By the same semi-discretization on the spatial variable as Example 4.3, and introducing generalized momenta $p = q'$, we obtain the corresponding Hamiltonian system with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T K q + U(q),$$

where $q(t) = (u_1(t), \dots, u_d(t))^T$ and $U(q) = \frac{1}{2}u_1^2 + \frac{1}{4}u_1^4 + \dots + \frac{1}{2}u_d^2 + \frac{1}{4}u_d^4$ with $u_i(t) \approx u(x_i, t)$, $x_i = i\Delta x, i = 1, \dots, d$, $\Delta x = L/d$,

$$K = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}, \tag{4.3}$$

and the initial conditions are

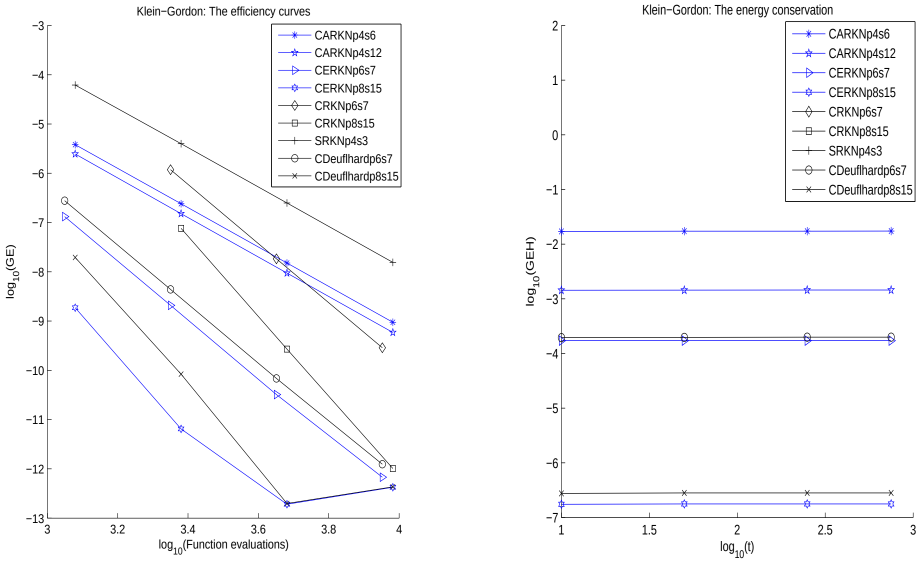
$$q(0) = \Big(0.9\big(1 + \cos(\frac{2\pi i}{d})\big)\Big)_{i=1}^{d}, \quad p(0) = \Big(0\Big)_{i=1}^{d}.$$

We take $d = 32$, and integrate the problem in the interval $[0, 10]$ with stepsizes $h = 1/2^j$ for the methods CERKNp8s15, CRKNp8s15, CDeuflhardp8s15, $h = 1/2^{j+1}$ for CERKNp6s7, CRKNp6s7, CDeuflhardp6s7, $h = 6/(15 \times 2^j)$ for CARKNp4s6, $h = 12/(15 \times 2^j)$ for CARKNp4 -s12, and $h = 3/(15 \times 2^j)$ for SRKNp4s3, where $j = 3, 4, 5, 6$.

Fig. 4.4(a) shows the error of the position q at $t_{end} = 10$ versus the computational effort. We then integrate the problem with stepsize $h = 0.08$ in the interval $[0, t_{end}]$, $t_{end} = 10 \times 5^i$, $i = 0, 1, 2, 3$. Fig. 4.4(b) shows the energy errors of different methods.

From the numerical results shown in Figs. 4.1-4.4, it follows that overall, for the problems under consideration the symmetric and symplectic composition methods based on ARKN and ERKN methods (extended Störmer-Verlet method, Deuflhard's method) give more efficient and accurate qualitative features than the classical symmetric and symplectic composition methods based on the RKN method (Störmer-Verlet method). In addition, the classical method SRKNp4s3 gives the poorest results on both the efficiency and energy conservation. This fact shows that taking account of the oscillatory structure is a significant factor to be considered in the numerical integration of oscillatory Hamiltonian systems. On the other hand, from Fig. 4.1 and Fig. 4.4, it is clear that for the problems 1 and 4, the symmetric and symplectic composition method CRKNp8s15 of order eight is more efficient than the ARKN-based symmetric and symplectic composition methods CARKNp4s6 and CARKNp4s12 of order four. This means that apart from symplecticity, symmetry, adaption to oscillation, the algebraic order cannot be ignored when designing efficient numerical methods.

For a large stepsize, it can be seen from the results of the numerical experiments that the new composition methods based on ARKN and ERKN methods perform very well. However, the traditional composition methods give unsatisfied qualitative behavior. Therefore, the symmetric



(a) (b)

Fig. 4.4. Results for Example 4.4. (a): The logarithm of the global error (GE) over the integration interval against the logarithm of the number of function evaluations. (b): The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{end})$.

and symplectic composition methods based on ARKN and ERKN methods is more suitable for long-term integration of oscillatory Hamiltonian systems.

5. Conclusions

For solving a multi-frequency and multi-dimensional oscillatory second-order initial value problem of the form $q'' + Kq = f(q)$, multi-frequency and multi-dimensional ARKN integrators and multi-frequency and multi-dimensional ERKN integrators are incorporated with the special structure brought by the linear term Kq. These integrators exactly integrate the multi-frequency oscillatory homogeneous system $q'' + Kq = 0$. The sympleticity conditions of multi-frequency and multi-dimensional ERKN integrators were presented in [27]. This paper derived the symplecticity conditions for multi-frequency and multi-dimensional ARKN integrators. Furthermore, the symplecticity conditions for the adjoint integrators of multi-frequency and multi-dimensional symplectic ARKN integrators and symplectic ERKN integrators were analyzed, respectively. We showed that the adjoint method of the one-stage symplectic ARKN method is still symplectic. The adjoint integrator of a multi-frequency and multi-dimensional symplectic ERKN integrator is also symplectic. Based on these properties, we analyzed and derived four new high-order symplectic and symmetric methods by the composition of ARKN and ERKN integrators. The numerical results were accompanied which support the theory analysis and show that the new composition methods are more efficient than the composition methods of traditional RKN methods when applied to multi-frequency and multi-dimensional oscillatory Hamiltonian systems. Last but not least, we again point out that a symplectic ARKN method or a symplectic ERKN method for a single-frequency oscillatory Hamiltonian system cannot ensure itself to be again a symplectic method when applied to a multi-frequency and multi-dimensional oscillatory Hamiltonian system.

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