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ON ENERGY CONSERVATION BY TRIGONOMETRIC INTEGRATORS IN THE LINEAR CASE WITH APPLICATION TO WAVE EQUATIONS*

(Dedicated to Ernst Hairer on the occasion of his seventieth birthday and to Christian Lubich on the occasion of his sixtieth birthday.)

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Abstract

Trigonometric integrators for oscillatory linear Hamiltonian differential equations are considered. Under a condition of Hairer & Lubich on the filter functions in the method, a modified energy is derived that is exactly preserved by trigonometric integrators. This implies and extends a known result on all-time near-conservation of energy. The extension can be applied to linear wave equations.

Mathematics subject classification: 65P10, 65L05, 37M15.
Key words: Oscillatory Hamiltonian systems, Trigonometric integrators, Energy conservation, Long-time behaviour, Modified energy.

1. Introduction

Trigonometric integrators form a popular class of numerical methods for oscillatory second-order differential equations; see [16, Chapter XIII]. The various available trigonometric integrators differ (only) by the filter functions that are used inside the methods. One way to choose filter functions was put forward by Hairer & Lubich in [14], which led to the well-known trigonometric integrators of Hairer & Lubich [14] and Grimm & Hochbruck [13]. It is a condition on the filter functions (see (3.3) below) that can be proven to imply very good energy conservation by the corresponding trigonometric integrators on long time intervals: In the case of *linear* oscillatory Hamiltonian differential equations, all-time near-conservation of energy can be proven for *all* step-sizes; see [14]. In other words, there are no numerical resonances (in the linear case) that show up in other trigonometric integrators on long time intervals.

In the present note, we consider trigonometric integrators under the mentioned condition on the filter functions of Hairer & Lubich [14] in the mentioned situation of linear oscillatory Hamiltonian differential equations. We show that there exists a *modified energy* that is *exactly* preserved by the numerical method. This modified energy is close to the original energy, which yields a new proof and an extension of the mentioned result of [14] on all-time near-conservation of energy for all step-sizes.

This extension can be applied to linear wave equations. We use it to prove all-time near-conservation of energy for a spectral semi-discretization of linear wave equations, again without any restriction on the time step-size, neither of CFL-type nor of resonance-excluding nature.

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This seems to be the first long-time result for temporal discretizations of Hamiltonian partial differential equations that is completely uniform in the time step-size.

2. Oscillatory Hamiltonian Systems

We consider oscillatory Hamiltonian systems of the form

$$\ddot{q} = -\Omega^2 q + g(q), \qquad q = q(t) \in \mathbb{C}^d. \tag{2.1}$$

In this equation, the matrix

$$\Omega = \operatorname{diag}(\omega_j)_{j=1}^d \in \mathbb{R}^{d\times d}$$

is a diagonal matrix containing nonnegative, possibly large frequencies $\omega_j \in \mathbb{R}$. We denote by ω the smallest nonzero frequency:

$$\omega = \min_{j:\,\omega_j>0} \omega_j. \tag{2.2}$$

The term

$$g(q) = -\nabla U(q)$$

in (2.1) stems from a (sufficiently regular, in particular real differentiable) potential $U\colon \mathbb{C}^d \to \mathbb{R}$. The complex gradient ∇ with respect to $q \in \mathbb{C}^d$ is defined as $\nabla = \nabla_x + \mathrm{i}\nabla_y$ with the real part $x \in \mathbb{R}^d$ and the imaginary part $y \in \mathbb{R}^d$ of $q = x + \mathrm{i}y$.[1)] We will be interested in the case that (2.1) is a linear equation, i.e.,

$$g(q) = -Aq, \qquad U(q) = \tfrac{1}{2} q^* A q, \qquad A \in \mathbb{C}^{d\times d} \text{ self-adjoint}, \tag{2.3}$$

where $*$ denotes the conjugate transpose.

The total energy of the Hamiltonian system (2.1) is given by

$$H(q,\dot{q}) = \tfrac{1}{2}\|\Omega q\|^2 + \tfrac{1}{2}\|\dot{q}\|^2 + U(q), \tag{2.4}$$

where $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{C}^d$.

3. Trigonometric Integrators

Trigonometric integrators form a popular class of numerical methods for oscillatory Hamiltonian systems (2.1). These integrators make use of the fact that the equation $\mathrm{d}^2q/\mathrm{d}t^2 = -\Omega^2 q$ is easy to solve since Ω is diagonal. (In contrast, the complete equation $\mathrm{d}^2q/\mathrm{d}t^2 = -\Omega^2 q - Aq$ (in the linear situation (2.3)) is, in general, much more difficult since it involves a possibly full matrix A, see also Section 7.)

We consider here symmetric trigonometric integrators with the step-size h (see [16, Chapter XIII]):

$$q_{n+1} = \cos(h\Omega)q_n + h\,\operatorname{sinc}(h\Omega)\dot{q}_n + \tfrac{1}{2}h^2\,\operatorname{sinc}(h\Omega)\Psi_1 g(\Phi q_n), \tag{3.1a}$$

$$\dot{q}_{n+1} = -\Omega\sin(h\Omega)q_n + \cos(h\Omega)\dot{q}_n + \tfrac{1}{2}h\big(\cos(h\Omega)\Psi_1 g(\Phi q_n) + \Psi_1 g(\Phi q_{n+1})\big). \tag{3.1b}$$

Throughout the paper, we assume $h \le 1$. In the method (3.1), we use filter operators

$$\Psi_1 = \psi_1(h\Omega) \qquad \text{and} \qquad \Phi = \phi(h\Omega)$$

[1)] We remark that the choice of a complex setting is with a view towards the application to wave equations in the final part of the paper.