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Long Time Energy and Kinetic Energy Conservations 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.

AMS subject classifications: 65P10, 65L05

Key words: Highly oscillatory conservative systems, modulated Fourier expansion, exponential integrators, long-time conservation.

1. Introduction

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

$$y'(t) = Q\nabla H\big(y(t)\big), \quad y(0) = y_0 \in \mathbb{R}^d, \quad t \in [0,T], \tag{1.1}$$

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

$$H(y) = \frac{1}{2\epsilon} y^{\intercal} M y + V(y). \tag{1.2}$$

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Here ϵ is a small parameter satisfying $0 < \epsilon \ll 1$, M is a $d \times d$ real 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 (1.1) is a conservative system with the first integral H: i.e.,

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

The kinetic energy of the system (1.1) is given by

$$K(y) = \frac{1}{2\epsilon} y^\intercal M y.$$

For brevity, by letting

$$\Omega = \frac{1}{\epsilon} QM, \quad g\big(y(t)\big) = Q\nabla V\big(y(t)\big),$$

the system (1.1) can be rewritten as

$$y'(t) = \Omega y(t) + g\big(y(t)\big), \quad y(0) = y_0 \in \mathbb{R}^d. \tag{1.3}$$

It is well known that the exact solution of (1.1) or (1.3) can be represented by the variation-of-constants formula

$$y(t) = e^{t\Omega} y_0 + t \int_0^1 e^{(1-\tau)t\Omega} g\big(y(\tau t)\big) d\tau. \tag{1.4}$$

In the analysis of this paper, it is assumed that the matrix Ω is 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 [22]).

The highly oscillatory system (1.3) often arises in a wide range of applications such as in engineering, astronomy, mechanics, physics and molecular dynamics (see, e.g. [11, 20, 22, 25, 31, 38, 39]). There are also some semidiscrete PDEs such as semilinear Schrödinger equations fit this form [3,4,6,34]. In recent decades, as an efficient approach to integrating (1.3), exponential integrators have been widely investigated and developed, and the reader is referred to [1,2,12,16,21,23,24,28,33,35] for example. A systematic survey of exponential integrators is referred to [22]. One important advantage of exponential integrators is that they make well use of the variation-of-constants formula (1.4), and can perform 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 [18]. 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, 20, 36], for an implicit-explicit method in [27, 32], for heterogeneous multiscale methods in [30] and for