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NUMERICAL ENERGY CONSERVATION FOR MULTI-FREQUENCY OSCILLATORY DIFFERENTIAL EQUATIONS

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Abstract.

The long-time near-conservation of the total and oscillatory energies of numerical integrators for Hamiltonian systems with highly oscillatory solutions is studied in this paper. The numerical methods considered are second-order symmetric trigonometric integrators and the Störmer–Verlet method. Previously obtained results for systems with a single high frequency are extended to the multi-frequency case, and new insight into the long-time behaviour of numerical solutions is gained for resonant frequencies. The results are obtained using modulated multi-frequency Fourier expansions and the Hamiltonian-like structure of the modulation system. A brief discussion of conservation properties in the continuous problem is also included.

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1 Introduction

This article studies the conservation of invariants and almost-invariants along numerical approximations of solutions that are highly oscillatory. We consider Hamiltonian systems with Hamiltonian function

$$H(x,\dot x) = \frac{1}{2}\sum_{j=0}^{\ell}\Big(\|\dot x_j\|^2 + \frac{\lambda_j^2}{\varepsilon^2}\,\|x_j\|^2\Big) + U(x), \tag{1.1}$$

where $x = (x_0, x_1, \ldots, x_\ell)$ with $x_j \in \mathbb{R}^{d_j}$, $\lambda_0 = 0$ and $\lambda_j \geq 1$ are distinct real numbers, ε is a small positive parameter, and $U(x)$ is a smooth potential function. Our aim is to extend the results of [5] (see also Chapter XIII of [6]) to the multi-frequency case $\ell > 1$.

Following [1] we consider the resonance module

$$\mathcal{M} = \{k \in \mathbb{Z}^\ell : k_1\lambda_1 + \ldots + k_\ell\lambda_\ell = 0\} \tag{1.2}$$

and we denote the *oscillatory energy* of the jth frequency by

$$I_j(x,\dot x) = \frac{1}{2}\Big(\|\dot x_j\|^2 + \frac{\lambda_j^2}{\varepsilon^2}\,\|x_j\|^2\Big). \tag{1.3}$$

In [1] it is shown that under a diophantine non-resonance condition outside $\mathcal{M}$ the quantities

$$I_\mu(x,\dot x) = \sum_{j=1}^{\ell} \frac{\mu_j}{\lambda_j}\, I_j(x,\dot x) \tag{1.4}$$

are approximately preserved along every bounded solution of the Hamiltonian system that has a total energy bounded independently of ε, on exponentially long time intervals of size $\mathcal{O}(\mathrm{e}^{c/\varepsilon})$ if the potential $U(x)$ is analytic and

$$\mu = (\mu_1,\dots,\mu_\ell) \quad \text{is orthogonal to } \mathcal{M}. \tag{1.5}$$

Since $\mu=\lambda$ is always orthogonal to $\mathcal{M}$, the total oscillatory energy $\sum_{j=1}^{\ell} I_j(x,\dot x)$ of the system is approximately preserved independently of the resonance module $\mathcal{M}$. Subtracting this expression from the total energy (1.1), we see that also the *smooth energy*

$$K(x,\dot x) = \frac{1}{2}\|\dot x_0\|^2 + U(x) \tag{1.6}$$

is approximately preserved. With an ε-independent bound of the total energy $H(x,\dot x)$ we have $x_j=\mathcal{O}(\varepsilon)$ for $j=1,\dots,\ell$, so that $K(x,\dot x)$ is close to the Hamiltonian of the reduced system in which all oscillatory degrees of freedom are taken out, $H_0(x_0,\dot x_0)=\frac{1}{2}\|\dot x_0\|^2 + U(x_0,0,\dots,0)$.

EXAMPLE 1.1. *To illustrate the conservation of the various energies, we consider a Hamiltonian (1.1) with* $\ell=3$, $\lambda=(1,\sqrt{2},2)$ *and we assume that the dimensions of* x_j *are all* 1 *with the exception of that of* $x_1=(x_{11},x_{12})$ *which is* 2. *We take* $\varepsilon^{-1}=\omega=70$, *the potential*

$$U(x) = (0.001x_0 + x_{11} + x_{12} + x_2 + x_3)^4, \tag{1.7}$$

and $x(0)=(1,0.3\varepsilon,0.8\varepsilon,-1.1\varepsilon,0.7\varepsilon)$, $\dot x(0)=(-0.75,0.6,0.7,-0.9,0.8)$ *as initial values. For* $\lambda=(1,\sqrt{2},2)$ *we can take* $\mu=(1,0,2)$ *and* $\mu=(0,\sqrt{2},0)$ *with (1.5). In Fig. 1.1 we plot the oscillatory energies for the individual components of the system. The corresponding frequencies are attached to the curves. We also plot the sum* I_1+I_3 *of the three oscillatory energies corresponding to the resonant frequencies* $1/\varepsilon$ *and* $2/\varepsilon$. *We see that* I_1+I_3 *as well as* I_2 *(which are* I_μ *for the above two vectors* μ *satisfying (1.5)) are well conserved over long times up to small oscillations of size* $\mathcal{O}(\varepsilon)$. *Already from the very beginning there is an energy exchange between the two components corresponding to the same frequency* $1/\varepsilon$, *and on a larger scale an energy exchange between* I_1 *and* I_3 *can be seen.*

If we replace the factor 0.001 *in the potential* $U(x)$ *of (1.7) by* 1, *then no visible exchange takes place between oscillatory energies corresponding to different frequencies, and all* I_j *are approximately preserved. This is probably due to the*

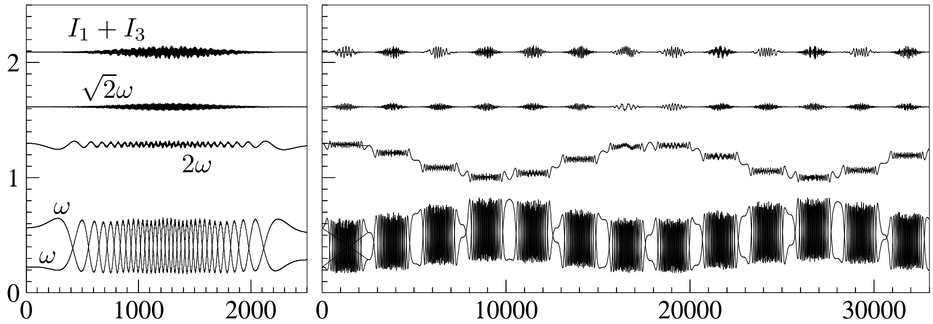

Figure 1.1: Oscillatory energies of the individual components (the frequencies $\lambda_j\omega = \lambda_j/\varepsilon$ are indicated) and the sum $I_1 + I_3$ of the oscillatory energies corresponding to the resonant frequencies ω and 2ω.

fact that quadratic terms in $U(x)$ can no longer be neglected and perturb the resonant frequencies. The same observation can be made if $U(x)$ is kept unchanged but $\lambda_1 = 1$ is replaced by $\lambda_1 = 1 + \varepsilon^2$.

In this article we study the long-time preservation of $H(x, \dot{x})$ and $I_\mu(x, \dot{x})$ along numerical solutions obtained by integrators that solve the linear part of the differential equation exactly and reduce to the Störmer–Verlet method if only the term for $\ell = 0$ is present in the sum (1.1). We begin with presenting the main results and we illustrate them with numerical experiments (Section 2). The proof of the main theorem is based on an extension of the technique of modulated Fourier expansions to the multi-frequency case (Section 3) and on the existence of formal invariants for the coefficient functions of this expansion (Section 4). In Section 5 we describe the extension of the long-time energy conservation results to the Störmer-Verlet method. We finally apply, in Section 6, the approach of modulated Fourier expansions to the analytical problem. We show that under the weak non-resonance condition

$$|k \cdot \lambda| \geq c\sqrt{\varepsilon} \quad \text{for } k \in \mathbb{Z}^\ell \setminus \mathcal{M} \text{ with } |k| \leq N \tag{1.8}$$

(where $k \cdot \lambda = k_1\lambda_1 + \ldots + k_\ell\lambda_\ell$ and $|k| = |k_1| + \ldots + |k_\ell|$) the expression $I_\mu(x, \dot{x})$ with $\mu \perp \mathcal{M}_N := \{k \in \mathcal{M} : |k| \leq N\}$ is approximately preserved over intervals of length $\mathcal{O}(\varepsilon^{-N+1})$. Condition (1.8) is the analogue of a non-resonance condition that will be required for the numerical discretization.

2 Main result and numerical experiments

The equations of motion for the Hamiltonian system (1.1) can be written as the system of second-order differential equations

$$\ddot{x} = -\Omega^2 x + g(x), \tag{2.1}$$

where $\Omega = \mathrm{diag}(\omega_j I)$ with $\omega_j = \lambda_j/\varepsilon$ and $g(x) = -\nabla U(x)$. We consider the class of numerical methods studied in [5] and [6, Chapter XIII]. With the step size h, these methods can be given in the two-step form (with subscripts now refering to the time step, not to components)

$$x_{n+1} - 2\cos(h\Omega)x_n + x_{n-1} = h^2 \Psi g(\Phi x_n). \tag{2.2}$$

Here $\Psi = \psi(h\Omega)$ and $\Phi = \phi(h\Omega)$, where the filter functions ψ and ϕ are real-valued bounded functions with $\psi(0) = \phi(0) = 1$. This is complemented by a velocity approximation given by

$$2h\,\mathrm{sinc}(h\Omega)\dot{x}_n = x_{n+1} - x_{n-1} \tag{2.3}$$

provided that $\mathrm{sinc}(h\Omega)$ is invertible. Here $\mathrm{sinc}(\xi) = \sin(\xi)/\xi$. This class of methods gives the exact solution for $g = 0$ and reduces to the Störmer–Verlet method for $\Omega = 0$. It includes as special cases various methods proposed and studied by Gautschi [4] ($\psi(\xi) = \mathrm{sinc}^2(\xi/2)$, $\phi(\xi) = 1$), Deuflhard [2] ($\psi(\xi) = \mathrm{sinc}(\xi)$, $\phi(\xi) = 1$), García-Archilla, Sanz-Serna and Skeel [3] ($\psi(\xi) = \mathrm{sinc}(\xi)\phi(\xi)$), and Hochbruck and Lubich [7] ($\psi(\xi) = \mathrm{sinc}^2(\xi/2)$). The interest in such methods comes from the fact that they can be used with long time steps for which $h\omega_j$ need not be small.

We note that the method can be rewritten as a symmetric one-step method $(x_n, \dot{x}_n) \mapsto (x_{n+1}, \dot{x}_{n+1})$ on substituting x_{n-1} from (2.3) into (2.2). We always assume that the second starting value x_1 for (2.2) is obtained in this way.

We are interested in the long-time near-conservation of the total energy $H(x, \dot{x})$ and the oscillatory energies $I_\mu(x, \dot{x})$ for $\mu \perp \mathcal{M}$ along numerical solutions $(x_n, \dot{x}_n)$ obtained with step sizes that are not small compared to ε. We make the following assumptions, cf. [6, p. 447]:

- The energy of the initial values is bounded independently of ε,

$$\frac{1}{2}\|\dot{x}_0\|^2 + \frac{1}{2}\|\Omega x_0\|^2 \le E\ . \tag{2.4}$$

- The numerical solution values Φx_n stay in a compact subset of a domain on which the potential U is smooth.

- We impose a lower bound on the step size: $h/\varepsilon \ge c_0 > 0$.

- We assume the numerical non-resonance condition

$$\Big|\sin\Big(\frac{h}{2\varepsilon}\,k\cdot\lambda\Big)\Big| \ge c\sqrt{h} \quad \text{for all } k \in \mathbb{Z}^\ell \setminus \mathcal{M} \text{ with } |k| \le N, \tag{2.5}$$

  for some $N \ge 2$ and $c > 0$.

- The filter function $\psi(\xi)$ satisfies, with $\xi_j = h\omega_j = h\lambda_j/\varepsilon$,

$$|\psi(\xi_j)| \le C\,\big|\mathrm{sinc}\big(\tfrac{1}{2}\,\xi_j\big)\big| \quad \text{for } j = 1, \dots, \ell. \tag{2.6}$$

Notice that these conditions guarantee first order convergence on finite time intervals (cf. Theorem XIII.4.1 of [6], page 427).

We then have the following main result of this paper which we split into two theorems. They extend Theorem 7.1 of [5] (or Theorem XIII.7.1 of [6]) to multi-frequency systems. In the first theorem we consider in addition the conditions

$$|\psi(\xi_j)| \le C \operatorname{sinc}^2\big(\tfrac{1}{2}\xi_j\big), \tag{2.7}$$

$$|\psi(\xi_j)| \le C\,|\phi(\xi_j)| \qquad \text{for } j = 1,\dots,\ell. \tag{2.8}$$

THEOREM 2.1. *Under the above conditions (2.4)–(2.6) and additionally (2.7) and (2.8), the numerical solution obtained by the method (2.2)–(2.3) satisfies*

$$\begin{aligned} H(x_n,\dot x_n) &= H(x_0,\dot x_0) + \mathcal{O}(h) && \text{for } 0 \le nh \le \sigma_0 h\cdot \min(\varepsilon^{-M+1}, h^{-N}) \\ I_j(x_n,\dot x_n) &= I_j(x_0,\dot x_0) + \mathcal{O}(h) && \text{for } 0 \le nh \le \sigma_j h\cdot \min(\varepsilon^{-M+1}, h^{-N}) \end{aligned}$$

for $j = 1,\dots,\ell$. Here, $M = \min\{|k| : 0 \ne k \in \mathcal{M}\}$, $\sigma_j = |\sigma(\xi_j)|$, and $\sigma_0 = \min\{1,\sigma_1,\dots,\sigma_\ell\}$, where $\sigma(\xi) = \operatorname{sinc}(\xi)\phi(\xi)/\psi(\xi)$. Without the condition (2.7) the statement is still true with the error term $\mathcal{O}(h)$ replaced by $\mathcal{O}(\sqrt{h})$. The constants symbolized by $\mathcal{O}$ are independent of n, h, ε, λ_j satisfying the above conditions, but depend on N and the constants in the conditions.

Note, $\sigma_0 \ge c_1\,\varepsilon/\sqrt{h}$ with $c_1 > 0$ by (2.5) and (2.8). For the non-resonant case $\mathcal{M} = \{0\}$ we have $M = \infty$ and hence the length of the interval with energy conservation is only restricted by (2.5). Notice that always $M \ge 3$, and that $M = 3$ only in the case of a 1:2 resonance among the λ_j. For a 1:3 resonance we have $M = 4$ and in all other cases $M \ge 5$.

Considering the modified energies

$$H^*(x,\dot x) = H(x,\dot x) + \sum_{j=1}^{\ell}\big(\sigma(\xi_j) - 1\big)\, I_j(x,\dot x) \tag{2.9}$$

$$I_\mu^*(x,\dot x) = \sum_{j=1}^{\ell} \sigma(\xi_j)\,\frac{\mu_j}{\lambda_j}\, I_j(x,\dot x) \tag{2.10}$$

with $\xi_j = h\lambda_j/\varepsilon$ and $\sigma(\xi) = \operatorname{sinc}(\xi)\phi(\xi)/\psi(\xi)$, we can prove their conservation over even longer time intervals. Here we consider the additional condition

$$|\phi(\xi_j)| \le C\,\big|\operatorname{sinc}\big(\tfrac{1}{2}\xi_j\big)\big| \quad \text{for } j = 1,\dots,\ell. \tag{2.11}$$

THEOREM 2.2. *Under the conditions (2.4)–(2.6) and additionally (2.11), the numerical solution obtained by the method (2.2)–(2.3) satisfies*

$$\left.\begin{aligned} H^*(x_n,\dot x_n) &= H^*(x_0,\dot x_0) + \mathcal{O}(h) \\ I_\mu^*(x_n,\dot x_n) &= I_\mu^*(x_0,\dot x_0) + \mathcal{O}(h) \end{aligned}\right. \qquad \text{for} \quad 0 \le nh \le h^{-N+1}$$

for $\mu \in \mathbb{R}^\ell$ with $\mu \perp \mathcal{M}_N = \{k \in \mathcal{M} : |k| \le N\}$. Without the condition (2.11) the statement is still true with the error term $\mathcal{O}(h)$ replaced by $\mathcal{O}(\sqrt{h})$. The *constants symbolized by $\mathcal{O}$ are independent of n, h, ε, λ_j satisfying the above conditions, but depend on N and the constants in the conditions.*

Since $\mu = \lambda$ is always orthogonal to $\mathcal{M}$ and to $\mathcal{M}_N$, the relation

$$K(x, \dot{x}) = H^*(x, \dot{x}) - I_\lambda^*(x, \dot{x})$$

for the smooth energy (1.6) implies

$$K(x_n, \dot{x}_n) = K(x_0, \dot{x}_0) + \mathcal{O}(h) \qquad \text{for} \quad 0 \le nh \le h^{-N+1}. \tag{2.12}$$

The analysis of Sections 3 and 4 below shows that this estimate is true without the assumptions (2.7), (2.8), and (2.11).

Notice that for $\sigma(\xi) = 1$ (or equivalently $\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi)$) the modified energies (2.9) and (2.10) are identical to the original energies (1.1) and (1.4). The condition $\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi)$ is known to be equivalent to the symplecticity of the one-step method $(x_n, \dot{x}_n) \mapsto (x_{n+1}, \dot{x}_{n+1})$, but its appearance in the above theorem is caused by a different mechanism which is not in any obvious way related to symplecticity.

Numerical experiment. We consider the initial value problem described in the introduction, we apply several numerical methods, and we compare the oscillatory energies along the numerical solution with those of the exact solution.

As a first method we take (2.2) with $\phi(\xi) = 1$ and $\psi(\xi) = \operatorname{sinc}(\xi)$, and we apply it to the differential equation with large step sizes so that $h\omega = h/\varepsilon$ takes the values 1, 2, 4, and 8. Figure 2.1 shows the various oscillatory energies which can be compared to the exact values in Fig. 1.1. For all step sizes, the oscillatory energy corresponding to the frequency $\sqrt{2}\omega$ and the sum $I_1 + I_3$ are well conserved on long time intervals. Oscillations in these expressions increase with h. The energy exchange between resonant frequencies is close to that of the exact solution for $h = 1/\omega$. It changes for larger step sizes. We have not plotted the total energy $H(x_n, \dot{x}_n)$ nor the smooth energy $K(x_n, \dot{x}_n)$ of (1.6). Both are well conserved over long times. The total energy shows oscillations of a size similar to that of I_2 or $I_1 + I_3$. The size of the oscillations in $K(x_n, \dot{x}_n)$ is smaller and independent of the chosen values for the step size.

We repeat this experiment with the method where $\phi(\xi) = 1$ and $\psi(\xi) = \operatorname{sinc}^2(\xi/2)$ (Fig. 2.2). Only the oscillatory energy corresponding to $\sqrt{2}\omega$ is approximately conserved over long times. It is not surprising that neither the expression $I_1 + I_3$ nor the total energy (not shown) are conserved, because the defining functions of the method do not satisfy $\sigma(\xi) = 1$. In fact, if we plotted the modified energy (2.10), good conservation would be observed. Also the smooth energy $K(x_n, \dot{x}_n)$ is well conserved.

Figure 2.3 shows the corresponding result for the method with $\phi(\xi) = \operatorname{sinc}(\xi)$ and $\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi)$. Since $\sigma(\xi) = 1$, the oscillatory energy for $\sqrt{2}\omega$ and also $I_1 + I_3$ are well conserved. However, the energy exchange between the resonant frequencies is not correctly reproduced.

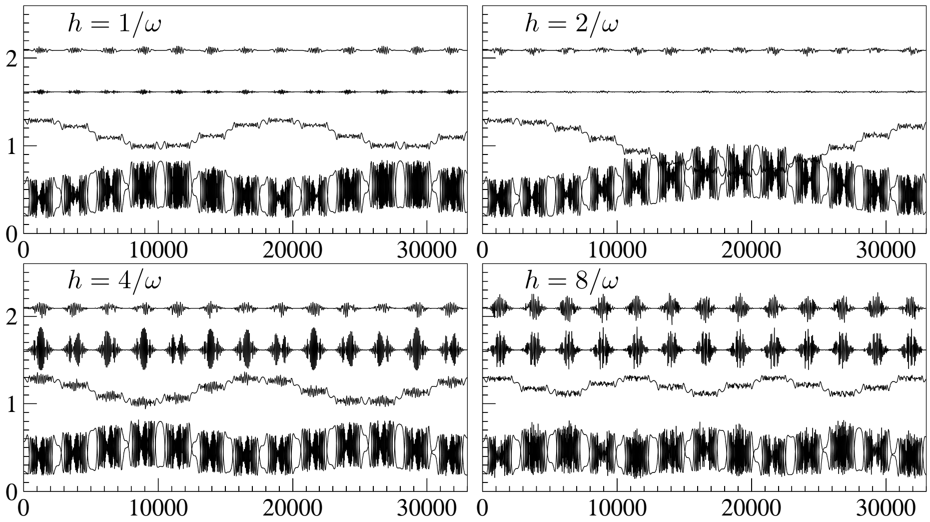

Figure 2.1: Oscillatory energies as in Fig. 1.1 along the numerical solution of (2.2) with $\phi(\xi) = 1$ and $\psi(\xi) = \operatorname{sinc}(\xi)$. Notice that for this method $\sigma(\xi) = 1$.

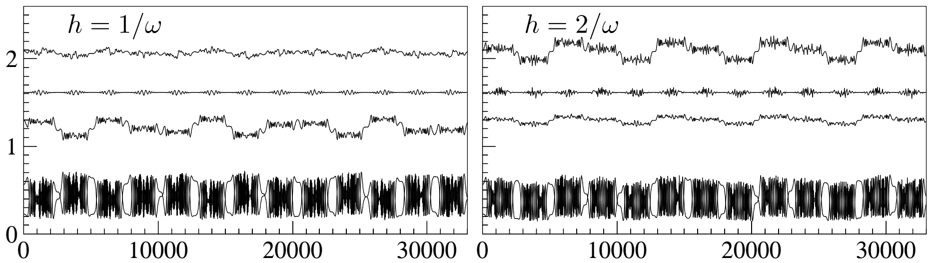

Figure 2.2: Oscillatory energies as in Fig. 1.1 along the numerical solution of (2.2) with $\phi(\xi) = 1$ and $\psi(\xi) = \operatorname{sinc}^2(\xi/2)$.

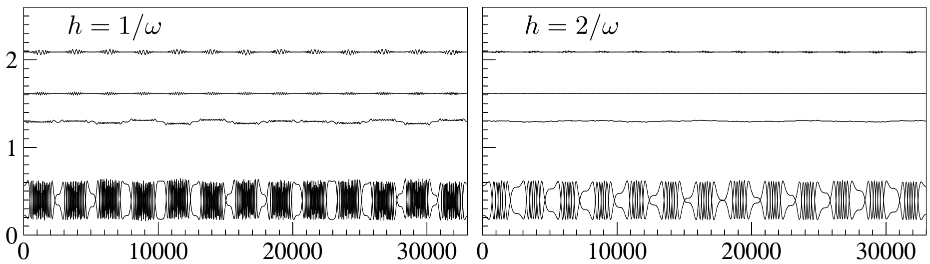

Figure 2.3: Oscillatory energies as in Fig. 1.1 along the numerical solution of (2.2) with $\phi(\xi) = \operatorname{sinc}(\xi)$ and $\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi)$.

3 Modulated Fourier expansions

For a given vector $\lambda = (\lambda_1, \dots, \lambda_\ell)$ and for the resonance module $\mathcal{M}$ defined by (1.2), we let $\mathcal{K}$ be a set of representatives of the equivalence classes in $\mathbb{Z}^\ell/\mathcal{M}$ which are chosen such that for each $k \in \mathcal{K}$ the sum $|k| = |k_1|+\ldots+|k_\ell|$ is minimal in the equivalence class $[k] = k + \mathcal{M}$, and that with $k \in \mathcal{K}$, also $-k \in \mathcal{K}$. We denote, for N of (2.5),

$$\mathcal{N} = \{k \in \mathcal{K} : |k| < N\}, \qquad \mathcal{N}^* = \mathcal{N} \setminus \{(0,\dots,0)\}. \tag{3.1}$$

The following result establishes a modulated Fourier expansion for the numerical solution. It is the multi-frequency version of Theorem XIII.5.2 of [6]. Its proof follows the lines of the proof of that theorem, with rather obvious adaptations.

Theorem 3.1. *Consider the numerical solution of the system (2.1) by the method (2.2) with step size h. Under the conditions (2.4)–(2.6), the numerical solution admits an expansion*

$$x_n \;=\; y(t) + \sum_{k\in\mathcal{N}^*} \mathrm{e}^{\mathrm{i}k\cdot\omega t} z^k(t) + \Psi \cdot \mathcal{O}(t^2 h^N) \tag{3.2}$$

with $\omega = \lambda/\varepsilon$, uniformly for $0 \le t = nh \le T$ and ε and h satisfying $h/\varepsilon \ge c_0 > 0$. The modulation functions together with all their derivatives (up to some arbitrarily fixed order) are bounded by

$$\begin{aligned} y_0 \;&=\; \mathcal{O}(1), \qquad & y_j \;&=\; \mathcal{O}\Big(\frac{\varepsilon^2\psi(\xi_j)}{\mathrm{sinc}^2(\xi_j/2)}\Big)\\ z_j^{\pm\langle j\rangle} \;&=\; \mathcal{O}(\varepsilon), \qquad & \dot z_j^{\pm\langle j\rangle} \;&=\; \mathcal{O}\Big(\frac{\varepsilon^2\psi(\xi_j)}{\mathrm{sinc}(\xi_j)}\Big)\\ z_j^k \;&=\; \mathcal{O}\big(h\varepsilon^{|k|}\psi(\xi_j)\big) \quad \text{for } k \ne \pm\langle j\rangle && \end{aligned} \tag{3.3}$$

for $j = 1,\dots,\ell$. Here, $\langle j\rangle = (0,\dots,1,\dots,0)$ is the jth unit vector. The last estimate holds also for z_0^k for all $k \in \mathcal{N}^*$.

Moreover, the function y is real-valued and $z^{-k} = \overline{z^k}$ for all $k \in \mathcal{N}^*$. The constants symbolized by the $\mathcal{O}$-notation are independent of h, ε and λ_j with (2.5), but they depend on E, N, c, and T.

In terms of the difference operator of the method (2.2),

$$\begin{aligned} L(hD) \;&:=\; \mathrm{e}^{hD} - 2\cos h\Omega + \mathrm{e}^{-hD} \;=\; 2\big(\cos(\mathrm{i}hD) - \cos h\Omega\big)\\ &=\; 4\,\sin\big(\tfrac12 h\Omega + \tfrac12 \mathrm{i}hD\big)\sin\big(\tfrac12 h\Omega - \tfrac12 \mathrm{i}hD\big) \end{aligned} \tag{3.4}$$

(with D denoting the differentiation operator), the functions $y(t)$ and $z^k(t)$ are constructed such that, up to terms of size $\Psi \cdot \mathcal{O}(h^{N+2})$,

$$\begin{aligned} L(hD)y &= h^2\Psi\Big(g(\Phi y) + \sum_{s(\alpha)\sim 0} \frac{1}{m!}\, g^{(m)}(\Phi y)(\Phi z)^\alpha\Big)\\ L(hD + \mathrm{i}hk\cdot\omega)z^k &= h^2\Psi \sum_{s(\alpha)\sim k} \frac{1}{m!}\, g^{(m)}(\Phi y)(\Phi z)^\alpha. \end{aligned} \tag{3.5}$$

Here, the sums on the right-hand side are over all $m \geq 1$ and over multi-indices $\alpha = (\alpha_1, \ldots, \alpha_m)$ with $\alpha_j \in \mathcal{N}^*$, for which the sum $s(\alpha) = \sum_{j=1}^m \alpha_j$ satisfies the relation $s(\alpha) \sim k$, which means $s(\alpha) - k \in \mathcal{M}$. The notation $(\Phi z)^\alpha$ is short for the m-tuple $(\Phi z^{\alpha_1}, \ldots, \Phi z^{\alpha_m})$. We remark that the equations (3.5) arise from the fact that for $y^k(t) = \mathrm{e}^{\mathrm{i}k\cdot\omega t} z^k(t)$ we have

$$L(hD) y^k(t) = \mathrm{e}^{\mathrm{i}k\cdot\omega t} L(hD + \mathrm{i}hk\cdot\omega) z^k(t), \tag{3.6}$$

and from collecting all terms with the same factor $\mathrm{e}^{\mathrm{i}k\cdot\omega t}$ on the right-hand side after a Taylor expansion of the nonlinearity around Φy.

A similar expansion to that for x_n exists also for the velocity approximation $\dot{x}_n$, cf. [6, Theorem XIII.5.3].

Theorem 3.2. *Under the conditions of Theorem 3.1, the velocity approximation admits an expansion*

$$\dot{x}_n \;=\; v(t) + \sum_{k\in\mathcal{N}^*} \mathrm{e}^{\mathrm{i}k\cdot\omega t} w^k(t) + \mathcal{O}(t^2 h^{N-1}) \tag{3.7}$$

uniformly for $0 \leq t = nh \leq T$. The modulation functions together with all their derivatives up to arbitrary order satisfy

$$\begin{aligned} v_0 &= \dot{y}_0 + \mathcal{O}(h^2), \qquad v_j \;=\; \mathcal{O}\Big(\frac{\varepsilon^2\psi(\xi_j)}{\mathrm{sinc}^2(\xi_j/2)\,\mathrm{sinc}(\xi_j)}\Big) \\ w_j^{\pm\langle j\rangle} &= \pm\mathrm{i}\omega_j z_j^{\pm\langle j\rangle} + \mathcal{O}\Big(\frac{\varepsilon^2\psi(\xi_j)}{\mathrm{sinc}^2(\xi_j)}\Big) \\ w_j^k &= \mathcal{O}\Big(\frac{h\varepsilon^{|k|}\psi(\xi_j)}{\mathrm{sinc}(\xi_j)}\Big) \qquad \textit{for}\;\; k \neq \pm\langle j\rangle. \end{aligned} \tag{3.8}$$

Moreover, $w^{-k} = \overline{w^k}$ for all $k \in \mathcal{N}^*$. The constants symbolized by the $\mathcal{O}$-notation are independent of h, ε and λ_j with (2.5), but they depend on E, N, c, and T.

As a consequence of Theorems 3.1 and 3.2, the oscillatory energy (1.3) along the numerical solution takes the form

$$I_j(x_n, \dot{x}_n) = 2\omega_j^2\, \|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}\Big(\frac{\varepsilon\psi(\xi_j)}{\mathrm{sinc}^2(\xi_j/2)}\Big) + \mathcal{O}\big(h\psi(\xi_j)\big) \tag{3.9}$$

for $t = nh \leq T$. The assumptions (2.5) and (2.6) thus yield the estimate $I_j(x_n, \dot{x}_n) = 2\omega_j^2\, \|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}(\sqrt{h})$ and, together with (2.7), we get the sharper formula $I_j(x_n, \dot{x}_n) = 2\omega_j^2\, \|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}(\varepsilon)$.

4 Almost-invariants

The coefficients of the modulated Fourier expansion of the numerical solution have almost-invariants that are related to the Hamiltonian H and the oscillatory energies I_μ with $\mu \perp \mathcal{M}$. This comes as a consequence of the fact that the system (3.5) still has a close-to-Hamiltonian structure. To see this, we introduce

$$\mathbf{y} = (y^k)_{k\in\mathcal{N}}, \qquad \mathbf{z} = (z^k)_{k\in\mathcal{N}}$$

with $y^0(t) = z^0(t) = y(t)$ and $y^k(t) = \mathrm{e}^{\mathrm{i}k\cdot\omega t} z^k(t)$ for $k \in \mathcal{N}$, where y and z^k are the modulation functions of Theorem 3.1. We introduce the extended potential

$$\mathcal{U}(\mathbf{y}) \;=\; U(\Phi y^0) + \sum_{s(\alpha)\sim 0} \frac{1}{m!}\, U^{(m)}(\Phi y^0)(\Phi \mathbf{y})^\alpha \;, \tag{4.1}$$

where the sum is again taken over all $m \geq 1$ and all multi-indices $\alpha = (\alpha_1, \ldots, \alpha_m)$ with $\alpha_j \in \mathcal{N}^*$ for which $s(\alpha) = \sum_j \alpha_j \in \mathcal{M}$. It then follows from (3.5) that the functions $y^k(t)$ satisfy

$$\Psi^{-1}\Phi\, h^{-2} L(hD)\, y^k \;=\; -\nabla_{-k}\,\mathcal{U}(\mathbf{y}) + \Phi \cdot \mathcal{O}(h^N), \tag{4.2}$$

where ∇_{-k} denotes the gradient with respect to the variable y^{-k}. This system has various almost-invariants, as we show next.

4.1 The energy-type almost-invariant of the modulation system

We multiply (4.2) by $(\dot y^{-k})^T$ and sum over $k \in \mathcal{N}$ to obtain

$$\sum_{k\in\mathcal{N}} (\dot y^{-k})^T \Psi^{-1}\Phi\, h^{-2} L(hD) y^k + \frac{d}{dt}\mathcal{U}(\mathbf{y}) \;=\; \mathcal{O}(h^N).$$

Since we know bounds of the modulation functions z^k and of their derivatives from Theorem 3.1, we switch to the quantities z^k and we get the equivalent relation

$$\sum_{k\in\mathcal{N}} (\dot z^{-k} - \mathrm{i}k\cdot\omega z^{-k})^T \Psi^{-1}\Phi h^{-2} L(hD + \mathrm{i}hk\cdot\omega) z^k + \frac{d}{dt}\,\mathcal{U}(\mathbf{z}) = \mathcal{O}(h^N). \tag{4.3}$$

As in [6, p. 444] we obtain that the left-hand side of (4.3) can be written as the time derivative of a function $\mathcal{H}^*[\mathbf{z}](t)$ which depends on the values at t of the modulation-function vector $\mathbf{z}$ and its first N time derivatives. The relation (4.3) thus becomes

$$\frac{d}{dt}\mathcal{H}^*[\mathbf{z}](t) \;=\; \mathcal{O}(h^N).$$

Together with the estimates (3.3) and the decomposition (3.4), this construction of $\mathcal{H}^*$ yields the following multi-frequency extension of Lemma XIII.6.4 of [6].

LEMMA 4.1. *Under the assumptions of Theorem 3.1, the modulation functions* $\mathbf{z} = (z^k)_{k\in\mathcal{N}}$ *of the numerical solution satisfy*

$$\mathcal{H}^*[\mathbf{z}](t) \;=\; \mathcal{H}^*[\mathbf{z}](0) \;+\; \mathcal{O}(th^N) \tag{4.4}$$

for $0 \leq t \leq T$. *Moreover, with* $\sigma(\xi) = \mathrm{sinc}(\xi)\phi(\xi)/\psi(\xi)$ *we have*

$$\begin{aligned}\mathcal{H}^*[\mathbf{z}](t) \;=\; \frac{1}{2}\,\|\dot y_0(t)\|^2 + \sum_{j=1}^{\ell} \sigma(h\omega_j)\, 2\omega_j^2\, \|z_j^{\langle j\rangle}(t)\|^2 + U(\Phi y(t))\\ + \mathcal{O}(h^2) + \mathcal{O}(\varepsilon\sqrt{h}).\end{aligned} \tag{4.5}$$

By (3.9) and condition (2.11), which gives $|\sigma(\xi_j)\psi(\xi_j)/\mathrm{sinc}^2(\frac{1}{2}\xi_j)| \le C$ for $\xi_j = h\omega_j$, the relation (4.5) yields

$$\mathcal{H}^*[\mathbf{z}](t) \;=\; H^*(x_n, \dot{x}_n) + \mathcal{O}(h) \tag{4.6}$$

at $t = nh \le T$, with $H^*(x,\dot{x})$ of (2.9). Without the condition (2.11) the error is of size $\mathcal{O}(\sqrt{h})$.

4.2 The momentum-type almost-invariants of the modulation system

The equations (4.2) have further almost-invariants that result from invariance properties of the extended potential $\mathcal{U}$, similarly as the conservation of angular momentum results from an invariance of the potential U in a mechanical system by Noether's theorem. For $\mu \in \mathbb{R}^\ell$ and $\mathbf{y} = (y^k)_{k\in\mathcal{N}}$ we set

$$S_\mu(\tau)\mathbf{y} = (\mathrm{e}^{\mathrm{i}k\cdot\mu\tau} y^k)_{k\in\mathcal{N}}, \qquad \tau \in \mathbb{R}$$

so that, by the multi-linearity of the derivative, the definition (4.1) yields

$$\mathcal{U}\big(S_\mu(\tau)\mathbf{y}\big) \;=\; U(\Phi y^0) + \sum_{s(\alpha)\sim 0} \frac{\mathrm{e}^{\mathrm{i}s(\alpha)\cdot\mu\tau}}{m!}\, U^{(m)}(\Phi y^0)(\Phi\mathbf{y})^\alpha \;, \tag{4.7}$$

If $\mu \perp \mathcal{M}$, then the relation $s(\alpha) \sim 0$ implies $s(\alpha)\cdot\mu = 0$, and hence the expression (4.7) is independent of τ. It therefore follows that

$$0 = \frac{d}{d\tau}\Big|_{\tau=0} \mathcal{U}(S_\mu(\tau)\mathbf{y}) = \sum_{k\in\mathcal{N}} \mathrm{i}(k\cdot\mu)\,\big(y^k\big)^T \nabla_k \mathcal{U}(\mathbf{y})$$

for all vectors $\mathbf{y} = (y^k)_{k\in\mathcal{N}}$. If μ is not orthogonal to $\mathcal{M}$, some terms in the sum of (4.7) depend on τ. The same argument as before and the bounds (3.3) then yield

$$\sum_{k\in\mathcal{N}} \mathrm{i}(k\cdot\mu)\,\big(y^k\big)^T \nabla_k \mathcal{U}(\mathbf{y}) = \begin{cases} \mathcal{O}(\varepsilon^M) & \text{for arbitrary } \mu \\ \mathcal{O}(\varepsilon^{N+1}) & \text{for } \mu \perp \mathcal{M}_N \end{cases} \tag{4.8}$$

for the vector $\mathbf{y} = \mathbf{y}(t)$ as given by Theorem 3.1. Multiplying the relation (4.2) by $\frac{\mathrm{i}}{\varepsilon}(-k\cdot\mu)\big(y^{-k}\big)^T$ and summing over $k \in \mathcal{N}$, we obtain with (4.8) that

$$-\frac{\mathrm{i}}{\varepsilon}\sum_{k\in\mathcal{N}} (k\cdot\mu)(y^{-k})^T \Psi^{-1}\Phi\, h^{-2} L(hD) y^k \;=\; \mathcal{O}(h^N) + \mathcal{O}(\varepsilon^{M-1}).$$

The $\mathcal{O}(\varepsilon^{M-1})$ term can be removed for $\mu \perp \mathcal{M}_N$. Written in the z variables, this becomes

$$-\frac{\mathrm{i}}{\varepsilon}\sum_{k\in\mathcal{N}} (k\cdot\mu)(z^{-k})^T \Psi^{-1}\Phi\, h^{-2} L(hD + \mathrm{i}hk\cdot\omega) z^k \;=\; \mathcal{O}(h^N) + \mathcal{O}(\varepsilon^{M-1}). \tag{4.9}$$

As in (4.3), the left-hand expression can be written as the time derivative of a function $\mathcal{I}^*_\mu[\mathbf{z}](t)$ which depends on the values at t of the function $\mathbf{z}$ and its first N derivatives:

$$\frac{d}{dt}\mathcal{I}^*_\mu[\mathbf{z}](t) \;=\; \mathcal{O}(h^N) + \mathcal{O}(\varepsilon^{M-1}).$$

Together with the estimates of Theorem 3.1 this yields the following result.

LEMMA 4.2. *Under the assumptions of Theorem 3.1, the modulation functions* $\mathbf{z}$ *satisfy*

$$\mathcal{I}^*_\mu[\mathbf{z}](t) \;=\; \mathcal{I}^*_\mu[\mathbf{z}](0) \;+\; \mathcal{O}(th^N) + \mathcal{O}(t\varepsilon^{M-1}) \tag{4.10}$$

for all $\mu \in \mathbb{R}^\ell$ *and for* $0 \le t \le T$*. They satisfy*

$$\mathcal{I}^*_\mu[\mathbf{z}](t) \;=\; \mathcal{I}^*_\mu[\mathbf{z}](0) \;+\; \mathcal{O}(th^N) \tag{4.11}$$

for $\mu \perp \mathcal{M}_N$ *and* $0 \le t \le T$*. Moreover,*

$$\mathcal{I}^*_\mu[\mathbf{z}](t) \;=\; \sum_{j=1}^{\ell} \sigma(h\omega_j)\, \frac{\mu_j}{\lambda_j}\, 2\omega_j^2\, \|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}(\varepsilon\sqrt{h}), \tag{4.12}$$

where again $\sigma(\xi) = \mathrm{sinc}(\xi)\phi(\xi)/\psi(\xi)$.

By (3.9) and (2.11), the relation (4.12) implies

$$\mathcal{I}^*_\mu[\mathbf{z}](t) \;=\; I^*_\mu(x_n, \dot x_n) + \mathcal{O}(\varepsilon) \tag{4.13}$$

at $t = nh \le T$, with $I^*_\mu(x, \dot x)$ of (2.10). Without the assumption (2.11) we have an error of size $\mathcal{O}(\sqrt{h})$.

4.3 Proof of Theorems 2.1 and 2.2

With the proof of Theorem XIII.7.1 of [6, p. 447], which patches many short time intervals together, the estimates (4.4) and (4.6) yield directly the result for $H^*(x_n, \dot x_n)$ in Theorem 2.2. In the same way, (4.11) and (4.13) yield the result for $I^*_\mu(x_n, \dot x_n)$ in Theorem 2.2. Subtracting (4.12) with $\mu = \lambda$ from (4.5) yields the statement (2.12) for the smooth energy $K(x_n, \dot x_n)$. For the choice $\mu = \langle j\rangle$, the relations (4.10), (4.12) together with $|\sigma(h\omega_j)| \ge c_1\, \varepsilon/\sqrt{h}$ (which follows from (2.5) and (2.8)), and (3.9) with (2.7) yield the estimate for $I_j(x_n, \dot x_n)$ of Theorem 2.1. Combined with the estimate already shown for $K(x_n, \dot x_n)$, this finally gives the result for $H(x_n, \dot x_n)$ in Theorem 2.1.

5 Energy conservation of the Störmer–Verlet method

The Störmer–Verlet method applied to (2.1) reads

$$x_{n+1} - 2x_n + x_{n-1} = -h^2\Omega^2 x_n + h^2 g(x_n). \tag{5.1}$$

For linear stability it needs the step size restriction $h\omega_{\max} < 2$, where $\omega_{\max} = \max(\omega_j)$ with $\omega_j = \lambda_j/\varepsilon$. For such step sizes the method can be rewritten as a trigonometric method (2.2) with modified frequencies,

$$x_{n+1} - 2\cos(h\widetilde\Omega) x_n + x_{n-1} = h^2 g(x_n), \tag{5.2}$$

where

$$\widetilde{\Omega} = \mathrm{diag}(\widetilde{\omega}_j) \qquad \text{with} \qquad \sin\big(\tfrac{1}{2}h\widetilde{\omega}_j\big) = \tfrac{1}{2}h\omega_j. \tag{5.3}$$

This interpretation makes the Störmer–Verlet method accessible to the analysis of the preceding sections. Of course, the relevant resonance module is then that for the modified frequencies $\widetilde{\omega}_j$,

$$\widetilde{\mathcal{M}} = \{k \in \mathbb{Z}^\ell : k_1\widetilde{\omega}_1 + \ldots + k_\ell\widetilde{\omega}_\ell = 0\}, \tag{5.4}$$

which is in general entirely different from the resonance module $\mathcal{M}$ of the original system, unless both are 0. Moreover, the usual velocity approximation given by

$$2h\,\dot{x}_n = x_{n+1} - x_{n-1} \tag{5.5}$$

does not correspond to (2.3) with $\widetilde{\Omega}$ instead of Ω. As a consequence, the total and oscillatory energies $H(x_n, \dot{x}_n)$ and $I_j(x_n, \dot{x}_n)$ are not preserved up to $\mathcal{O}(h)$, but have $\mathcal{O}(h\omega_{\max})$ deviations even over short time intervals. Nevertheless, combining the results of Sections 3 and 4 with the arguments of [6, Theorem XIII.8.1], we obtain the long-time near-conservation of the modified energies

$$H^*(x,\dot{x}) = H(x,\dot{x}) + \frac{1}{2}\sum_{j=1}^{\ell}\gamma(\xi_j)\,\|\dot{x}_j\|^2 \tag{5.6}$$

$$I_j^*(x,\dot{x}) = I_j(x,\dot{x}) + \frac{1}{2}\gamma(\xi_j)\,\|\dot{x}_j\|^2 \tag{5.7}$$

with $\xi_j = h\omega_j = h\lambda_j/\varepsilon$ and $\gamma(\xi) = (1 - \frac{1}{4}\xi^2)^{-1} - 1$. In particular, this yields the near-conservation of the smooth energy (1.6),

$$K(x,\dot{x}) = H^*(x,\dot{x}) - \sum_{j=1}^{\ell} I_j^*(x,\dot{x}).$$

Moreover, by the arguments of [6, Theorem XIII.8.2], the Störmer–Verlet method also approximately preserves the time averages over intervals of a fixed length T of the total and oscillatory energies,

$$\overline{H}_n = \frac{h}{T}\sum_{|ih|\le T/2} H(x_{n+i}, \dot{x}_{n+i})$$

$$\overline{I}_{j,n} = \frac{h}{T}\sum_{|ih|\le T/2} I_j(x_{n+i}, \dot{x}_{n+i}).$$

Here we need the following assumptions in analogy to (2.4)–(2.6):

- The energy of the initial values has a bound independent of ε.
- The numerical solution values x_n stay in a compact subset of a domain on which the potential U is smooth.

- We impose lower and upper bounds on the step size:

$$0 < c_0 < h\omega_j < c_1 < 2 \qquad \text{for} \quad j = 1, \dots, \ell.$$

- We assume the numerical non-resonance condition

$$\Big|\sin\Big(\frac{1}{2}hk\cdot\widetilde{\omega}\Big)\Big| \ge c\sqrt{h} \quad \text{for all } k \in \mathbb{Z}^\ell \setminus \widetilde{\mathcal{M}} \text{ with } |k| \le N, \tag{5.8}$$

for some $N \ge 2$ and $c > 0$.

Theorem 5.1. *Under the above conditions, the smooth energy along the numerical solution* $(x_n, \dot{x}_n)$ *of the Störmer–Verlet method satisfies*

$$K(x_n, \dot{x}_n) = K(x_0, \dot{x}_0) + \mathcal{O}(h) \qquad \textit{for} \quad 0 \le nh \le h^{-N+1},$$

and the time averages of the total and oscillatory energies satisfy, for $j = 1, \dots, \ell$,

$$\begin{aligned} \overline{H}_n &= \overline{H}_0 + \mathcal{O}(h) \\ \overline{I}_{j,n} &= \overline{I}_{j,0} + \mathcal{O}(h) \end{aligned} \qquad \textit{for} \quad 0 \le nh \le h\,\min(\varepsilon^{-\widetilde{M}+1}, h^{-N}),$$

where $\widetilde{M} = \min\{|k| : 0 \ne k \in \widetilde{\mathcal{M}}\}$. *The constants symbolized by* $\mathcal{O}$ *are independent of* n, h, ε *with the above conditions.*

Numerical experiment. We apply the Störmer–Verlet method (5.1) to the problem of Example 1.1. The oscillatory energies along the numerical solution

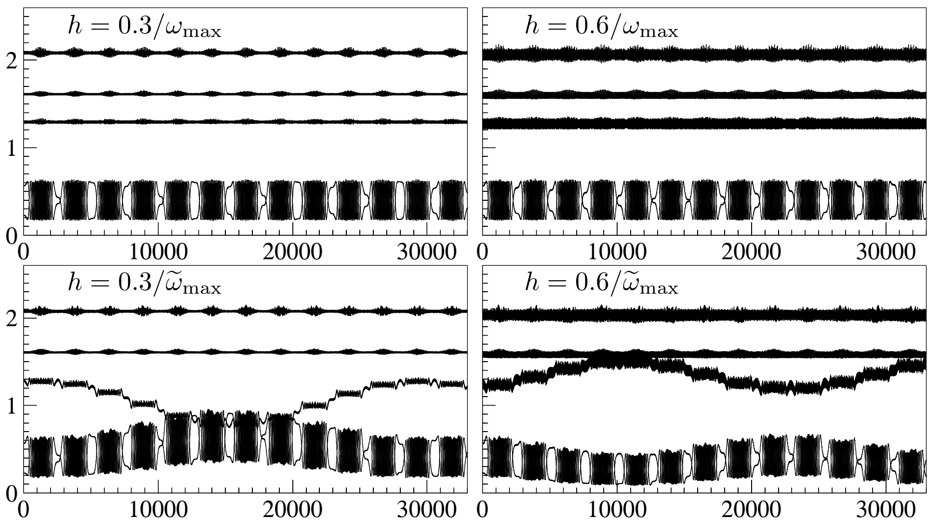

Figure 5.1: Oscillatory energies as in the figures of Section 2 for the Störmer–Verlet method; the two upper pictures correspond to $\omega_j = \lambda_j/\varepsilon$ with $\varepsilon = 1/70$ and $\lambda = (1, \sqrt{2}, 2)$; the two lower pictures correspond to $\omega_j = \sin(h\widetilde{\omega}_j/2)\cdot 2/h$ with $\widetilde{\omega}_j = \lambda_j/\varepsilon$ and the same λ_j and ε as before.

are shown in the upper two pictures of Fig. 5.1 for two different step sizes. Since for our choice of step sizes $\gamma(\xi_j)$ is not larger than 0.1, the perturbation terms of (5.7) can hardly be observed. In contrast to the exact solution (see Fig. 1.1), there is no energy exchange between the energies corresponding to resonant frequencies. If we perturb the frequencies ω_j in such a way that the modified frequencies $\widetilde{\omega}_j$ of (5.3) take the values $(1,\sqrt{2},2)/\varepsilon$, we recover the energy exchange in the numerical solution, though now there is no exchange in the continuous problem. This example demonstrates that in the presence of resonance the energy exchange is not correctly reproduced for step sizes with relatively large $h\omega_{\max}$.

6 Oscillatory energies along the exact solution

The techniques of Sections 3 and 4 can also be applied to the exact solution of the Hamiltonian system (1.1). This then yields the following result.

THEOREM 6.1. *Assume the energy bound (2.4) and let N be such that the non-resonance condition (1.8) is satisfied. As long as the exact solution of the system stays in a compact subset of a domain on which the potential $U(x)$ is smooth, we have*

$$I_j\big(x(t),\dot x(t)\big) \;=\; I_j\big(x(0),\dot x(0)\big)+\mathcal{O}(\varepsilon) \quad \text{for } 0\le t\le \varepsilon\cdot\min(\varepsilon^{-M+1},\varepsilon^{-N}) \tag{6.1}$$

for $j=1,\dots,\ell$. The integer $M=\min\{|k|:0\ne k\in\mathcal{M}\}$ is as in Theorem 2.1. We further have

$$I_\mu\big(x(t),\dot x(t)\big) \;=\; I_\mu\big(x(0),\dot x(0)\big)+\mathcal{O}(\varepsilon) \quad \text{for } 0\le t\le \varepsilon^{-N+1} \tag{6.2}$$

for $\mu\in\mathbb{R}^\ell$ with $\mu\perp\mathcal{M}_N=\{k\in\mathcal{M}:|k|\le N\}$. The constants symbolized by $\mathcal{O}$ are independent of t, ε, λ_j satisfying the above conditions, but depend on N and the constants in the conditions.

The statement (6.2) is in complete agreement with the results of [1] where estimates on exponentially long time intervals are provided for $\mu\perp\mathcal{M}$. The formula (6.1) gives information about the energy exchange in the presence of resonance.

The idea of the proof is to write the exact solution $x(t)$ of the problem as

$$x(t) \;=\; y(t)+\sum_{k\in\mathcal{N}^*}\mathrm{e}^{\mathrm{i}k\cdot\omega t}z^k(t)+\mathcal{O}(t^2\varepsilon^N). \tag{6.3}$$

In complete analogy to Theorem 3.1 the modulation functions $z^k(t)$ together with their derivatives are bounded on finite time intervals by

$$y_0=\mathcal{O}(1),\;\; y_j=\mathcal{O}(\varepsilon^2),\;\; z_j^{\pm\langle j\rangle}=\mathcal{O}(\varepsilon),\;\; \dot z_j^{\pm\langle j\rangle}=\mathcal{O}(\varepsilon^2),\;\; z_j^k=\mathcal{O}(\varepsilon^{|k|+1}). \tag{6.4}$$

They are determined such that $y^k(t)=\mathrm{e}^{\mathrm{i}k\cdot\omega t}z^k(t)$ satisfy

$$\ddot y^k+\Omega^2y^k \;=\; -\nabla_{-k}\mathcal{U}(\mathbf{y})+\mathcal{O}(\varepsilon^N), \tag{6.5}$$

which is the analogue of (4.2). Here, $\mathcal{U}(\mathbf{y})$ is defined as in (4.1) without the factors Φ. With (6.4) and (6.5) instead of (3.3) and (4.2), the analysis of Sections 3 and 4 proves the theorem.

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