Long-term analysis of exponential integrators for highly oscillatory conservative systems

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Abstract

In this paper, we investigate the long-time near-conservations of energy and kinetic energy by the widely used exponential integrators to highly oscillatory conservative systems. The modulated Fourier expansions of two kinds of exponential integrators have been constructed and the long-time numerical conservations of energy and kinetic energy are obtained by deriving two almost-invariants of the expansions. Practical examples of the methods are given and the theoretical results are confirmed and demonstrated by a numerical experiment.

Keywords: highly oscillatory conservative systems, modulated Fourier expansion, exponential integrators, long-time energy conservation

MSC: 65P10, 65L05

1 Introduction

In this paper, we are concerned with the long-term analysis of implicit exponential integrators for solving the systems of the form

\[ y'(t) = Q \nabla H(y(t)), \quad y(0) = y_0 \in \mathbb{R}^d, \quad t \in [0, T], \]  

where \( Q \) is a \( d \times d \) skew symmetric matrix, and \( H : \mathbb{R}^d \to \mathbb{R} \) is defined by

\[ H(y) = \frac{1}{2} y^\top \left( \frac{1}{\epsilon} M \right) y + V(y). \]  

Here \( \epsilon \) is a small parameter satisfying \( 0 < \epsilon \ll 1 \), \( M \) is a \( d \times d \) symmetric real matrix, and \( V : \mathbb{R}^d \to \mathbb{R} \) is a differentiable function. It is important to note that since \( Q \) is skew symmetric, the system (1) is a conservative system with the first integral \( H \): i.e.,

\[ H(y(t)) = H(y_0) \quad \text{for any} \quad t \in [0, T]. \]

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The kinetic energy of the system (1) is given by
\[
K(y) = \frac{1}{2} y^T \left( \frac{1}{\epsilon} M \right) y.
\]

For brevity, by letting
\[
\Omega = \frac{1}{\epsilon} Q M, \quad g(y(t)) = Q \nabla V(y(t)),
\]
the system (1) can be rewritten as
\[
y'(t) = \Omega y(t) + g(y(t)), \quad y(0) = y_0 \in \mathbb{R}^d.
\]

(3)

It is well known that the exact solution of (1) or (3) can be represented by the variation-of-constants formula
\[
y(t) = e^{t \Omega} y_0 + t \int_0^1 e^{(1-\tau)t \Omega} g(y(\tau t)) d\tau.
\]

(4)

In the analysis of this paper, it is assumed that the matrix \( \Omega \) is symmetric negative definite or skew-Hermitian with eigenvalues of large modulus. Under these conditions, the exponential \( e^{t \Omega} \) enjoys favourable properties such as uniform boundedness, independent of the time step \( t \) (see [19]).

The highly oscillatory system (3) often arises in a wide range of applications such as in engineering, astronomy, mechanics, physics and molecular dynamics (see, e.g. [17, 19, 31, 33, 34]). There are also some semidiscrete PDEs such as semilinear Schrödinger equations fit this form. In recent decades, as an efficient approach to integrating (3), exponential integrators have been widely investigated and developed, and the reader is referred to [1, 2, 4, 14, 18, 20, 23, 21, 27, 29, 30, 32] for example. A systematic survey of exponential integrators is referred to [19]. One important advantage of exponential integrators is that they make well use of the variation-of-constants formula (4), and can performance very well even for highly oscillatory problems.

On the other hand, an important aspect in the numerical simulation of conservative systems is the approximate conservation of the invariants over long times. In order to study the long-time behaviour for numerical methods/differential equations, modulated Fourier expansion was firstly developed in [15]. In the recent two decades, this technique has been used successfully in the long-time analysis for various numerical methods, such as for trigonometric integrators in [6, 7, 17, 28], for an implicit-explicit method in [22, 26], for heterogeneous multiscale methods in [25], and for splitting methods in [11, 13]. So far modulated Fourier expansion has been presented and developed as an important mathematical tool in the long-time analysis (see, e.g. [5, 6, 9, 12, 16]). However, for the well known exponential integrators, the technique of modulated Fourier expansions has only been used in the long-time analysis for cubic Schrödinger equations (see [4]). It is noted that, until now, the long-time analysis of exponential integrators for Hamiltonian ordinary differential equations has not been considered in the literature, which motivates this paper.

With this promise, in this paper, we present the long-time analysis of implicit exponential integrators for solving the highly oscillatory conservative system (1). The technique of modulated Fourier expansions will be used as an important tool in the analysis. This seems to be the first long-time result for exponential integrators of Hamiltonian ordinary differential equations.

We organize the rest of this paper as follows. In Section 2, two kinds of exponential integrators are considered for solving (1) and an illustrative numerical experiment is presented to show the long-time behaviour of these methods. Then in Section 3 we derive the modulated Fourier expansion for the first class of integrators and then obtain the long-time near conservations of energy and kinetic
energy by showing two almost-invariants. The analyses of long time conservations for the second class of exponential integrators are given in Section 4. Section 5 includes the conclusions of this paper.

2 Exponential integrators and numerical experiment

2.1 Two kinds of methods

In order to solve (3) effectively, exponential integrators are considered throughout this paper.

Definition 1 (See [19]). An $s$-stage exponential integrator for solving (3) is given by

$$
\begin{align*}
Y^{n+c_i} &= e^{c_i h\Omega}y^n + h \sum_{j=1}^{s} a_{ij}(h\Omega)g(Y^{n+c_j}), & i = 1, \ldots, s, \\
y^{n+1} &= e^{h\Omega}y^n + h \sum_{i=1}^{s} b_i(h\Omega)g(Y^{n+c_i}),
\end{align*}
$$

where $h$ is a stepsize, $c_i \in [0,1]$ for $i = 1, \ldots, s$ are real constants, and $b_i(h\Omega)$ and $a_{ij}(h\Omega)$ for $i, j = 1, \ldots, s$ are matrix-valued and bounded functions of $h\Omega$. The coefficients of this exponential integrator can be compactly arranged as a Butcher Tableau

$$
\begin{pmatrix}
c_1 & a_{11}(h\Omega) & \cdots & a_{1s}(h\Omega) \\
\vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1}(h\Omega) & \cdots & a_{ss}(h\Omega)
\end{pmatrix}
\begin{pmatrix}
c \\
b^T
\end{pmatrix} =
\begin{pmatrix}
c_1 \\
c_s
\end{pmatrix} + 
\begin{pmatrix}
a_{11}(h\Omega) \\
ap_{s1}(h\Omega)
\end{pmatrix} h\Omega + 
\begin{pmatrix}
a_{1s}(h\Omega) \\
a_{s1}(h\Omega)
\end{pmatrix} h\Omega + 
\begin{pmatrix}
a_{ss}(h\Omega) \\
a_{s1}(h\Omega)
\end{pmatrix} h\Omega.
$$

As the first example, approximating the integral in (4) leads to the following exponential integrator.

Definition 2 An exponential integrator for solving (4) is defined by

$$
y^{n+1} = e^{h\Omega}y^n + \frac{h}{2} \left( g(y^{n+1}) + e^{h\Omega}g(y^n) \right).$$

This integrator is symmetric and can be considered as a two-stage exponential integrator with the following Butcher Tableau

$$
\begin{pmatrix}
0 & 0 & 0 \\
1 & \frac{1}{2} e^{h\Omega} & \frac{1}{2}
\end{pmatrix}
\begin{pmatrix}
b^T
\end{pmatrix} =
\begin{pmatrix}
0 \\
\frac{1}{2} e^{h\Omega} \\
\frac{1}{2}
\end{pmatrix}.
$$

We denote it by EI-T.

Besides this integrator, in this paper, we also consider one-stage implicit exponential integrators, which are given as follows.

Definition 3 An one-stage implicit exponential integrator is defined by

$$
\begin{align*}
Y^{n+c_1} &= e^{c_1 h\Omega}y^n + h a_{11}(h\Omega)g(Y^{n+c_1}), \\
y^{n+1} &= e^{h\Omega}y^n + h b_1(h\Omega)g(Y^{n+c_1}),
\end{align*}
$$

This integrator is denoted by EI-O.
Table 1: Five one-stage implicit exponential integrators.

| Integrators | $c_1$ | $a_{11}(h\Omega)$ | $b_1(h\Omega)$ | Symmetric | Reversible | Symplectic |
|-------------|-------|--------------------|----------------|-----------|-----------|-----------|
| EI-O1       | $\frac{1}{2}$ | $\frac{1}{2}$ | $e^{\frac{1}{2}h\Omega}$ | Yes       | Yes       | Yes       |
| EI-O2       | $\frac{1}{2}$ | $\frac{1}{2}$ | $\varphi_1(h\Omega)$ | Non       | Non       | Non       |
| EI-O3       | $\frac{2}{3}$ | $\frac{1}{2}$ | $e^{\frac{1}{2}h\Omega}$ | Non       | Non       | Yes       |
| EI-O4       | $\frac{1}{2}$ | $\frac{1}{2}b_1(h\Omega/2)$ | $\varphi_1(h\Omega)$ | Yes       | Yes       | Non       |
| EI-O5       | $\frac{1}{2}$ | $\frac{1}{4}$ | $\frac{2}{3}e^{\frac{1}{2}h\Omega}$ | Non       | Non       | Yes       |

Five EI-O integrators are listed in Table 1 and it follows from [5] that EI-O1 and EI-O4 are both symmetric and reversible, and the others are neither symmetric nor reversible. About the symplecticness, the authors in [23] proved that if a Runge–Kutta (RK) method with the coefficients $c_i, \bar{b}_i, \bar{a}_{ij}$ is symplectic, then the exponential integrator of the coefficients

$$a_{ij}(h\Omega) = \bar{a}_{ij}e^{(c_i-c_j)h\Omega}, \quad b_i(h\Omega) = \bar{b}_i e^{(1-c_i)h\Omega}$$  

is symplectic. We note that the integrator EI-T can be written as a two-stage exponential integrator satisfying (8) and with

$$\begin{pmatrix} c & \bar{A} \\ \bar{b}^T \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

This shows that the integrator EI-T is not symplectic by considering that the trapezoidal rule is not symplectic. In the light of the symplecticness condition of one-stage RK method, one gets $b_1 = 2\bar{a}_{11}$. Therefore, a class of one-stage implicit symplectic exponential integrators is given by

$$a_{11}(h\Omega) = \bar{a}_{11}, \quad b_1(h\Omega) = 2\bar{a}_{11} e^{(1-c_1)h\Omega}.$$  

With this result, the properties of symplecticity are shown in Table 1.

2.2 Numerical experiments

As an example, we apply these methods to the following averaged system in wind-induced oscillation

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}' = \frac{1}{\epsilon} \begin{pmatrix} -\zeta & -\lambda \\ \lambda & -\zeta \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} x_1x_2 \\ \frac{1}{2}(x_1^2 - x_2^2) \end{pmatrix},$$

where $\zeta \geq 0$ is a damping factor and $\lambda$ is a detuning parameter. By setting

$$\zeta = r \cos(\theta), \quad \lambda = r \sin(\theta), \quad r \geq 0, \quad \theta = \pi/2,$$

we get...
this system can be transformed into the scheme with

\[
Q = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad M = \frac{1}{\epsilon} \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix}, \quad V = -\frac{1}{2}(x_1^2 + \frac{1}{3}x_1^3) - \frac{1}{2}(x_2^2 + \frac{1}{3}x_1^3).
\]

The energy of this system is given by

\[
H = \frac{1}{2}r(\bar{x}_1^2 + \bar{x}_2^2) - \frac{1}{2}(\bar{x}_1^2 + \frac{1}{3}x_1^3).
\]

We choose \( r = 1, \epsilon = 10^{-4} \) and use the initial values \( \bar{x}_1(0) = 1.1\sqrt{\epsilon}, \; \bar{x}_2(0) = \sqrt{\epsilon} \). This problem is solved in a long interval \([0, 10^6]\) with \( h = 0.5 \). The conservations of the energy and the kinetic energy for different integrators are presented in Figures 1-6.

From these results, it can be observed that EI-T and symplectic EI-O methods conserve the energy and the kinetic energy quite well over a long term. The integrator EI-O2 does not conserve the energy and the magnetic moment as well as the others. For the five EI-O integrators, it seems that the symplectiness condition plays an important role for the long-time conservations. We will explain the good numerical behaviours of EI-T and EI-O satisfying symplectiness condition theoretically by the modulated Fourier expansion of the integrators in the rest of this paper. For the method EI-O4 which does not satisfy symplectiness condition, it has a much better numerical behaviour than we expect. The theoretical reason for this will be further studied in future.

3 Long-time conservation of the method EI-T

In this section, we show the long-time conservations of the method EI-T by modulated Fourier expansion. Our analysis is limited to the case that \( \Omega \) is skew-Hermitian with eigenvalues of large modulus. The analysis for the case that \( \Omega \) is symmetric negative definite can be obtained in a same way.

3.1 Preliminaries

To do this, we first transform the system as follows. For the skew-Hermitian \( \Omega \), there exists a unitary matrix \( P \) and a diagonal matrix \( \Lambda \) such that \( \Omega = P\Lambda P^H \), where

\[
\Lambda = \frac{1}{\epsilon} \text{diag}(-\lambda_1 I_{d_1}, \ldots, -\lambda_1 I_{d_1}, -\lambda_0 I_{d_0}, \lambda_0 I_{d_0}, \lambda_1 I_{d_1}, \ldots, \lambda_l I_{d_l})
\] (10)

with \( \lambda_0 = 0 \) and \( \lambda_k > 0 \). Since \( \Omega = \frac{1}{\epsilon}QM \) with a skew symmetric matrix \( Q \) and a symmetric real matrix \( M \), the trance of \( \Omega \) is zero. This is the reason that why \( \Lambda \) is assumed to be the form (10). With the linear change of variable

\[
\tilde{y}(t) = P^H y(t),
\]

the system can be rewritten as

\[
\ddot{\tilde{y}}(t) = \tilde{\Omega}\tilde{y}(t) + \ddot{\tilde{y}}(\tilde{y}(t)), \quad \tilde{y}(0) = P^H y_0,
\]

where

\[
\tilde{\Omega} = \text{diag}(-\tilde{\omega}_1 I_{d_1}, \ldots, -\tilde{\omega}_1 I_{d_1}, -\tilde{\omega}_0 I_{d_0}, \tilde{\omega}_0 I_{d_0}, \tilde{\omega}_1 I_{d_1}, \ldots, \tilde{\omega}_l I_{d_l})
\]
Energy conservation with $h=0.5$

Kinetic energy conservation with $h=0.5$

Figure 1: EI-T: the logarithm of the errors against $t$.

Energy conservation with $h=0.5$

Kinetic energy conservation with $h=0.5$

Figure 2: EI-O1: the logarithm of the errors against $t$. 
Figure 3: EI-O2: the logarithm of the errors against $t$.

Figure 4: EI-O3: the logarithm of the errors against $t$. 
Figure 5: EI-O4: the logarithm of the errors against $t$.

Figure 6: EI-O5: the logarithm of the errors against $t$. 
with \( \tilde{\omega}_k = \frac{\omega_k}{\epsilon} \) and
\[
\tilde{g}(\tilde{y}) = P^H g(P\tilde{y}) = -\nabla \tilde{y} V(P\tilde{y}).
\]
The energy of this transformed system is given by
\[
H(y) = \frac{1}{2} y^T (\frac{1}{\epsilon} M) y + V(y) = \frac{1}{2} \tilde{y}^T \tilde{A} \tilde{y} + V(P\tilde{y}) := \tilde{H}(\tilde{y})
\]
and the kinetic energy becomes
\[
K(y) = \frac{1}{2} \tilde{y}^T \tilde{A} \tilde{y} := \tilde{K}(\tilde{y}).
\]
For solving this system, the EI-T scheme (6) has the following form
\[
\dot{y}^{n+1} = e^{ih\tilde{\Omega}} y^n + \frac{\hbar}{2} \left( \tilde{g}(y^{n+1}) + e^{ih\tilde{\Omega}} \dot{g}(y^n) \right).
\]
Let
\[
\lambda = (\lambda_1, \ldots, \lambda_l), \quad k = (k_1, \ldots, k_l), \quad k \cdot \lambda = k_1 \lambda_1 + \cdots + k_l \lambda_l,
\]
and the resonance module is denoted by
\[
\mathcal{M} = \{ k \in \mathbb{Z}^l : k \cdot \lambda = 0 \}.
\]
Moreover, the following notations will be used in this paper:
\[
\omega = (\omega_1, \ldots, \omega_l), \quad j = (0, \ldots, 1, \ldots, 0), \quad |k| = |k_1| + \cdots + |k_l|.
\]
Denote by \( \mathcal{K} \) a set of representatives of the equivalence classes in \( \mathbb{Z}^l \setminus \mathcal{M} \) which are chosen such that for each \( k \in \mathcal{K} \) the sum \(|k|\) is minimal in the equivalence class \([k] = k + \mathcal{M}\), and that with \( k \in \mathcal{K} \), also \(-k \in \mathcal{K}\). For the positive integer \( N \), it is denoted that
\[
\mathcal{N} = \{ k \in \mathcal{K} : |k| \leq N \}, \quad \mathcal{N}^* = \mathcal{N} \setminus \{(0, \ldots, 0)\}.
\]
In this paper, the vector \( y \) is denoted by
\[
y = (y_{-1}, \ldots, y_{-1}, y_0, y_1, \ldots, y_l)
\]
with \( q_{\pm j} \in \mathbb{R}^{d_j} \). The same notation is used for all the vectors with the same dimension as \( y \).

Following (17), we define the operator
\[
L(hD) = (e^{hD} - e^{ih\tilde{\Omega}})(e^{hD} + e^{ih\tilde{\Omega}})^{-1}
\]
with the differential operator \( D \). We consider the application of such an operator to functions of the form \( e^{i(k \cdot \omega)t} \). Furthermore, this operator has the following proposition which can be verified easily.

**Proposition 1** The Taylor expansions of \( L(hD) \) are given by
\[
L(hD) = -\tan\left(\frac{1}{2}h\tilde{\Omega}\right)i - (I + \cos(h\tilde{\Omega}))^{-1}i(hD) - 2 \csc^3(h\tilde{\Omega}) \sin^4\left(\frac{1}{2}h\tilde{\Omega}\right)i(hD)^2 - \cdots,
\]
\[
L(hD + ih(k \cdot \tilde{\omega})) = \tan\left(\frac{1}{2}h((k \cdot \tilde{\omega})I - \tilde{\Omega})\right)i - (I + \cos\left(h((k \cdot \tilde{\omega})I - \tilde{\Omega})\right))^{-1}i(hD)
\]
\[
\qquad + 2 \csc^3\left(h((k \cdot \tilde{\omega})I - \tilde{\Omega})\right) \sin^4\left(\frac{1}{2}h((k \cdot \tilde{\omega})I + \tilde{\Omega})\right)i(hD)^2 + \cdots.
\]
3.2 Modulated Fourier expansion

In this subsection, we derive the modulated Fourier expansion of EI-T integrator. Before doing that, we need the following assumptions which have also been used in [15, 5].

**Assumption 1**

- It is assumed that the initial value \( y^0 \) satisfies
  \[
  \frac{1}{2\epsilon} \| y^{0T} My^0 \|^2 + V(y^0) \leq E,
  \]  
  (19)
  where \( E \) is a constant independent of \( \epsilon \).

- The numerical solution is supposed to stay in a compact set on which the potential \( V \) is smooth.

- It is required a lower bound for the step size \( h/\epsilon \geq c_0 > 0 \).

- The numerical non-resonance condition is considered
  \[
  | \sin \left( \frac{h}{2\epsilon} (k \cdot \lambda) \right) | \geq c \sqrt{h} \text{ for } k \in \mathbb{Z} \setminus \mathcal{M} \text{ with } |k| \leq N
  \]  
  (20)
  for some \( N \geq 2 \) and \( c > 0 \).

**Theorem 1** Under the above assumptions and for \( 0 \leq t = nh \leq T \), the EI-T method \( (15) \) can be expressed by the following modulated Fourier expansion

\[
\tilde{y}_n = \tilde{\zeta}(t) + \sum_{k \in \mathbb{N}^*} e^{i(k \cdot \tilde{\omega})t} \tilde{\zeta}_k(t) + \tilde{R}_{h,N}(t),
\]  
(21)

where the remainder term is bounded by

\[
\tilde{R}_{h,N}(t) = O(th^{N-1}),
\]  
(22)

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

\[
\tilde{\zeta}_0(t) = O(1), \quad \tilde{\zeta}_{\pm j}(t) = O(\sqrt{h}),
\]
\[
\tilde{\zeta}_{-j}^{(-j)}(t) = O(\sqrt{h}), \quad \tilde{\zeta}_j^{(j)}(t) = O(\sqrt{h}) + \cdots,
\]  
(23)

\[
\tilde{\zeta}_k^{(j)}(t) = O \left( h^{\frac{|k|+1}{2}} \right), \quad k \neq -j, \quad \tilde{\zeta}_j^{(j)}(t) = O \left( h^{\frac{|k|+1}{2}} \right), \quad k \neq j,
\]

for \( j = 1, \ldots, l \). It is noted that \( \tilde{\zeta}_{-j}^{(-j)} = \tilde{\zeta}_j^{(j)} \). The constants symbolised by the notation depend on \( E, N, c_0 \) and \( T \), but are independent of \( h \) and \( \tilde{\omega} \).

**Proof** In the proof of this theorem, we will construct the function

\[
\tilde{y}_h(t) = \tilde{\zeta}(t) + \sum_{k \in \mathbb{N}^*} e^{i(k \cdot \tilde{\omega})t} \tilde{\zeta}_k(t)
\]  
(24)

with smooth coefficient functions \( \tilde{\zeta} \) and \( \tilde{\zeta}_k \) and show that there is only a small defect when \( \tilde{y}_h(t) \) is inserted into the numerical scheme \( (15) \).

- Construction of the coefficients functions.
Inserting (24) into (15) and using the operator $L(hD)$ and the Taylor series of the nonlinearity, we have

$$L(hD)\tilde{y}_h(t) = \frac{h}{2} \tilde{g}(\tilde{y}_h(t)) = \frac{h}{2} \left[ \tilde{g}(\tilde{z}(t)) + \sum_{k \in \mathbb{N}^*} e^{i(k \cdot \omega)t} \sum_{s(\alpha) = k} \frac{1}{m!} \tilde{g}^{(m)}(\tilde{z}(t))(\tilde{z}(t))^\alpha \right],$$

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 $s(\alpha) - k \in \mathcal{M}$. We note that an abbreviation for the $m$-tuple $(\zeta^{a_1}(t), \ldots, \zeta^{a_m}(t))$ is denoted by $(\tilde{\zeta}(t))^\alpha$.

Inserting the ansatz (24) and comparing the coefficients of $e^{i(k \cdot \omega)t}$ yields

$$L(hD)\tilde{z}(t) = \frac{h}{2} \left[ \tilde{g}(\tilde{z}(t)) + \sum_{s(\alpha) \sim k} \frac{1}{m!} \tilde{g}^{(m)}(\tilde{z}(t))(\tilde{z}(t))^\alpha \right],$$

$$L(hD + i(k \cdot \omega)h)\tilde{z}^k(t) = \frac{h}{2} \sum_{s(\alpha) \sim k} \frac{1}{m!} \tilde{g}^{(m)}(\tilde{z}(t))(\tilde{z}(t))^\alpha. \quad (25)$$

This formula gives the modulation system for the coefficients $\tilde{z}^k(t)$ of the modulated Fourier expansion. According to Proposition 1 the following ansatz of the modulated Fourier functions $\tilde{z}^k(t)$ can be obtained:

$$\begin{align*}
\tilde{z}_0(t) &= G_{00}(\cdot) + \cdots, \\
\tilde{z}_{\pm j}(t) &= \frac{\tilde{h}}{\tan(\frac{\pm j \omega}{2})} (G_{j0}(\cdot) + \cdots), \\
\tilde{z}_{-j}(t) &= F_{-j0}(\cdot) + \cdots, \\
\tilde{z}_{j}(t) &= F_{j0}(\cdot) + \cdots, \quad (26) \\
\tilde{z}^k_j(t) &= \frac{\tilde{h}}{\tan(\frac{k \omega + j \omega}{2})} (F_{-j0}(\cdot) + \cdots), \quad k \neq -j, \\
\tilde{z}^k_j(t) &= \frac{\tilde{h}}{\tan(\frac{k \omega - j \omega}{2})} (F_{j0}(\cdot) + \cdots), \quad k \neq j,
\end{align*}$$

where $j = 1, \ldots, l$ and the dots stand for power series in $\sqrt{h}$.

**Initial values.**

We determine the initial values for the differential equations by considering the conditions that (24) is satisfied without remainder term for $t = 0$. From $\tilde{y}_h(t) = \tilde{y}^0$, it follows that

$$\begin{align*}
\tilde{y}^0_0 &= \tilde{z}_0(0) + \mathcal{O}(\sqrt{h}), \\
\tilde{y}^0_j &= \tilde{z}_{-j}(0) + \mathcal{O}(\sqrt{h}), \\
\tilde{y}^0_j &= \tilde{z}_j(0) + \mathcal{O}(\sqrt{h}). \quad (27)
\end{align*}$$

Thus we get the initial values $\tilde{z}_0(0)$, $\tilde{z}_{-j}(0)$ and $\tilde{z}_j(0)$.

**Bounds of the coefficients functions.**

The bound (23) is immediately obtained on the base of the above initial values, the ansatz (26) and Assumption 1.
Defect.
By using the Lipschitz continuous of the nonlinearity and the standard convergence estimates, it is easy to prove the defect \[22\].

In the light of the linear transform \[11\], the modulated Fourier expansion for \(y^n\) is given as follows.

**Theorem 2** The numerical solution of the EI-T method \[6\] admits the following modulated Fourier expansion
\[
y^n = \zeta(t) + \sum_{k \in \mathbb{N}^*} e^{i(k \cdot \tilde{\omega})t} \zeta_k(t) + R_{h,N}(t),
\]
where \(\zeta(t) = P\tilde{\zeta}(t), \zeta_k(t) = P\tilde{\zeta}_k(t)\). The bounds of these functions and the remainders are the same as those given in Theorem \[1\]. Moreover, we have \(\zeta^{-k} = \overline{\zeta}^k\).

### 3.3 Long time energy conservation

In this subsection, we study long time energy conservation of EI-T integrator, which is derived by showing an almost-invariant of the functions of modulated Fourier expansions.

**Theorem 3** Let \(\tilde{\zeta} = (\zeta_k)_{k \in \mathbb{N}}\). Under the conditions of Theorem \[1\] there exists a function \(\tilde{H}[\tilde{\zeta}]\) such that
\[
\tilde{H}[\tilde{\zeta}](t) = \tilde{H}[\tilde{\zeta}](0) + O(th^N) \quad \text{for} \ 0 \leq t \leq T.
\]
Moreover, the function \(\tilde{H}[\tilde{\zeta}]\) can be expressed as
\[
\tilde{H}[\tilde{\zeta}] = \frac{1}{2} \sum_{j=-l,j \neq 0}^{l} \left( \tilde{\omega}_j (\tilde{\zeta}^{-j}_j)^T \tilde{\zeta}^{-j}_j + \tilde{\omega}_j (\tilde{\zeta}^j_j)^T \tilde{\zeta}^j_j \right) + V(PH\tilde{\zeta}(t)) + O(h).
\]

**Proof** From the proof of Theorem \[1\] it follows that
\[
L(hD)\tilde{y}_h^k(t) = \frac{h}{2} \tilde{g}(\tilde{y}_h(t)) + O(h^{N+1}),
\]
where we use the denotations
\[
\tilde{y}_h(t) = \sum_{k \in \mathbb{N}} \tilde{y}_h^k(t) \quad \text{with} \quad \tilde{y}_h^k(t) = e^{i(k \cdot \tilde{\omega})t} \tilde{\zeta}_k(t).
\]
Multiplication of this result with \(P\) yields
\[
PL(hD)PH\tilde{y}_h(t) = PL(hD)PH\tilde{y}_h(t) = \frac{h}{2} \tilde{g}(\tilde{y}_h(t)) + O(h^{N+1}) = \frac{h}{2} g(y_h(t)) + O(h^{N+1}),
\]
where
\[
y_h(t) = \sum_{k \in \mathbb{N}} y_h^k(t) \quad \text{with} \quad y_h^k(t) = e^{i(k \cdot \omega)t} \zeta_k(t).
\]
For the terms of \(\tilde{y}_h^k\), one gets
\[
PL(hD)PH\tilde{y}_h^k(t) = \frac{h}{2} \nabla_{y^k} V(\tilde{y}(t)) + O(h^{N+1}),
\]
where $\mathcal{V}(\tilde{y}(t))$ is defined as

$$\mathcal{V}(\tilde{y}(t)) = V(y^0_h(t)) + \sum_{s(\alpha)=0}^1 \frac{1}{m!} V^{(m)}(y^0_h(t))(y_h(t))^\alpha$$  \hspace{1cm} (32)

with

$$\tilde{y}(t) = (y^k_h(t))_{k \in \mathbb{N}^*}.$$  

Multiplying (31) with $(\tilde{y}^{-k}_h(t))^T$ and summing up gives

$$\frac{2}{h} \sum_{k \in \mathbb{N}} (\tilde{y}^{-k}_h(t))^T P_L(hD)P^H H^k y_h(t) + \frac{d}{dt} \mathcal{V}(\tilde{y}(t)) = O(h^N).$$

By switching to the quantities $\zeta^k$, we obtain

$$O(h^N) = \frac{2}{h} \sum_{k \in \mathbb{N}} (\tilde{\zeta}^{-k}(t) - i(k \cdot \omega)\tilde{\zeta}^{-k}(t))^T P_L(hD + ih(k \cdot \omega))P^H \zeta^k(t) + \frac{d}{dt} \mathcal{V}(\tilde{\zeta}(t))$$

$$= \frac{2}{h} \sum_{k \in \mathbb{N}} (\tilde{\zeta}^k(t) - i(k \cdot \omega)\tilde{\zeta}^k(t))^T P_L(hD + ih(k \cdot \omega))P^H \zeta^k(t) + O(h^N)$$

$$= \frac{2}{h} \sum_{k \in \mathbb{N}} (\tilde{\zeta}^k(t) - i(k \cdot \omega)\tilde{\zeta}^k(t))^T P^H P_L(hD + ih(k \cdot \omega))P^H \zeta^k(t) + O(h^N)$$

$$= \frac{2}{h} \sum_{k \in \mathbb{N}} (\tilde{\zeta}^k(t) - i(k \cdot \omega)\tilde{\zeta}^k(t))^T L(hD + ih(k \cdot \omega))\tilde{\zeta}^k(t) + O(h^N).$$  \hspace{1cm} (33)

By the Taylor expansions of $L(hD)$ given in Proposition 11 and the “magic formulas” on p. 508 of [17], it is easy to check that $\text{Im}(\tilde{\zeta}^k(t))^T L(hD + ih(k \cdot \omega))\tilde{\zeta}^k(t)$ and $\text{Im}(i(k \cdot \omega)\tilde{\zeta}^k(t))^T L(hD + ih(k \cdot \omega))\tilde{\zeta}^k(t)$ are both total derivatives. Therefore, the imaginary part of the right-hand side of (33) is the total derivative. There exists a function $\hat{\mathcal{H}}$ such that $\frac{d}{dt} \hat{\mathcal{H}}[\zeta](t) = O(h^N)$ and the statement (24) is obtained by an integration.

The construction (24) of $\hat{\mathcal{H}}$ is shown by considering the previous analysis and the bounds of Theorem 11.

The first main result about the long time energy conservation of EI-T is given as follows.

**Theorem 4** Under the conditions of Theorem 3 one obtains

$$\hat{\mathcal{H}}[\zeta](t) = H(y^n) + O(h)$$

for $0 \leq t = nh \leq T$. Moreover, for the long time energy conservation of EI-T, we have

$$H(y^n) = H(y^0) + O(h)$$

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

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In the light of the bounds given in Theorem 1, we deduce that
\[
H(y^n) = \tilde{H}(y^n) = \frac{1}{2} \sum_{j=-l_j \neq 0}^l \left( \tilde{\omega}_j (\tilde{\zeta}_{-j}^{-(j)})^T \tilde{\zeta}_{-j}^{-(j)} + \tilde{\omega}_j (\tilde{\zeta}_j^{(j)})^T \tilde{\zeta}_j^{(j)} \right) + V(P^H \tilde{\zeta}(t)) + O(h). \tag{34}
\]

A comparison between (30) and (34) yields the first result of this theorem. The second statement of this theorem is easily obtained by following the same way used in Section XIII of [17].

### 3.4 Long time kinetic energy conservation

We now turn to the long time conservation of kinetic energy. Define the vector functions of \( \tilde{\zeta}(\lambda, t) \) as
\[
\tilde{\zeta}(\lambda, t) = (e^{i(k \cdot \tilde{\omega}) \lambda} \tilde{\zeta}_k(t))_{k \in \mathbb{N}}.
\]
Then it can be observed from the definition (32) that \( V(\tilde{\zeta}(\lambda, t)) \) does not depend on \( \lambda \). Thus, the following result is obtained
\[
0 = \frac{d}{d\lambda} \mid_{\lambda=0} V(\tilde{\zeta}(\lambda, t)) = \sum_{k \in \mathbb{N}} i(k \cdot \tilde{\omega})(\tilde{\zeta}_{-k}^{-(k)})^T \nabla_{\tilde{\zeta}_{-k}^{-(k)}} V(\tilde{\zeta}(t))
\]
\[
= \frac{-2}{\hbar} \sum_{k \in \mathbb{N}} i(k \cdot \tilde{\omega})(\tilde{\zeta}_{-k}^{-(k)})^T P L(hD + i\hbar(k \cdot \tilde{\omega}))P^H \tilde{\zeta}_{-k}^{(k)}(t) + O(h^N)
\]
\[
= \frac{-2}{\hbar} \sum_{k \in \mathbb{N}} i(k \cdot \tilde{\omega})(\tilde{\zeta}_{k}^{(k)})^T P L(hD + i\hbar(k \cdot \tilde{\omega}))P^H \tilde{\zeta}_{k}^{(k)}(t) + O(h^N)
\]
\[
= \frac{-2}{\hbar} \sum_{k \in \mathbb{N}} i(k \cdot \tilde{\omega})(\tilde{\zeta}_{k}^{(k)})^T L(hD + i\hbar(k \cdot \tilde{\omega}))\hat{\tilde{\zeta}}_{k}(t) + O(h^N).
\]

Similar to the analysis of the above subsection, it can be verified that the right hand size of (35) is a total derivative. Therefore, we get the second almost-invariant as follows.

**Theorem 5** Under the conditions of Theorem 1 for \( 0 \leq t \leq T \), there exists a function \( \tilde{\mathcal{M}}[\tilde{\zeta}] \) such that
\[
\tilde{\mathcal{M}}[\tilde{\zeta}](t) = \tilde{\mathcal{M}}[\tilde{\zeta}](0) + O(t h^N), \tag{36}
\]
where
\[
\tilde{\mathcal{M}}[\tilde{\zeta}] = \frac{1}{2} \sum_{j=-l_j \neq 0}^l \left( \tilde{\omega}_j (\tilde{\zeta}_{-j}^{-(j)})^T \tilde{\zeta}_{-j}^{-(j)} + \tilde{\omega}_j (\tilde{\zeta}_j^{(j)})^T \tilde{\zeta}_j^{(j)} \right) + O(h). \tag{37}
\]

Then, we obtain the result about the long time kinetic energy conservation of EI-T.

**Theorem 6** Under the conditions of Theorem 3 we have
\[
\tilde{\mathcal{M}}[\tilde{\zeta}](t) = K(y^n) + O(h)
\]
for $0 \leq t = nh \leq T$. Moreover, for the long time kinetic energy conservation of EI-T, it is true that

$$K(y^n) = K(y^0) + O(h)$$

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

4 Long-time conservation of the EI-O integrators

For solving the transformed system (12), the EI-O integrators (7) are given as

$$\begin{align*}
\hat{Y}^{n+1} &= e^{ci\hat{\Omega} t} \hat{y}^n + h a_{11}(i\hbar \hat{\Omega}) \hat{F}(\hat{Y}^{n+1}), \\
\hat{y}^{n+1} &= e^{ih\hat{\Omega} t} \hat{y}^n + h b_1(i\hbar \hat{\Omega}) \hat{F}(\hat{Y}^{n+1}).
\end{align*}$$

(38)

In this section, we study the long-time conservations of these one-stage implicit EI-O integrators. It is assumed that these integrators satisfy the condition (9) in the analysis of this section.

We start by defining another three operators

$$\begin{align*}
\hat{L}_1(hD) &= (e^{hD} - e^{ih\hat{\Omega}})(e^{i(1-c_1)h\hat{\Omega} e^{c_1hD}})^{-1}, \\
\hat{L}_2(hD) &= (e^{-i(1-c_1)h\hat{\Omega} e^{c_1hD}} + e^{ic_1h\hat{\Omega} e^{c_1hD}}), \\
\hat{L}(hD) &= (\hat{L}_1 \circ \hat{L}_2^{-1})\hat{\phi}(hD).
\end{align*}$$

(39)

It can be checked easily that they have the following important property.

**Proposition 2** For the operator $\hat{L}(hD)$ given in (39), it is true that

$$\hat{L}(hD) = L(hD),$$

(40)

where $L(hD)$ is defined in (18). Therefore, $\hat{L}(hD)$ has the same Taylor series as given in Proposition 1.

4.1 Modulated Fourier expansion

For the EI-O integrator (38), we assume that the modulated Fourier expansions of $\hat{Y}^{n+1}$ and $\hat{y}^n$ are

$$\begin{align*}
\hat{Y}_h(t + c_1 h) &= \tilde{Y}(t + c_1 h) + \sum_{k \in \mathbb{N}^*} e^{i(k \cdot \omega) t + c_1 h} \tilde{Y}^{k}(t + c_1 h), \\
\hat{y}_h(t) &= \tilde{\zeta}(t) + \sum_{k \in \mathbb{N}^*} e^{i(k \cdot \omega) t} \tilde{\zeta}^{k}(t),
\end{align*}$$

(41)

respectively, where $t = nh$. Considering the scheme of the EI-O integrator (38), we have

$$\begin{align*}
\hat{Y}^{n+1} &= e^{c_1i\hbar \hat{\Omega}} \hat{y}^n + a_{11}(i\hbar \hat{\Omega}) b_1^{-1}(i\hbar \hat{\Omega})(\hat{y}^{n+1} - e^{i\hbar \hat{\Omega}} \hat{y}_n) \\
&= \frac{1}{2} b_1^{-1}(i\hbar \hat{\Omega}) \hat{y}^{n+1} + (e^{c_1i\hbar \hat{\Omega}} - \frac{1}{2} b_1^{-1}(i\hbar \hat{\Omega}) e^{i\hbar \hat{\Omega}}) \hat{y}_n \\
&= \frac{1}{2} e^{-(1-c_1)i\hbar \hat{\Omega}} \hat{y}^{n+1} + (e^{c_1i\hbar \hat{\Omega} e^{(1-c_1)i\hbar \hat{\Omega}}} - \frac{1}{2} e^{i\hbar \hat{\Omega}}) e^{-(1-c_1)i\hbar \hat{\Omega}} \hat{y}_n \\
&= \frac{1}{2} e^{-(1-c_1)i\hbar \hat{\Omega}} \hat{y}^{n+1} + \frac{1}{2} e^{c_1i\hbar \hat{\Omega}} \hat{y}_n,
\end{align*}$$

(39)
where the condition (9) is used here. Inserting the modulated Fourier expansions into these equations, we obtain

\[
\tilde{Y}_h(t + c_1 h) = \frac{1}{2} \left( e^{-(1-c_1)ih\tilde{\Omega}_h} \tilde{y}_h(t + c_1 h + (1 - c_1)h) + \frac{1}{2} e^{c_1ih\tilde{\Omega}_h} \tilde{y}_h(t + c_1 h - c_1 h) \right). \tag{42}
\]

Changing the time from \(t + c_1 h\) to \(t\) yields

\[
\tilde{Y}_h(t) = \frac{1}{2} \hat{L}_2(hD) \tilde{y}_h(t), \tag{43}
\]

which leads to

\[
\tilde{Y}(t) = \frac{1}{2} \hat{L}_2(hD) \tilde{\zeta}(t), \tag{44}
\]

\[
\tilde{Y}^k(t) = \frac{1}{2} \hat{L}_2(hD + ih(k \cdot \tilde{\omega})) \tilde{\zeta}^k(t).
\]

As an example of this connection, one has

\[
\tilde{Y} - \langle j \rangle - j(t) = \tilde{\zeta} - \langle j \rangle - j(t) + O(h),
\]

\[
\tilde{Y} \langle j \rangle j(t) = \tilde{\zeta} \langle j \rangle j(t) + O(h), \tag{45}
\]

for \(j = 1, \ldots, l\), which will be used in the next subsection.

On the other hand, by the definition of \(\hat{L}_1(hD)\), the second equality of (38) can be expressed as

\[
\hat{L}_1(hD) \tilde{y}_h(t) = h \tilde{F}(\tilde{Y}_h(t)). \tag{46}
\]

Combining (43) with (46) implies

\[
\frac{h}{4} \hat{L}(hD) \tilde{Y}_h(t) = \tilde{F}(\tilde{Y}_h(t)). \tag{47}
\]

Therefore, it is obtained

\[
\hat{L}(hD) \tilde{Y}_0 = \frac{h^2}{4} \left( \tilde{F}(\tilde{Y}_0) + \sum_{s(\alpha) = 0} \frac{1}{m!} \tilde{F}^{(m)}(\tilde{Y}_0)(\tilde{Y})^\alpha \right),
\]

\[
\hat{L}(hD + i(k \cdot \tilde{\omega})h) \tilde{Y}^k = \frac{h^2}{4} \sum_{s(\alpha) = k} \frac{1}{m!} \tilde{F}^{(m)}(\tilde{Y}_0)(\tilde{Y})^\alpha, \tag{48}
\]

which gives the modulation system for the coefficients \(\tilde{Y}_h\). The modulation system for the coefficient \(\tilde{\zeta}_h\) can be obtained by considering (44).

**Remark 1** It can be observed that the formula (48) is quite similar to (25). Therefore, with the property (41), a result similar to Theorem 1 about the bounds of the coefficient functions \(\tilde{Y}_h\) can be obtained. Then the bounds of the coefficient functions \(\tilde{\zeta}_h\) can be derived by considering (44). Therefore, the modulated Fourier expansions of EI-O integrators (38) are formulated as follows.
Theorem 7  Under the conditions given in Assumption 7 and for $0 \leq t = nh \leq T$, the EI-O integrators admit the following modulated Fourier expansions
\[
\tilde{Y}^{n+c_1} = \tilde{Y}(t + c_1h) + \sum_{k \in \mathbb{N}^*} e^{i(k\tilde{\omega})(t+c_1h)}\tilde{Y}^k(t + c_1h) + O(th^{N-1}),
\]
\[
\tilde{y}^n = \tilde{\zeta}(t) + \sum_{k \in \mathbb{N}^*} e^{i(k\tilde{\omega})t}\tilde{\zeta}^k(t) + O(th^{N-1}),
\]
where the coefficient functions $\tilde{Y}^k$ as well as all their derivatives have the same bounds as $\tilde{Y}^k$. The relationship between $\tilde{Y}^k$ and $\zeta^k$ is given by (44). For the EI-O integrators, their modulated Fourier expansions are given by
\[
Y^{n+c_1} = Y(t + c_1h) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)(t+c_1h)}Y^k(t + c_1h) + O(th^{N-1}),
\]
\[
y^n = \zeta(t) + \sum_{k \in \mathbb{N}^*} e^{i(k\omega)t}\zeta^k(t) + O(th^{N-1}),
\]
where $t = nh$, $Y^k = P\tilde{Y}^k$ and $\zeta^k = P\tilde{\zeta}^k$.

4.2 Long-time conservation results

By the same way as stated in Section 3, we can derive two almost invariants of the EI-O integrators. Based on these results, the long-time conservation results can be obtained. In what follows, we only present the results and skip all the proofs for brevity.

Theorem 8  Letting $\vec{\tilde{Y}}(t) = (\tilde{Y}^k)_{k \in \mathbb{N}}$ and under the conditions of Assumption 7 and 9, there exist two functions $\vec{\mathcal{H}}[\vec{\tilde{Y}}]$ and $\vec{\mathcal{M}}[\vec{\tilde{Y}}]$ such that
\[
\vec{\mathcal{H}}[\vec{\tilde{Y}}](t) = \begin{pmatrix} \vec{\tilde{H}}[\vec{\tilde{Y}}] \end{pmatrix} + O(th^N),
\]
\[
\vec{\mathcal{M}}[\vec{\tilde{Y}}](t) = \begin{pmatrix} \vec{\mathcal{M}}[\vec{\tilde{Y}}] \end{pmatrix} + O(th^N)
\]
for $0 \leq t \leq T$. Moreover, they can be expressed as
\[
\vec{\tilde{H}}[\vec{\tilde{Y}}] = \frac{1}{2} \sum_{j=-l,j \neq 0}^l \left( \bar{\omega}_j (\tilde{Y}_{-j})^T \tilde{Y}_{-j} + \bar{\omega}_j (\tilde{Y}_{j})^T \tilde{Y}_{j} \right) + V(P^H \tilde{Y}) + O(h),
\]
\[
\vec{\mathcal{M}}[\vec{\tilde{Y}}] = \frac{1}{2} \sum_{j=-l,j \neq 0}^l \left( \bar{\omega}_j (\tilde{Y}_{-j})^T \tilde{Y}_{-j} + \bar{\omega}_j (\tilde{Y}_{j})^T \tilde{Y}_{j} \right) + O(h).
\]
In the light of (45), these two almost invariants can be expressed
\[
\vec{\tilde{H}} = \frac{1}{2} \sum_{j=-l,j \neq 0}^l \left( \bar{\omega}_j (\tilde{\zeta}_{-j})^T \tilde{\zeta}_{-j} + \bar{\omega}_j (\tilde{\zeta}_{j})^T \tilde{\zeta}_{j} \right) + V(P^H \tilde{\zeta}) + O(h),
\]
\[
\vec{\mathcal{M}} = \frac{1}{2} \sum_{j=-l,j \neq 0}^l \left( \bar{\omega}_j (\tilde{\zeta}_{-j})^T \tilde{\zeta}_{-j} + \bar{\omega}_j (\tilde{\zeta}_{j})^T \tilde{\zeta}_{j} \right) + O(h).
\]
We are now in the position to present the main results of EI-O integrators.

**Theorem 9** It is assumed that all the conditions of Theorem 8 are satisfied. Then for the long time energy and kinetic energy conservations of EI-O integrators, we have

\[
H(y^n) = H(y^0) + O(h), \\
K(y^n) = K(y^0) + O(h)
\]

for \(0 \leq nh \leq h^{-N+1}\). The constants symbolized by \(O\) depend on \(N, T\) and the constants in the assumptions, but are independent of \(n, h, \epsilon\).

## 5 Conclusions

In this paper, we have studied the long-time energy and kinetic energy near-conservations of exponential integrators for solving highly oscillatory conservative systems. Two kinds of exponential integrators have been presented and their modulated Fourier expansions have been developed. By using the technique of modulated Fourier expansions, it is proved that the symmetric EI-T and the symplectic EI-O integrators approximately conserve the energy and kinetic energy over long times.

Last but not least, it is noted that we have tried to derive the long time result for explicit exponential integrators. Unfortunately, it does not work since the operator \(L(hD)\) determined by explicit exponential integrators does not have good property. Although implicit exponential integrators need more computation in comparison with explicit schemes, they are indeed used and analysed by many publications (see [3, 4, 5, 10]).

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