Long-time energy analysis of extended RKN integrators for multi-frequency highly oscillatory Hamiltonian systems

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Abstract

In this paper, we study the long-time near conservation of the total and oscillatory energies for extended RKN (ERKN) integrators when applied to multi-frequency highly oscillatory Hamiltonian systems. We consider one-stage explicit symmetric integrators and show their long-time behaviour of numerical energy conservations by using modulated multi-frequency Fourier expansions. Numerical experiments are carried out and the numerical results demonstrate the remarkable long-time near conservation of the energies for the ERKN integrators and support our theoretical analysis presented in this paper.

Keywords: Long-time energy conservation Modulated Fourier expansions Muti-frequencies highly oscillatory systems Hamiltonian systems Extended RKN integrators

MSC: 65P10 65L05

1 Introduction

The study of numerical energy preservation is an important aspect of numerical analysis in the sense of structure-preserving algorithms when applied to Hamiltonian systems. This paper is devoted to multi-frequency highly oscillatory Hamiltonian systems with the following Hamiltonian function

\[ H(q, p) = \frac{1}{2} \sum_{j=0}^{l} \left( \|p_j\|^2 + \frac{\lambda_j^2}{\epsilon^2} \|q_j\|^2 \right) + U(q), \]

where \( q = (q_0, q_1, \ldots, q_l) \), \( p = (p_0, p_1, \ldots, p_l) \) with \( q_j, p_j \in \mathbb{R}^{d_j} \), \( \lambda_0 = 0 \) and \( \lambda_j \geq 1 \) for \( j \geq 1 \) are distinct real numbers, \( \epsilon \) is a small positive parameter, and \( U(q) \) is a smooth potential function. We pay attention to the multi-frequency case where \( l > 1 \). As is known, this system has the oscillatory energy of the \( j \)th frequency as

\[ I_j(q, p) = \frac{1}{2} \left( \|p_j\|^2 + \frac{\lambda_j^2}{\epsilon^2} \|q_j\|^2 \right), \]

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and its total oscillatory energy is given by $I(q, p) = \sum_{j=1}^{l} I_j(q, p)$. Letting

$$\lambda = (\lambda_1, \ldots, \lambda_l), \quad k = (k_1, \ldots, k_l), \quad k \cdot \lambda = k_1 \lambda_1 + \cdots + k_l \lambda_l,$$

and denoting the resonance module by

$$\mathcal{M} = \{ k \in \mathbb{Z}^l : k \cdot \lambda = 0 \},$$

it follows from the analysis in [1] that the quantities

$$I_\mu(q, p) = \sum_{j=1}^{l} \frac{\mu_j}{\lambda_j} I_j(q, p) \quad \text{with } \mu \text{ orthogonal to } \mathcal{M}$$

are approximately preserved under a diophantine non-resonance condition outside $\mathcal{M}$. Here, it is clear that $I_{\lambda} = I(q, p)$.

This kind of multi-frequency highly oscillatory systems often arises in various fields such as applied mathematics, molecular biology, astronomy, and classical mechanics (see, e.g. [14, 16, 25, 30]). In recent years, many effective numerical methods have been developed and see, e.g. [9, 11, 15, 18, 22, 23, 26] as well as the references contained therein. In [29], the authors formulated a kind of trigonometric integrators called as extended Runge–Kutta–Nyström (ERKN) integrators for solving multi-frequency highly oscillatory systems. Some important properties of these integrators were further studied in [27, 28, 30]. Very recently, the long-time energy conservation of ERKN integrators for highly oscillatory Hamiltonian systems with one frequency was researched in [24]. On the basis of this work, this paper is devoted to the numerical energy analysis of ERKN integrators for multi-frequency highly oscillatory Hamiltonian systems.

For the analysis of energy preservation, modulated Fourier expansions are an elementary and useful analytical tool. It was firstly developed in [10] and then was used as an important mathematical tool in studying the long-time behaviour of numerical methods for differential equations (see, e.g. [2, 3, 4, 5, 6, 7, 8, 12, 13, 17, 19, 20, 21, 24]). The long-time analysis of some trigonometric integrators for multi-frequency oscillatory Hamiltonian systems has been given in [6]. In this paper we extend the long-time energy preservation results of [6, 24] to the ERKN integrators for multi-frequency cases. As is known, resonance frequencies may exist for multi-frequency oscillatory Hamiltonian systems. Hence, compared with the analysis of one-frequency case in [24], a new and important aspect of multi-frequency case is possible resonance among the frequencies, which is similar to the analysis made in [6].

The remainder of this paper is organised as follows. In Section 2 we briefly summarise ERKN integrators for the multi-frequency Hamiltonian systems [1] and present some preliminaries. The modulated Fourier expansion of ERKN integrators are derived and analysed in Section 3 and two almost-invariants of the modulated Fourier expansions are studied in Section 4. Then Section 5 presents the main result concerning the long-time near energy conservation. Numerical experiments are accompanied in Section 6. The last section is concerned with the conclusions of this paper.
2 Preliminaries

2.1 ERKN integrators

Rewrite the highly oscillatory system (1) as a system of second-order differential equations

\[ q'' = -\Omega^2 q + g(q), \quad q(0) = q^0, \quad p(0) = p^0, \]

where \( \Omega = \text{diag}(\omega_0, \omega_1, \ldots, \omega_d) \) with \( \omega_j = \lambda_j/\epsilon \) and \( g(q) = -\nabla U(q) \). A kind of trigonometric integrators called as ERKN integrators has been developed (see, e.g., [29]), and the one-stage ERKN explicit scheme will be discussed in detail in this paper.

**Definition 1** (See [29]) A one-stage explicit ERKN integrator for (3) is defined by

\[
\begin{align*}
Q^{n+c_1} &= \phi_0(c_1^2 V)q^n + h c_1 \phi_1(c_1^2 V)p^n, \\
q^{n+1} &= \phi_0(V)q^n + h \phi_1(V)p^n + h^2 b_1(V)g(Q^{n+c_1}), \\
p^{n+1} &= -h\Omega^2 \phi_1(V)q^n + \phi_0(V)p^n + h b_1(V)g(Q^{n+c_1}),
\end{align*}
\]

where \( h \) is a stepsize, \( c_1 \) is real constant satisfying \( 0 \leq c_1 \leq 1 \), \( b_1(V) \) and \( \bar{b}_1(V) \) are matrix-valued and uniformly bounded functions of \( V \equiv h^2 \Omega^2 \), and

\[
\phi_j(V) := \sum_{k=0}^{\infty} \frac{(-1)^k V^k}{(2k+j)!}, \quad j = 0, 1, \ldots.
\]

The following three results of ERKN integrators will be useful in this paper.

**Theorem 1** (See [29, 30]) The one-stage explicit ERKN integrator (4) is of order two if and only if

\[
b_1(V) = \phi_1(V) + \mathcal{O}(h^2), \quad c_1 b_1(V) = \phi_2(V) + \mathcal{O}(h), \quad \bar{b}_1(V) = \phi_2(V) + \mathcal{O}(h).
\]

**Theorem 2** (See [30]) If and only if

\[
c_1 = 1/2, \quad \bar{b}_1(V) = \phi_1(V)b_1(V) - \phi_0(V)\bar{b}_1(V), \quad \phi_0(c_1^2 V)\bar{b}_1(V) = c_1 \phi_1(c_1^2 V)b_1(V),
\]

then the one-stage explicit ERKN integrator (4) is symmetric.

**Theorem 3** (See [30]) If there exists a real number \( d_1 \) such that

\[
\phi_0(V)b_1(V) + V\phi_1(V)\bar{b}_1(V) = d_1 \phi_0(c_1^2 V), \quad d_1 \in \mathbb{R},
\]

\[
\phi_1(V)b_1(V) - \phi_0(V)\bar{b}_1(V) = c_1 d_1 \phi_1(c_1^2 V),
\]

then the one-stage explicit ERKN integrator (4) is symplectic.

2.2 Notations

Let \( V = h^2 \Omega^2 \). It follows from (5) that

\[
\phi_0(V) = \cos(h\Omega), \quad \phi_1(V) = \text{sinc}(h\Omega) := (h\Omega)^{-1} \sin(h\Omega).
\]
Throughout this paper, we use the notations $\bar{b}_j(h\Omega)$ and $b_j(h\Omega)$ to denote the coefficients appearing in the ERKN method \cite{3}. Moreover, we also adopt the following notations which appeared in \cite{3}:

$$\omega = (\omega_1, \ldots, \omega_l), \quad \langle j \rangle = (0, \ldots, 1, \ldots, 0), \quad |k| = |k_1| + \cdots + |k_l|.$$ 

For the resonance module \cite{2}, we let $K$ be a set of representatives of the equivalence classes in $\mathbb{Z}^l \setminus \mathcal{M}$ which are chosen such that for each $k \in K$ the sum $|k|$ is minimal in the equivalence class $[k] = k + \mathcal{M}$, and that with $k \in K$, also $-k \in K$. We denote, for the positive integer $N$,

$$\mathcal{N} = \{ k \in K : |k| \leq N \}, \quad \mathcal{N}^* = \mathcal{N} \setminus \{(0, \ldots, 0)\}. \quad (7)$$

In this paper, we use the following operator which has been defined in \cite{14}

$$\mathcal{L}(hD) := e^{hD} - 2 \cos(h\Omega) + e^{-hD} = 2\left( \cos(ihD) - \cos(h\Omega) \right)$$

$$= 4 \sin\left(\frac{1}{2}h\Omega + \frac{1}{2}ihD\right) \sin\left(\frac{1}{2}h\Omega - \frac{1}{2}ihD\right),$$

where $D$ is the differential operator. It is easy to verify that $(hD)^m x(t) = h^m x^{(m)}(t)$ for $m = 0, 1, \ldots$, and $e^{hD} x(t) = x(t + h)$.

We consider the application of such an operator to functions of the form $e^{i(k \cdot \omega) t}$. By Leibniz’ rule of calculus, one has

$$(hD)^m e^{i(k \cdot \omega)t} z(t) = e^{i(k \cdot \omega)t} (hD + i(k \cdot \omega)h)^m z(t),$$

which yields $f(hD)e^{i(k \cdot \omega)t} z(t) = e^{i(k \cdot \omega)t} f(hD + i(k \cdot \omega)h)z(t)$, where

$$f(hD + i(k \cdot \omega)h)z(t) = \sum_{m=0}^{\infty} \frac{f^{(m)}(i(k \cdot \omega)h)}{m!} h^m z^{(m)}(t).$$

Furthermore, we have the following proposition of the operator.

**Proposition 1** The Taylor expansions of $\mathcal{L}(hD)$ and $\mathcal{L}(hD + i(k \cdot \omega)t)$ are

$$\mathcal{L}(hD) = 4 \sin^2(h\Omega/2) - I(ihD)^2 + \ldots,$$

$$\mathcal{L}(hD + i(k \cdot \omega)h) = (2 \cos((k \cdot \omega)h)I - 2 \cos(h\Omega)) + 2 \sin((k \cdot \omega)h)I(ihD)$$

$$- \cos((k \cdot \omega)h)I(ihD)^2 + \ldots.$$ 

3 **Modulated Fourier expansion of the integrators**

Before presenting the analysis of long-time conservation, we make the following assumptions. The first four assumptions have been considered in \cite{3}.

**Assumption 1** • The initial values are assumed to satisfy

$$\frac{1}{2} \|p^0\|^2 + \frac{1}{2} \|\Omega q^0\|^2 \leq E.$$  

• It is assumed that the numerical solution $Q^{n+c_1}$ stays in a compact set on which the potential $U$ is smooth.
A lower bound is posed for the stepsize $h/\epsilon \geq c_0 > 0$.

Assume that the following numerical non-resonance condition holds

$$|\sin(\frac{h}{2\epsilon}(k \cdot \lambda))| \geq c\sqrt{h} \quad \text{for} \quad k \in \mathbb{Z}^l \setminus \mathcal{M} \quad \text{with} \quad |k| \leq N$$

for some $N \geq 2$ and $c > 0$. In this paper, the $N'$ given in (7) is defined for this $N$.

The ERKN integrators are required to satisfy the symmetry conditions (6). Moreover, it is assumed that

$$|b_1(h\omega_j)| \leq C_2|sinc(h\omega_j/2)|,$$

for $j = 1, \ldots, l$.

\textbf{Remark 1} It is clear that we consider the numerical non-resonance condition (8) in the analysis of this paper, which is the same as that in [7]. We also noted that the long-term analysis of some integrators for oscillatory systems under minimal non-resonance conditions has recently been presented in [4]. The long-time analysis of ERKN integrators under minimal non-resonance conditions will be our next work in the near future.

We will establish a modulated Fourier expansion for the ERKN integrators by the following theorem. It is the multi-frequency version of [24]. Its proof follows the lines of the proof of the corresponding theorem given in [24] but with rather obvious adaptations. In the proof of this theorem, we just briefly highlight the main differences and ignore the same derivations for brevity.

\textbf{Theorem 4} Suppose that Assumption (4) is true. The ERKN integrator (5) admits the expansions

$$q^n = \zeta(t) + \sum_{k \in N^*} e^{i(k \cdot \omega)t} \zeta^k(t) + R_{h,N}(t),$$

$$p^n = \eta(t) + \sum_{k \in N^*} e^{i(k \cdot \omega)t} \eta^k(t) + S_{h,N}(t),$$

for $0 \leq t = nh \leq T$. The remainder terms are bounded by

$$R_{h,N}(t) = \mathcal{O}(th^{N-1}), \quad S_{h,N}(t) = \mathcal{O}(th^{N-1}),$$

and the coefficient functions as well as all their derivatives are bounded by

$$\zeta_0(t) = \mathcal{O}(1), \quad \eta_0(t) = \mathcal{O}(1),$$

$$\zeta_j(t) = \mathcal{O}\left(\frac{h^2 b_1(h\omega_j)}{\sin^2(\frac{2\omega_j}{h})}\right) = \mathcal{O}(h), \quad \eta_j(t) = \mathcal{O}\left(\frac{h^2 b_1(h\omega_j)}{\sin^2(\frac{2\omega_j}{h})}\right) = \mathcal{O}(h),$$

$$\zeta_{\pm}^{(j)}(t) = \mathcal{O}\left(\frac{h}{\sin(\frac{2\omega_j}{h})}\right) = \mathcal{O}(h^{3/2}), \quad \eta_{\pm}^{(j)}(t) = \mathcal{O}\left(\frac{h}{\sin(\frac{2\omega_j}{h})}\right) = \mathcal{O}(h^{3/2}),$$

$$\zeta_{\pm}^{(j)}(t) = \mathcal{O}(\epsilon), \quad \eta_{\pm}^{(j)}(t) = \mathcal{O}(\epsilon),$$

$$\zeta^k_j(t) = \mathcal{O}(he^{[k]}), \quad \eta^k_j(t) = \mathcal{O}(he^{[k]}),$$

$$\zeta^k_j(t) = \mathcal{O}(he^{[k]}b_1(h\omega_j)) = \mathcal{O}(he^{[k]}), \quad \eta^k_j(t) = \mathcal{O}(he^{[k]}b_1(h\omega_j)) = \mathcal{O}(he^{[k]}),$$

for $j = 1, \ldots, l$. Moreover, we have $\zeta^{-k} = \overline{\zeta^k}$ and $\eta^{-k} = \overline{\eta^k}$. The constants symbolised by the notation are independent of $h$ and $\omega$, but depend on $E$, $N$, $c_0$ and $T$. 

\[\text{Remark 1}\] It is clear that we consider the numerical non-resonance condition (8) in the analysis of this paper, which is the same as that in [7]. We also noted that the long-term analysis of some integrators for oscillatory systems under minimal non-resonance conditions has recently been presented in [4]. The long-time analysis of ERKN integrators under minimal non-resonance conditions will be our next work in the near future.

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$$\zeta_{\pm}^{(j)}(t) = \mathcal{O}\left(\frac{h}{\sin(\frac{2\omega_j}{h})}\right) = \mathcal{O}(h^{3/2}), \quad \eta_{\pm}^{(j)}(t) = \mathcal{O}\left(\frac{h}{\sin(\frac{2\omega_j}{h})}\right) = \mathcal{O}(h^{3/2}),$$

$$\zeta_{\pm}^{(j)}(t) = \mathcal{O}(\epsilon), \quad \eta_{\pm}^{(j)}(t) = \mathcal{O}(\epsilon),$$

$$\zeta^k_j(t) = \mathcal{O}(he^{[k]}), \quad \eta^k_j(t) = \mathcal{O}(he^{[k]}),$$

$$\zeta^k_j(t) = \mathcal{O}(he^{[k]}b_1(h\omega_j)) = \mathcal{O}(he^{[k]}), \quad \eta^k_j(t) = \mathcal{O}(he^{[k]}b_1(h\omega_j)) = \mathcal{O}(he^{[k]}),$$

for $j = 1, \ldots, l$. Moreover, we have $\zeta^{-k} = \overline{\zeta^k}$ and $\eta^{-k} = \overline{\eta^k}$. The constants symbolised by the notation are independent of $h$ and $\omega$, but depend on $E$, $N$, $c_0$ and $T$. 

\[\text{Remark 1}\] It is clear that we consider the numerical non-resonance condition (8) in the analysis of this paper, which is the same as that in [7]. We also noted that the long-term analysis of some integrators for oscillatory systems under minimal non-resonance conditions has recently been presented in [4]. The long-time analysis of ERKN integrators under minimal non-resonance conditions will be our next work in the near future.
Proof. We will prove that there exist two functions

\[ q_h(t) = \zeta(t) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t} \zeta^k(t), \quad p_h(t) = \eta(t) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t} \eta^k(t) \]

(11)

with smooth coefficients \( \zeta, \zeta^k, \eta, \eta^k \), such that, for \( t = nh \),

\[ q^n = q_h(t) + \mathcal{O}(h^N), \quad p^n = p_h(t) + \mathcal{O}(h^N). \]

Construction of the coefficients functions.

• For the first term of (11), we look for the function

\[ q^{n+\frac{1}{2}} := \tilde{q}_h(t + \frac{h}{2}) = \xi(t + \frac{h}{2}) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t} \xi^k(t + \frac{h}{2}) \]

(12)

for \( Q^{n+\frac{1}{2}} \) in the numerical integrator (4). Inserting (11) and (12) into the first term of (4) and comparing the coefficients of \( e^{i(k\omega)t} \), one gets

\[ \xi(t + \frac{h}{2}) = \cos\left(\frac{1}{2} h \Omega \right) \zeta(t) + \frac{1}{2} h \text{sinc}\left(\frac{1}{2} h \Omega \right) \eta(t), \]

\[ \xi^k(t + \frac{h}{2}) = \cos\left(\frac{1}{2} h \Omega \right) \zeta^k(t) + \frac{1}{2} h \text{sinc}\left(\frac{1}{2} h \Omega \right) \eta^k(t). \]

• For the second term of (4), by the symmetry of the integrator, we obtain

\[ q^{n+1} - 2 \cos(h\Omega) q^n + q^{n-1} = h^2 \tilde{b}_1(h\Omega) \left[ g(q^{n+\frac{1}{2}}) + g(q^{n-\frac{1}{2}}) \right], \]

(13)

where \( q^{n-\frac{1}{2}} \) is defined by \( q^{n-\frac{1}{2}} := \tilde{q}_h(t - \frac{h}{2}) = \xi(t - \frac{h}{2}) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t} \xi^k(t - \frac{h}{2}) \) with

\[ \xi(t - \frac{h}{2}) = \cos\left(\frac{1}{2} h \Omega \right) \zeta(t) - \frac{1}{2} h \text{sinc}\left(\frac{1}{2} h \Omega \right) \eta(t), \]

\[ \xi^k(t - \frac{h}{2}) = \cos\left(\frac{1}{2} h \Omega \right) \zeta^k(t) - \frac{1}{2} h \text{sinc}\left(\frac{1}{2} h \Omega \right) \eta^k(t). \]

Inserting the expansions into (13), we obtain

\[ q_h(t + h) - 2 \cos(h\Omega) q_h(t) + q_h(t - h) = h^2 \tilde{b}_1(h\Omega) \left[ g(\tilde{q}_h(t + \frac{h}{2})) + g(\tilde{q}_h(t - \frac{h}{2})) \right]. \]

By the operator \( \mathcal{L}(hD) \) and the Taylor series, we can rewrite the above formula as

\[ \mathcal{L}(hD)q_h(t) = h^2 \tilde{b}_1(h\Omega) \left[ g(\tilde{q}_h(t + \frac{h}{2})) + g(\tilde{q}_h(t - \frac{h}{2})) \right] \]

\[ = h^2 \tilde{b}_1(h\Omega) \left[ g(\xi(t + \frac{h}{2}) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t} \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))^\alpha \right] \]

\[ + g(\xi(t - \frac{h}{2}) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t} \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))^\alpha \right] \]

\[ \left[ g(\tilde{q}_h(t + \frac{h}{2})) + g(\tilde{q}_h(t - \frac{h}{2})) \right]. \]
where the sums are over all \( m \geq 1 \) and over multi-indices \( \alpha = (\alpha_1, \ldots, \alpha_m) \) with \( \alpha_j \in \mathbb{N}^* \), and the relation \( s(\alpha) \sim k \) means \( s(\alpha) - k \in \mathcal{M} \). Here, an abbreviation for the \( m \)-tuple \( (\xi^{\alpha_1}(t), \ldots, \xi^{\alpha_m}(t)) \) is denoted by \( (\xi(t))^\alpha \).

Inserting the ansatz \((11)\) and comparing the coefficients of \( e^{i(k \cdot \omega)t} \) yields

\[
\mathcal{L}(hD)\zeta(t) = h^2 \bar{b}_1(h\Omega) \left[ g(\xi(t + \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right]
+ g(\xi(t - \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \right],
\]

\[
\mathcal{L}(hD + i(k \cdot \omega)h)\zeta(t) = h^2 \bar{b}_1(h\Omega) \left[ \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right]
+ g(\xi(t - \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \right].
\]

According to the results of \( \mathcal{L}(hD) \) and \( \mathcal{L}(hD + i(k \cdot \omega)h) \) given in Proposition \([1]\) the dominating terms of \( \mathcal{L}(hD)\zeta_0(t) \) and \( \mathcal{L}(hD)\zeta_j(t) \) are \( h^2 D^2 \zeta_0(t) \) and \( 4 \sin^2(h\omega_j/2)\zeta_j(t) \), respectively. Thus, we obtain

\[
\zeta_0(t) = \frac{h^2 \bar{b}_1(0)}{h^2} \left[ g(\xi(t + \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right]
+ g(\xi(t - \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \right],
\]

\[
\zeta_j(t) = \frac{h^2 \bar{b}_1(h\omega_j)}{4 \sin^2(h\omega_j)} \left[ g(\xi(t + \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right]
+ g(\xi(t - \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \right], j = 1, \ldots, l.
\]

Similarly, the dominating terms of \( \mathcal{L}(hD + i((k \cdot \omega)h)\zeta_j(t) \) for all \( k \in \mathbb{N}^* \) are \((2 - 2 \cos((k \cdot \omega)h))\zeta_j^j(t) \), and the dominating terms of \( \mathcal{L}(hD + i((k \cdot \omega)h)\zeta_j^\pm(t) \) for \( j = 1, \ldots, l \) are \( 2 \sin(\pm(j) \cdot \omega)h)) I(ihD)\zeta_j^\pm(t) \). We also get the dominating terms of \( \mathcal{L}(hD + i(k \cdot \omega)h)\zeta_k^j(t) \) for \( k \neq \pm(j) \):
\[
(2 \cos((k \cdot \omega)h) - 2 \cos(h\omega_j)) \zeta_j^k(t).
\]

Thus, we have
\[
\zeta_0^k(t) = \frac{h^2 b_1(0)}{2 - 2 \cos((k \cdot \omega)h)} \left( \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right.
\]
\[
+ \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \biggr)\biggr],
\]
\[
\zeta_j^k(t) = \frac{h^2 b_1(h\omega_j)}{2 \sin(\pm \omega_j h)} \left( \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right.
\]
\[
+ \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \biggr)\biggr],
\]
\[
\zeta_{j}^{\pm}(t) = \frac{h^2 b_1(h\omega_j)}{2 \sin(\pm \omega_j h)} \left( \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right.
\]
\[
+ \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \biggr)\biggr].
\]

- For the third term of (14), one arrives at
\[
p_h(t + h) - 2 \cos(h\omega_j)p_h(t) + p_n(t - h) = hb_1(h\Omega) [g(\xi(t + \frac{h}{2})) - g(\xi(t - \frac{h}{2}))].
\]

With regard to the coefficient functions \(\eta^k(t)\), it is true that
\[
\eta_0(t) = \frac{h b_1(0)}{h^2} \left( g(\xi(t + \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right.
\]
\[
- g(\xi(t - \frac{h}{2})) - \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \biggr)\biggr],
\]
\[
\eta_j(t) = \frac{h b_1(h\omega_j)}{4 \sin^2(\frac{h}{2} \omega_j)} \left( g(\xi(t + \frac{h}{2})) + \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right.
\]
\[
- g(\xi(t - \frac{h}{2})) - \sum_{s(\alpha) \sim 0} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \biggr)\biggr],
\]
\[
\eta_{j}^{\pm}(t) = \frac{h b_1(h\omega_j)}{2 - 2 \cos((k \cdot \omega)h)} \left( \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right.
\]
\[
- \sum_{s(\alpha) \sim k} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \biggr)\biggr].
\]
Furthermore, we note that it holds that

\[ \frac{\eta_j^\pm(t)}{2 \sin(\pm \omega_j h)} \left( \sum_{m=0}^{\infty} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right. \]

\[- \sum_{m=0}^{\infty} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \left. \right)_j, \]

\[ \eta_j^k(t) = \frac{\hbar b_1(h \omega_j)}{(2 \cos((k \cdot \omega) h) - 2 \cos(h \omega_j))} \left( \sum_{m=0}^{\infty} \frac{1}{m!} g^{(m)}(\xi(t + \frac{h}{2}))(\xi(t + \frac{h}{2}))^\alpha \right. \]

\[- \sum_{m=0}^{\infty} \frac{1}{m!} g^{(m)}(\xi(t - \frac{h}{2}))(\xi(t - \frac{h}{2}))^\alpha \left. \right)_j. \]

We now obtain the ansatz of all the modulated Fourier functions. Since the series in the ansatz usually diverge, in this paper we truncate them after the \( \mathcal{O}(h^{N+1}) \) terms (see [10, 13]).

**Initial values.** It follows from the conditions \( p_h(0) = p^0 \) and \( q_h(0) = q^0 \) that

\[ p^0 = \eta(0) + \sum_{k \in \mathbb{N}^\ast} \eta_k^k(0) + \mathcal{O}(h^N), \quad q^0 = \zeta(0) + \sum_{k \in \mathbb{N}^\ast} \zeta_k(0) + \mathcal{O}(h^N). \]

This implies

\[ p^0_0 = \eta_0(0) + \mathcal{O}(h), \quad q^0_0 = \zeta_0(0) + \mathcal{O}(h), \quad (16) \]

and

\[ p^0_j = \eta_j(0) + \eta_j^\pm(0) + \mathcal{O}(h \epsilon), \quad q^0_j = \zeta_j(0) + \zeta_j^\pm(0) + \mathcal{O}(h \epsilon), \]

which lead to

\[ 2 \Re(\eta_j^j(0)) = p^0_j - \eta_j(0) + \mathcal{O}(h \epsilon), \quad 2 \Re(\zeta_j(0)) = q^0_j - \zeta_j(0) + \mathcal{O}(h \epsilon). \quad (17) \]

Furthermore, we note that it holds that \( p_h(h) = p^1 \) and \( q_h(h) = q^1 \). Using the integrator \(|14|\), we have

\[ q^1 - q^0 = \hbar p^0 + h^2 \tilde{b}_1(0)(g(q^0_\pm))_0, \quad p^1_0 - p^0_0 = \hbar b_1(0)(g(q^0_\pm))_0. \]

Hence, we arrive at

\[ \dot{\zeta}_0(0) = \eta_0(0) + \hbar \tilde{b}_1(0)(g(q^0_\pm))_0 + \mathcal{O}(1), \quad \eta_0(0) = \tilde{b}_1(0)(g(q^0_\pm))_0 + \mathcal{O}(1). \quad (18) \]

The formulae \(|10|\) and \(|18|\) yield the initial values \( \zeta_0(0), \zeta_0(0), \eta_0(0), \eta_0(0) \). Therefore,

\[ \zeta_0(t) = \mathcal{O}(1), \quad \eta_0(t) = \mathcal{O}(1). \]

Considering again the integrator \(|4|\) implies

\[ q^1_j = \cos(h \Omega) q^0 = h \text{sinc}(h \Omega)p^0 + h^2 \tilde{b}_1(h \Omega)g(q^0_\pm). \]

On the other hand, a calculation gives

\[ q^1_j - \cos(h \omega_j) q^0_j = q_j(h) - \cos(h \omega_j)q_j(0) = \zeta_j(h) + \sum_{k \in \mathbb{N}^\ast} e^{i k \omega h} \zeta_j^k(h) \]

\[- \cos(h \omega_j) \left( \zeta_j(0) + \sum_{k \in \mathbb{N}^\ast} \zeta_j^k(0) \right) = \zeta_j(h) + e^{i \omega h} \zeta_j(0) + e^{-i \omega h} \zeta_j(0) \quad (19) \]

\[- \cos(h \omega_j) \left( \zeta_j(0) + \zeta_j^j(0) + \zeta_j^{-j}(0) \right) + \mathcal{O}(h \epsilon), \]
which leads to
\[ q_j^1 - \cos(h\omega_j)q_j^0 = (1 - \cos(h\omega_j))\zeta_j(0) + i\sin(h\omega_j)(\zeta_j^{(j)}(0) - \zeta_j^{- (j)}(0)) + O(h^2) + O(h\epsilon) \]
by expanding the functions \( \zeta_j(h), \zeta_j^{(j)}(h) \) and \( \zeta_j^{- (j)}(h) \) at \( h = 0 \). From the fact that \( 1 - \cos(h\omega_j) = \frac{1}{2}h^2\omega_j^2\text{sinc}^2(\omega_j/2) \), it follows that
\[ (1 - \cos(h\omega_j))\zeta_j(0) = \frac{1}{2}h^2\omega_j^2\text{sinc}^2(h\omega_j/2)\zeta_j(0) = 2\sin^2(h\omega_j/2)\zeta_j(0). \]

In the light of the second formula of (14), we get another expression of the above result
\[ (1 - \cos(h\omega_j))\zeta_j(0) = \frac{1}{2}h^2\omega_j^2\text{sinc}^2(h\omega_j/2)\zeta_j(0) = 2\sin^2(h\omega_j/2)\zeta_j(0). \]

Then (19) has the following form
\[
i\sin(h\omega_j)(\zeta_j^{(j)}(0) - \zeta_j^{- (j)}(0)) = h\text{sinc}(h\omega_j)p_j^0 + h^2\hat{b}_1(h\omega_j)(g(q_j^0))_j + g(\xi(-\frac{h}{2})) + \sum_{s(\alpha)\sim 0} g^{(m)}(\xi(\frac{h}{2}))\alpha \]
\[ + \sum_{s(\alpha)\sim 0} g^{(m)}(\xi(-\frac{h}{2}))\alpha \]
which yields
\[ 2\text{Im}(\zeta_j^{(j)}(0)) = \omega^{-1}p_j^0 + O(\epsilon). \quad (20) \]
Similarly, it can be obtained that
\[ 2\text{Im}(\eta_j^{(j)}(0)) = -\omega_jq_j^0 + O(\epsilon). \quad (21) \]
The conditions (17), (20) and (21) present the desired initial values \( \zeta_j^{\pm (j)}(0) \) and \( \eta_j^{\pm (j)}(0) \). This analysis implies
\[ \zeta_j^{\pm (j)}(t) = O(\epsilon), \quad \eta_j^{\pm (j)}(t) = O(1). \]

**Bounds.** Based on the ansatz, the initial values and Assumption [1] it is easy to get the bounds of modulated Fourier functions.

**Defect.** The defect (9) can be obtained by using the Lipschitz continuous of the nonlinearity \( g \), a discrete Gronwall lemma and the standard convergence estimates (see [10], [24] and Chap. XIII of [14] for more details).

We then complete the proof of this theorem. □
4 Almost-invariants of the integrators

In this section, we show that the ERKN integrators have two almost-invariants.

4.1 The first almost-invariant

Let \(\mathbf{\zeta} = (\zeta^k)_{k \in \mathbb{N}}\) and \(\mathbf{\eta} = (\eta^k)_{k \in \mathbb{N}}\). The first almost-invariant is given as follows.

**Theorem 5** Under the conditions of Theorem 4, there exists a function \(\mathcal{R}^k[\mathbf{\zeta}, \mathbf{\eta}]\) such that

\[
\mathcal{R}^k[\mathbf{\zeta}, \mathbf{\eta}](t) = \mathcal{R}^k[\mathbf{\zeta}, \mathbf{\eta}](0) + \mathcal{O}(th^N)
\]

for \(0 \leq t \leq T\). Moreover, \(\mathcal{R}\) can be expressed in

\[
\mathcal{R}^k[\mathbf{\zeta}, \mathbf{\eta}] = \sum_{j=1}^{L} \frac{2\omega_j^2 \text{sinc}(\omega_j)}{2b_1(\omega_j)} \left( \frac{1}{\omega_j} \right)^{\mathcal{R}_j} \mathbf{\zeta}^j
\]

\[
+ \sum_{j=1}^{L} 2h^2 \omega_j^2 \text{sinc}(\omega_j) \left( \frac{1}{\omega_j} \right)^{\mathcal{R}_j} \mathbf{\eta}^j + U(\Omega(t)) + \mathcal{O}(h).
\]

**Proof.** It follows from the proof of Theorem 4 that

\[
\begin{align*}
\dot{q}_h(t + \frac{h}{2}) &= \cos\left(\frac{1}{2}h\Omega\right)q_h(t) + \frac{1}{2}h\text{sinc}\left(\frac{1}{2}h\Omega\right)p_h(t), \\
\dot{q}_h(t - \frac{h}{2}) &= \cos\left(\frac{1}{2}h\Omega\right)q_h(t) - \frac{1}{2}h\text{sinc}\left(\frac{1}{2}h\Omega\right)p_h(t), \\
\mathcal{L}(hD)q_h(t) &= h^2b_1(h\Omega)(g(q_h(t + \frac{h}{2})) + g(q_h(t - \frac{h}{2}))) + \mathcal{O}(h^N), \\
\mathcal{L}(hD)p_h(t) &= hb_1(h\Omega)(g(q_h(t + \frac{h}{2})) - g(q_h(t - \frac{h}{2}))) + \mathcal{O}(h^N),
\end{align*}
\]

where the following denotations are used:

\[
q_h(t) = \sum_{k \in \mathbb{N}} q^k(t), \quad p_h(t) = \sum_{k \in \mathbb{N}} p^k(t), \quad \tilde{q}_h(t \pm \frac{h}{2}) = \sum_{k \in \mathbb{N}} \tilde{q}_h^k(t \pm \frac{h}{2})
\]

with

\[
q^k_h(t) = e^{i(k\omega)t}\zeta^k(t), \quad p^k_h(t) = e^{i(k\omega)t}\eta^k(t), \quad \tilde{q}_h^k(t \pm \frac{h}{2}) = e^{i(k\omega)t}\xi^k(t \pm \frac{h}{2}).
\]

This yields

\[
\begin{align*}
\tilde{q}_h^k(t + \frac{h}{2}) &= \cos\left(\frac{1}{2}h\Omega\right)q^k_h(t) + \frac{1}{2}h\text{sinc}\left(\frac{1}{2}h\Omega\right)p^k_h(t), \\
\tilde{q}_h^k(t - \frac{h}{2}) &= \cos\left(\frac{1}{2}h\Omega\right)q^k_h(t) - \frac{1}{2}h\text{sinc}\left(\frac{1}{2}h\Omega\right)p^k_h(t), \\
\mathcal{L}(hD)q^k_h(t) &= -h^2b_1(h\Omega)\left(\nabla_{q^k} U(\tilde{q}(t + \frac{h}{2})) + \nabla_{q^k} U(\tilde{q}(t - \frac{h}{2}))\right) + \mathcal{O}(h^N), \\
\mathcal{L}(hD)p^k_h(t) &= -hb_1(h\Omega)\left(\nabla_{q^k} U(\tilde{q}(t + \frac{h}{2})) - \nabla_{q^k} U(\tilde{q}(t - \frac{h}{2}))\right) + \mathcal{O}(h^N),
\end{align*}
\]

\[\tag{22}\]
where $\mathcal{U}(\tilde{q})$ is defined as

$$\mathcal{U}(\tilde{q}(t \pm \frac{h}{2})) = U(\tilde{q}_h(t \pm \frac{h}{2})) + \sum_{s(\alpha) = 0}^{1} \frac{1}{m!} U^{(m)}(\tilde{q}_h(t \pm \frac{h}{2}))(\tilde{q}_h(t \pm \frac{h}{2}))$$

with $\tilde{q}(t \pm \frac{h}{2}) = (\tilde{q}_h^k(t \pm \frac{h}{2}))_{k \in N}$. Hence, the following result is obtained

$$\frac{1}{2} \frac{d}{dt} \left( \mathcal{U}(\tilde{q}(t + \frac{h}{2})) + \mathcal{U}(\tilde{q}(t - \frac{h}{2})) \right) = \frac{1}{2} \sum_{k \in N} \left[ (\tilde{q}_h^k(t))^T \nabla_{q^k \to q} \mathcal{U}(\tilde{q}(t + \frac{h}{2})) + (\tilde{q}_h^k(t - \frac{h}{2}))^T \nabla_{q^k \to q} \mathcal{U}(\tilde{q}(t - \frac{h}{2})) \right]

= \frac{1}{2} \sum_{k \in N} \left[ \left( \cos(\frac{1}{2}h\Omega)\tilde{q}_h^{-k}(t) + \frac{1}{2} h \text{sinc}(\frac{1}{2}h\Omega)\tilde{p}_h^{-k}(t) \right)^T \nabla_{q^k \to q} \mathcal{U}(\tilde{q}(t + \frac{h}{2})) + \left( \cos(\frac{1}{2}h\Omega)\tilde{q}_h^{-k}(t) - \frac{1}{2} h \text{sinc}(\frac{1}{2}h\Omega)\tilde{p}_h^{-k}(t) \right)^T \nabla_{q^{-k} \to q} \mathcal{U}(\tilde{q}(t - \frac{h}{2})) \right].$$

By the last two equations of [22], this formula becomes

$$\frac{1}{2} \frac{d}{dt} \left( \mathcal{U}(\tilde{q}(t + \frac{h}{2})) + \mathcal{U}(\tilde{q}(t - \frac{h}{2})) \right) = \frac{1}{2} \sum_{k \in N} \left[ (\tilde{q}_h^{-k}(t))^T \cos(\frac{1}{2}h\Omega)(-h^2b_1(h\Omega))^{-1} L(hD)\tilde{q}_h^{-k}(t) + \frac{1}{2} h \text{sinc}(\frac{1}{2}h\Omega)(-hb_1(h\Omega))^{-1} L(hD)\tilde{p}_h^{-k}(t) \right] + \mathcal{O}(h^N).$$

Rewrite it in the quantities $\zeta_h^k(t)$, $\eta_h^k(t)$

$$\frac{1}{2} \frac{d}{dt} \left( \mathcal{U}(\xi_h(t + \frac{h}{2})) + \mathcal{U}(\xi_h(t - \frac{h}{2})) \right) = \frac{1}{2} \sum_{k \in N} \left[ (\zeta_h^{-k}(t) - i(k \cdot \omega)\zeta_h^{-k}(t))^T \cos(\frac{1}{2}h\Omega)(h^2b_1(h\Omega))^{-1} L(hD + i(k \cdot \omega)h)\zeta_h^{-k}(t) + \frac{1}{2} h \text{sinc}(\frac{1}{2}h\Omega)(hb_1(h\Omega))^{-1} L(hD + i(k \cdot \omega)h)\eta_h^{-k}(t) \right] + \mathcal{O}(h^N),$$

$$\frac{1}{2} h \text{sinc}(\frac{1}{2}h\Omega)(hb_1(h\Omega))^{-1} L(hD + i(k \cdot \omega)h)\eta_h^{-k}(t) = \mathcal{O}(h^N),$$

where $\xi_h(t \pm \frac{h}{2}) = (\xi_h^k(t \pm \frac{h}{2}))_{k \in N}$.

With the analysis given in Section XIII of [14], it is known that the left-hand side of [24] is a total derivative and its construction is given as follows. According to the “magic formulas” on p.
508 of \[14\] and the bounds of Theorem 4, we have

\[
\mathcal{H}[\zeta, \eta] = \frac{1}{4b_1} \zeta_0^2 + \sum_{j=1}^{l} 2\omega_j^2 \text{sinc}(h\omega_j) \left( \frac{\cos(\frac{1}{2}h\omega_j)}{2b_1(h\omega_j)} \right) \zeta_j^{(j)} \eta_j^{(j)} \\
+ \frac{1}{l} \left( U(\xi(t + \frac{1}{2}h)) + U(\xi(t - \frac{1}{2}h)) \right) + \mathcal{O}(h)
\]

\[
= \frac{1}{4b_1} \eta_{h,1}^2 + \sum_{j=1}^{l} 2\omega_j^2 \text{sinc}(h\omega_j) \left( \frac{\cos(\frac{1}{2}h\omega_j)}{2b_1(h\omega_j)} \right) \zeta_j^{(j)} \eta_j^{(j)} \\
+ \frac{1}{l} U(\xi(t)) + \mathcal{O}(h),
\]

where the fact that \( \dot{\zeta}_{h,1} = \eta_{h,1} + \mathcal{O}(h) \) is used. The proof is complete.

\[\square\]

4.2 The second almost-invariant

For \( \mu \in \mathbb{R}^l \) and \( \bar{q}(t \pm \frac{1}{2}h) = (\bar{q}_h^k(t \pm \frac{1}{2}h))_{k \in \mathbb{N}} \), let

\[ S_\mu(\tau)\bar{q}(t \pm \frac{1}{2}h) = (e^{i(k\cdot\mu)\tau}\bar{q}_h^k(t \pm \frac{1}{2}h))_{k \in \mathbb{N}}, \quad \tau \in \mathbb{R}. \]

Inserting \( S_\mu(\tau)\bar{q}(t \pm \frac{1}{2}h) \) into (23) yields

\[
U(S_\mu(\tau)\bar{q}(t \pm \frac{1}{2}h)) = U(\bar{q}_h(t \pm \frac{1}{2}h)) + \sum_{s(\alpha) \sim 0} \frac{e^{i(s(\alpha)\cdot\mu)\tau}}{m!} U^{(m)}(\bar{q}_h(t \pm \frac{1}{2}h))
\]

\[ (e^{i(\alpha_1\cdot\mu)\tau}\bar{q}_h^1(t \pm \frac{1}{2}h), \ldots, e^{i(\alpha_m\cdot\mu)\tau}\bar{q}_h^m(t \pm \frac{1}{2}h)). \]

If \( \mu \perp \mathcal{M} \), then it follows from the relation \( s(\alpha) \sim 0 \) that \( s(\alpha) \cdot \mu = 0 \). This means that the expression (25) is independent of \( \tau \). Therefore, we have

\[
0 = \frac{d}{d\tau} \big|_{\tau=0} U(S_\mu(\tau)\bar{q}(t \pm \frac{1}{2}h)) = \sum_{k \in \mathbb{N}} i(k \cdot \mu)(\bar{q}_h^k(t \pm \frac{1}{2}h))^T \nabla_{\bar{q}} U(\bar{q}(t \pm \frac{1}{2}h)).
\]

If \( \mu \) is not orthogonal to \( \mathcal{M} \), this means that some terms in the sum of (24) depend on \( \tau \). For these terms with \( s(\alpha) \in \mathcal{M} \) and \( s(\alpha) \cdot \mu \not= 0 \), we have \( |s(\alpha)| \geq M = \min\{|k| : 0 \neq k \in \mathcal{M}\} \) and if \( \mu \perp \mathcal{M}_N := \{k \in \mathcal{M} : |k| \leq N\} \), then \( |s(\alpha)| \geq N + 1 \). This result as well as the bounds (10) then implies

\[
\sum_{k \in \mathbb{N}} i(k \cdot \mu)(\bar{q}_h^k(t \pm \frac{1}{2}h))^T \nabla_{\bar{q}} U(\bar{q}(t \pm \frac{1}{2}h)) = \begin{cases} \mathcal{O}(\epsilon^M), & \text{for arbitrary } \mu, \\ \mathcal{O}(\epsilon^{N+1}), & \text{for } \mu \perp \mathcal{M}_N. \end{cases}
\]
Therefore, we obtain

\[
O(h^N) + O(e^{M-1}) = \frac{i}{\epsilon} \left[ \frac{d}{dt} \left\{ \tau \to U(S_\mu(\tau) \tilde{q}(t + \frac{1}{2} h)) + U(S_\mu(\tau) \tilde{q}(t - \frac{1}{2} h)) \right\} \right]
\]

\[
= \frac{1}{\epsilon} \sum_{k \in \mathbb{N}} \left( \langle \tilde{q}_k(t + \frac{1}{2} h) \rangle \right)^T \nabla \tilde{q} U(\tilde{q}(t + \frac{1}{2} h)) + \langle \tilde{q}_k(t - \frac{1}{2} h) \rangle^T \nabla \tilde{q} U(\tilde{q}(t - \frac{1}{2} h)) \right),
\]

and the \(O(e^{M-1})\) term can be removed for \(\mu \perp \mathcal{N}\).

In a similar way to the proof of Theorem 5, the above analysis yields the following second almost-invariant.

**Theorem 6** Under the conditions of Theorem 5 there exists a function \(\tilde{I}_\mu[\vec{\zeta}, \vec{\eta}]\) such that

\[
\tilde{I}_\mu[\tilde{\vec{q}}, \tilde{\vec{p}}](t) = \tilde{I}_\mu[\tilde{\vec{q}}, \tilde{\vec{p}}](0) + O(th^N) + O(t \epsilon^{M-1})
\]

for all \(\mu \in \mathbb{R}^l \) and \(0 \leq t \leq T\). They satisfy

\[
\tilde{I}_\mu[\tilde{\vec{q}}, \tilde{\vec{p}}](t) = \tilde{I}_\mu[\tilde{\vec{q}}, \tilde{\vec{p}}](0) + O(th^N)
\]

for \(\mu \perp \mathcal{N}\) and \(0 \leq t \leq T\). Moreover, \(\tilde{I}\) can be expressed in

\[
\tilde{I}_\mu[\tilde{\vec{q}}, \tilde{\vec{p}}] = \sum_{j=1}^{l} 2 \omega^2 j \text{sinc}(h \omega_j) \left( \frac{\cos(h \omega_j)}{2b_1(h \omega_j)} \frac{\mu_j}{\lambda_j} (\vec{\zeta}_j^{(j)})^T \vec{\zeta}_j \right)
\]

\[
+ \sum_{j=1}^{l} 2h^2 \omega^2 j \text{sinc}(h \omega_j) \left( \frac{\text{sinc}(h \omega_j)}{2b_1(h \omega_j)} \frac{\mu_j}{\lambda_j} (\vec{\eta}_j^{(j)})^T \vec{\eta}_j \right) + O(h).
\]

### 5 Long-time near-conservation of total and oscillatory energy

Based on the previous analysis of this paper and following [6, 24] and Section XIII of [14], it is easy to obtain the following result.

**Theorem 7** Under the conditions of Theorem 6 and the additional condition

\[
\text{sinc}(h \Omega) \left( \frac{\cos(h \Omega)}{2b_1(h \Omega)} + h^2 \Omega^2 \text{sinc}(h \Omega) \frac{1}{2b_1(h \Omega)} \right) = I, \quad (26)
\]

it holds that

\[
\tilde{\mathcal{H}}[\tilde{\vec{q}}, \tilde{\vec{p}}](nh) = H(q_n, p_n) + O(h),
\]

\[
\tilde{I}_{(j)}[\tilde{\vec{q}}, \tilde{\vec{p}}](nh) = I_j(q_n, p_n) + O(h), \quad (27)
\]

where the constants symbolized by \(O\) depend on \(N, T\) and the constants in the assumptions.

**Remark 2** It is noted that the symmetry condition \(\tilde{I}\) and the condition \(26\) determine a symmetric and symplectic ERKN integrator (ERKN3 presented in next section). The appearance of \(26\) is obtained by requiring the almost-invariants \(\tilde{\mathcal{H}}\) and \(\tilde{I}_{(j)}\) to be close to the energies \(H\) and \(I_j\), respectively. The mechanism is not in any obvious way related to symplecticity. The same coincidence happens in the analysis of trigonometric integrators in [17].
The near conservation of $H$ and $I$ over long time intervals is given by the following theorem.

**Theorem 8** Under the conditions of Theorem 7, we have

\[
H(q^n, p^n) = H(q^0, p^0) + O(h),
\]

\[
I_j(q^n, p^n) = I_j(q^0, p^0) + O(h)
\]

for $0 \leq nh \leq h^{-N+1}$ and $j = 1, 2, \ldots, l$. The constants symbolized by $O$ are independent of $n$, $h$, $\Omega$, but depend on $N$, $T$ and the constants in the assumptions.

To be able to treat the ERKN integrators which are symmetric but do not satisfy (26), we consider the modified energies

\[
H^*(q, p) = H(q, p) + \sum_{j=1}^{l} (\sigma(\xi_j) - 1) I_j(q, p)
\]

and

\[
I^*_\mu(q, p) = \sum_{j=1}^{l} \sigma(\xi_j) \frac{\mu}{\lambda_j} I_j(q, p),
\]

where $\sigma$ is defined by

\[
\sigma(\xi_j) := \text{sinc}(\xi_j) \frac{\cos(\frac{1}{2}\xi_j)}{2b_1(\xi_j)} + \xi_j^2 \text{sinc}(\xi_j) \frac{\frac{1}{2}\text{sinc}(\frac{1}{2}\xi_j)}{2b_1(\xi_j)} = \frac{\cos(\frac{1}{2}\xi_j)}{b_1(\xi_j)}.
\]

We then obtain the following result.

**Theorem 9** Under the conditions of Theorem 7 and that $\bar{b}_1 = \frac{1}{2}$, it holds that

\[
\hat{H}[\vec{\zeta}, \vec{\eta}](nh) = H^*(q_n, p_n) + O(h),
\]

\[
\hat{I}_\mu[\vec{\zeta}, \vec{\eta}](nh) = I^*_\mu(q_n, p_n) + O(h),
\]

Moreover, we have

\[
H^*(q^n, p^n) = H^*(q^0, p^0) + O(h),
\]

\[
I^*_\mu(q^n, p^n) = I^*_\mu(q^0, p^0) + O(h)
\]

for $0 \leq nh \leq h^{-N+1}$, $\mu \in \mathbb{R}^l$ and $\mu \perp M_N$. The constants symbolized by $O$ are independent of $n$, $h$, $\Omega$, but depend on $N$, $T$ and the constants in the assumptions.

### 6 Numerical examples

As examples, we present four practical one-stage explicit ERKN integrators whose coefficients are given in Table 1. From Theorem 1, it follows that all these integrators are of order two. According to Theorems 2 and 3, the symmetry and symplecticness for these integrators are shown in Table 1.

In order to illustrate the numerical conservation of energies for these four integrators, a Hamiltonian with $l = 3$, $\lambda = (1, \sqrt{2}, 2)$ is considered (see [6]). It follows from the discussion in [6] that there is the $1:2$ resonance between $\lambda_3$ and $\lambda_3$: $M = \{-2k_3, 0, k_3) : k_3 \in \mathbb{Z}\}$. For this problem,
the dimension of $q_1 = (q_{11}, q_{12})$ is assumed to be 2 and all the other $q_j$ are assumed to be 1. We choose $\epsilon^{-1} = \omega = 70$, the potential

$$U(q) = (0.001q_0 + q_{11} + q_{22} + q_2 + q_3)^4,$$

and

$$q(0) = (1, 0.3\epsilon, 0.8\epsilon, -1.1\epsilon, 0.7\epsilon), \quad p(0) = (-0.75, 0.6, 0.7, -0.9, 0.8)$$

as initial values. For $\lambda = (1, \sqrt{2}, 2)$, we consider

$$\mu = (1, 0, 2) \quad \text{and} \quad \mu = (0, \sqrt{2}, 0)$$

for $I_\mu$ and the corresponding results are

$$I_\mu = I_1 + I_3 \quad \text{and} \quad I_\mu = I_2.$$

The system is integrated in the interval $[0, 10000]$ with $h = 0.01$. First the errors of the total energy $H$ and oscillatory energy $I$ and $I_2$ against $t$ for ERKN3 and the errors of the modified energies $H^*, I^*$, $I^*_2$ for ERKN1 are shown in Fig. 1. Then we present the energies and the modified energies for ERKN 2 and 4 in Figs. 2 and 3, respectively.

From the numerical results, it follows that the non-symmetric ERKN1 can not preserve the energies and the symmetric and symplectic ERKN3 can approximately conserve the energies very well over long times. For the symmetric ERKN 2 and 4 not satisfying the condition (26), they approximately conserve the modified energies better than the original energies.

## 7 Conclusions

This paper studied the long-time behaviour of ERKN integrators for multi-frequency highly oscillatory Hamiltonian systems. The modulated multi-frequency Fourier expansion of ERKN integrators were developed and by which, we showed the long-time numerical energy conservation of the integrators. Our next work will be devoted to the long-time analysis of ERKN integrators for multi-frequency highly oscillatory Hamiltonian systems under minimal non-resonance conditions.
Figure 1: The errors against $t$ for ERKN 1 (up) and 3 (down).

Figure 2: The errors of energies (up) and modified energies (down) against $t$ for ERKN 2.
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