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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 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.

AMS subject classification (2000): 65L05, 65P10.

Key words: Gautschi-type numerical methods, Störmer–Verlet method, Hamiltonian systems, modulated Fourier expansion, energy conservation, oscillatory solutions.

1 Introduction.

An important aspect in the numerical treatment of Hamiltonian systems is the approximate conservation of the total energy over long times, as well as the near-conservation of further invariants and of almost-invariants (adiabatic invariants) that are present in oscillatory systems with multiple time scales. For symplectic methods used with step sizes h that are much smaller than the inverse of the highest frequency ω in the linearized system, long-time near-conservation of the total energy and of adiabatic invariants are obtained with the help of backward error analysis, which interprets the numerical method as the (almost) exact flow of a modified Hamiltonian system, up to exponentially small terms $\mathcal{O}(\mathrm{e}^{-c/(h\omega)})$; see [3, 8, 13, 14] and [11, Ch. IX].

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This very useful technique is, however, not applicable for methods used with (large) step sizes for which the product $h\omega$ is bounded away from 0. In molecular dynamics, the Störmer–Verlet method is often used with $h\omega \approx \frac{1}{2}$, and in wave equations with the Courant number $h\omega \approx 1$. Specially constructed long-time-step methods, such as the trigonometric integrators in [5–7, 12] and [11, Ch. XIII], are designed to be used with large $h\omega$.

For a class of nonlinear model problems with a single constant high frequency ω, long-time near-conservation of the total and oscillatory energy by trigonometric integrators and the Störmer–Verlet method, used with $h\omega$ bounded away from 0, has been studied in [9, 10] and [11, Ch. XIII]. The basic tool are modulated Fourier expansions, which represent the exact and numerical solution by a series of oscillatory exponentials $\mathrm{e}^{\mathrm{i}k\omega t}$ (with integer k) multiplied with slowly varying coefficient functions. The system determining the coefficient functions has a near-Hamiltonian structure that permits to conclude to the almost-conservation of the total and oscillatory energy along the numerical solution (and along the exact solution, see also [4]). The near-conservation of the oscillatory energy along the exact solution can also be proved using coordinate transforms of Hamiltonian perturbation theory [1]. However, this does not seem possible for the numerical discretization, in particular because symplecticity of the numerical method is not required (it may even be an obstacle to the correct slow energy exchange, see [11, Sects. XIII.2.4 and XIII.4.2]), whereas the symmetry of the methods plays an essential role.

In this paper we extend the long-time energy preservation results of [9, 10] and [11, Ch. XIII] to oscillatory systems with several high frequencies. Modulated Fourier expansions are again the basic analytical tool. A new aspect is possible resonance among the frequencies.

We begin with a description of the analytical problem (Section 2), for which various energies are approximately conserved. We then present the main results and illustrate them with numerical experiments (Section 3). We show the long-time preservation of the total and oscillatory energies along numerical solutions obtained by trigonometric integrators that solve the linear part of the differential equation exactly and reduce to the Störmer–Verlet method if no high frequencies are present. The proof of the main theorem is based on the extension of the technique of modulated Fourier expansions to the multi-frequency case (Section 4) and on the existence of formal invariants for the coefficient functions of this expansion (Section 5). In these proofs we assume some familiarity of the reader with the corresponding proofs for the single-frequency case and, to keep the presentation within a reasonable length, we thus concentrate on those aspects which are new in the multi-frequency case. In Section 6 we describe the extension of the long-time energy conservation results to the Störmer–Verlet method. We finally apply, in Section 7, the approach of modulated Fourier expansions to the analytical problem.

2 Oscillatory energies and resonances.

We consider Hamiltonian systems with Hamiltonian function

$$H(x,\dot x) = \frac12 \sum_{j=0}^{\ell} \left(\|\dot x_j\|^2 + \frac{\lambda_j^2}{\varepsilon^2}\|x_j\|^2 \right) + U(x), \tag{2.1}$$

where $x = (x_0, x_1, \dots, x_\ell)$ with $x_j \in \mathbb{R}^{d_j}$, $\lambda_0 = 0$ and $\lambda_j \ge 1$ are distinct real numbers, ε is a small positive parameter, and $U(x)$ is a smooth potential function. We are interested in the multi-frequency case $\ell > 1$.

Following [2] we consider the resonance module

$$\mathcal{M} = \{k \in \mathbb{Z}\ell : k_1\lambda_1 + \cdots + k_\ell\lambda_\ell = 0\} \tag{2.2}$$

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

$$I_j(x,\dot x) = \frac12 \left(\|\dot x_j\|^2 + \frac{\lambda_j^2}{\varepsilon^2}\|x_j\|^2 \right). \tag{2.3}$$

In [2] it is shown that under a diophantine non-resonance condition outside $\mathcal{M}$ the quantities

$$I_\mu(x,\dot x) = \sum_{j=1}^{\ell} \frac{\mu_j}{\lambda_j} I_j(x,\dot x) \tag{2.4}$$

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

$$\mu = (\mu_1, \dots, \mu_\ell) \quad \text{is orthogonal to } \mathcal{M}. \tag{2.5}$$

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 (2.1), we see that also the *smooth energy*

$$K(x,\dot x) = \frac12 \|\dot x_0\|^2 + U(x) \tag{2.6}$$

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, $H_0(x_0,\dot x_0) = \frac12\|\dot x_0\|^2 + U(x_0, 0, \dots, 0)$.

In Section 7 we apply the approach of modulated Fourier expansions to the analytical problem. We show that under the weak non-resonance condition

$$|k\cdot\lambda| \ge c\sqrt{\varepsilon} \quad \text{for } k \in \mathbb{Z}^\ell \setminus \mathcal{M} \text{ with } |k| \le N \tag{2.7}$$

(where $k\cdot\lambda = k_1\lambda_1 + \cdots + k_\ell\lambda_\ell$ and $|k| = |k_1| + \cdots + |k_\ell|$) the expression $I_\mu(x,\dot x)$ with $\mu \perp \mathcal{M}_N := \{k \in \mathcal{M} : |k| \le N\}$ is approximately preserved over intervals of length $\mathcal{O}(\varepsilon^{-N+1})$. Condition (2.7) is the analogue of a non-resonance condition that will be required for the numerical discretization.

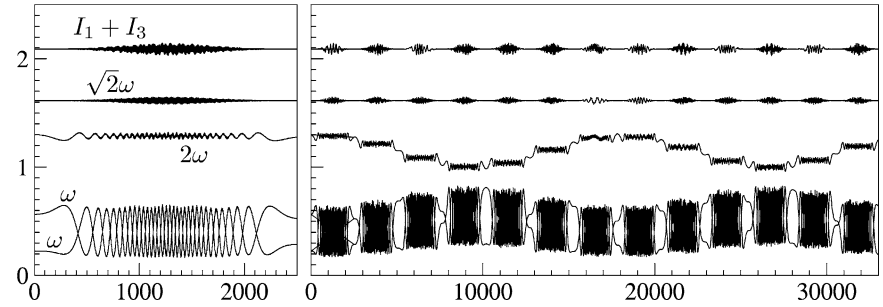

Figure 2.1: Oscillatory energies of the individual components (the frequencies $\lambda_j\omega = \lambda_j/\varepsilon$ are indicated) and the sum $I_1 + I_3$ of the oscillatory energies corresponding to the resonant frequencies ω and 2ω.

EXAMPLE 2.1. To illustrate the conservation of the various energies, we consider a Hamiltonian (2.1) with $\ell = 3$, $\lambda = (1, \sqrt{2}, 2)$. Note the 1:2 resonance between λ_1 and λ_3 : $\mathcal{M} = \{(-2k_3, 0, k_3) : k_3 \in \mathbb{Z}\}$. 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

$$U(x) = (0.001x_0 + x_{11} + x_{12} + x_2 + x_3)^4, \tag{2.8}$$

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 (2.5). In Figure 2.1 we plot the oscillatory energies for the individual components of the system along a solution which has been computed with very high accuracy and can be considered as exact. 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 (2.5)) 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 (2.8) 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 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 $\lambda_1 = 1 + \varepsilon^2$.

3 Main result and numerical experiments.

The equations of motion for the Hamiltonian system (2.1) can be written as the system of second-order differential equations

$$\ddot{x} = -\Omega^2 x + g(x), \tag{3.1}$$

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 [10] and [11, 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)

$$x_{n+1} - 2\cos(h\Omega)x_n + x_{n-1} = h^2\Psi g(\Phi x_n). \tag{3.2}$$

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

$$2h\,\mathrm{sinc}(h\Omega)\dot{x}_n = x_{n+1} - x_{n-1} \tag{3.3}$$

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 [7] ($\psi(\xi) = \mathrm{sinc}^2(\xi/2)$, $\phi(\xi) = 1$), Deuflhard [5] ($\psi(\xi) = \mathrm{sinc}(\xi)$, $\phi(\xi) = 1$), García-Archilla et al. [6] ($\psi(\xi) = \mathrm{sinc}(\xi)\phi(\xi)$), and Hochbruck and Lubich [12] ($\psi(\xi) = \mathrm{sinc}^2(\xi/2)$). 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 (3.3) into (3.2). We always assume that the second starting value x_1 for (3.2) 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. [11, p. 447]:

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

$$\frac{1}{2}\|\dot{x}_0\|^2 + \frac{1}{2}\|\Omega x_0\|^2 \le E. \tag{3.4}$$

- 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

$$\left|\sin\left(\frac{h}{2\varepsilon}\, k\cdot\lambda\right)\right| \ge c\sqrt{h} \quad \text{for all } k \in \mathbb{Z}^\ell \setminus \mathcal{M} \text{ with } |k| \le N, \tag{3.5}$$

  for some $N \ge 2$ and $c > 0$.
- The filter functions ψ and ϕ are bounded real-valued functions. The function ψ satisfies, with $\xi_j = h\omega_j = h\lambda_j/\varepsilon$,

$$|\psi(\xi_j)| \le C\left|\mathrm{sinc}\left(\frac{1}{2}\xi_j\right)\right| \quad \text{for } j = 1, \dots, \ell. \tag{3.6}$$

The bounded-energy condition (3.4) is already essential for the analytical theory. The lower bound on the time step primarily reflects our interest to use large time steps. This condition could be weakened to, e.g., $\sqrt{h} > \varepsilon$, with slight modifications in the results. For $h \ll \varepsilon$ the numerical behaviour can be studied with the help of backward error analysis.

Condition (3.5) is the analogue for the numerical discretization of the non-resonance condition (2.7), and it is the multi-frequency extension of condition (XIII.5.10) of [11] for the single-frequency case. Notice that condition (3.5) excludes resonances between the inverse step size and the frequencies, but does not exclude resonances among the frequencies as described by the resonance module $\mathcal{M}$. The condition excludes that $\xi_j = h\lambda_j/\varepsilon$ is close to an integral multiple of π. The integer $N \geq 2$ will limit the time scale $\mathcal{O}(h^{-N+1})$ on which we can ensure near-preservation of energies.

Condition (3.6) is weaker than the three conditions on the filter functions imposed in Section XIII.7 of [11], which guarantee second-order convergence on finite time intervals by Theorem XIII.4.1 of [11], page 427. By a straightforward extension of that theorem to the multi-frequency case considered here, it can be seen that condition (3.6) together with the other conditions above guarantee first order convergence on finite time intervals. Condition (3.6) is, in fact, sufficient for obtaining long-time energy preservation in the single-frequency case, with the same proofs as in [11, Ch. XIII]. All these conditions on the filter functions are usually satisfied when $\xi_j = h\lambda_j/\varepsilon$ is bounded away from an integral multiple of π, and the case of ξ_j very close to a multiple of π is anyway excluded by condition (3.5).

We have the following main result of this paper which we split into two theorems. They extend Theorem 7.1 of [10] (or Theorem XIII.7.1 of [11]) to multi-frequency systems. In the first theorem we consider in addition the conditions

$$|\psi(\xi_j)| \leq C\,\mathrm{sinc}^2\left(\frac{1}{2}\xi_j\right), \tag{3.7}$$

$$|\psi(\xi_j)| \leq C|\phi(\xi_j)| \quad \text{for } j = 1, \ldots, \ell. \tag{3.8}$$

THEOREM 3.1. *Under the above conditions* (3.4)–(3.6) *and additionally* (3.7) *and* (3.8)*, the numerical solution obtained by the method* (3.2)–(3.3) *satisfies*

$$\begin{aligned} H(x_n, \dot{x}_n) &= H(x_0, \dot{x}_0) + \mathcal{O}(h) \ \text{ for } 0 \leq nh \leq \sigma_0 h \cdot \min(\varepsilon^{-M+1}, h^{-N}), \\ I_j(x_n, \dot{x}_n) &= I_j(x_0, \dot{x}_0) + \mathcal{O}(h) \ \text{ for } 0 \leq nh \leq \sigma_j h \cdot \min(\varepsilon^{-M+1}, h^{-N}) \end{aligned}$$

for $j = 1, \ldots, \ell$. *Here,* $M = \min\{|k| : 0 \neq k \in \mathcal{M}\}$, $\sigma_j = |\sigma(\xi_j)|$, *and* $\sigma_0 = \min\{1, \sigma_1, \ldots, \sigma_\ell\}$, *where* $\sigma(\xi) = \mathrm{sinc}(\xi)\phi(\xi)/\psi(\xi)$. *Without the condition* (3.7) *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, $\sigma_0 \geq c_1\varepsilon/\sqrt{h}$ with $c_1 > 0$ by (3.5) and (3.8). 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 (3.5). Notice that always $M \geq 3$, 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 $M \geq 5$.

Considering the modified energies

$$H^*(x, \dot{x}) \;=\; H(x, \dot{x}) + \sum_{j=1}^{\ell} \big(\sigma(\xi_j) - 1\big) I_j(x, \dot{x}) \tag{3.9}$$

$$I^*_\mu(x, \dot{x}) \;=\; \sum_{j=1}^{\ell} \sigma(\xi_j) \frac{\mu_j}{\lambda_j} I_j(x, \dot{x}) \tag{3.10}$$

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

$$|\phi(\xi_j)| \leq C \left| \operatorname{sinc}\left(\frac{1}{2}\xi_j\right) \right| \quad \text{for } j = 1, \ldots, \ell. \tag{3.11}$$

THEOREM 3.2. *Under the conditions* (3.4)–(3.6) *and additionally* (3.11)*, the numerical solution obtained by the method* (3.2)–(3.3) *satisfies*

$$\begin{aligned} H^*(x_n, \dot{x}_n) &= H^*(x_0, \dot{x}_0) + \mathcal{O}(h) \\ I^*_\mu(x_n, \dot{x}_n) &= I^*_\mu(x_0, \dot{x}_0) + \mathcal{O}(h) \end{aligned} \quad \textit{for } 0 \leq nh \leq h^{-N+1}$$

for $\mu \in \mathbb{R}^\ell$ with $\mu \perp \mathcal{M}_N = \{k \in \mathcal{M} : |k| \leq N\}$. Without the condition (3.11) *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 (2.6) implies

$$K(x_n, \dot{x}_n) = K(x_0, \dot{x}_0) + \mathcal{O}(h) \quad \text{for } 0 \leq nh \leq h^{-N+1}. \tag{3.12}$$

The analysis of Sections 4 and 5 below shows that this estimate is true without the assumptions (3.7), (3.8), and (3.11).

Notice that for $\sigma(\xi) = 1$ (or equivalently $\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi)$) the modified energies (3.9) and (3.10) are identical to the original energies (2.1) and (2.4). 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

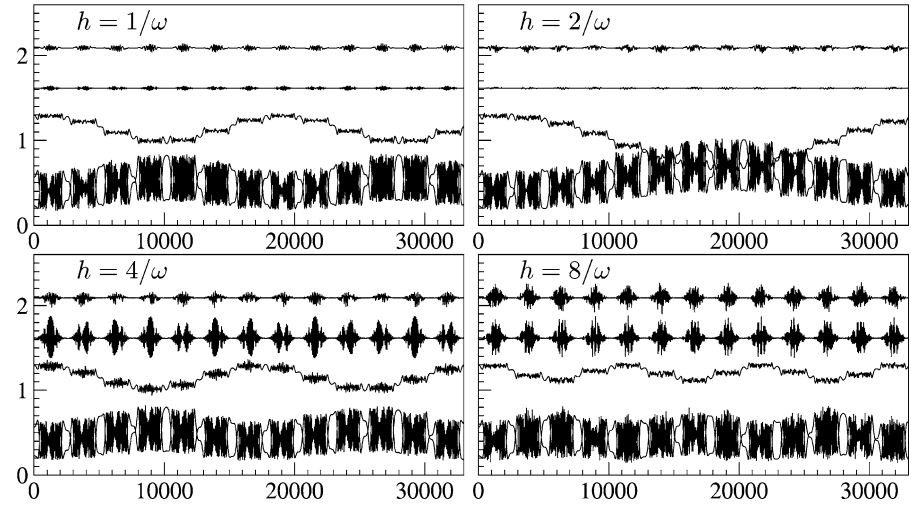

Figure 3.1: Oscillatory energies as in Figure 2.1 along the numerical solution of (3.2) with $\phi(\xi) = 1$ and $\psi(\xi) = \mathrm{sinc}(\xi)$. Notice that for this method $\sigma(\xi) = 1$.

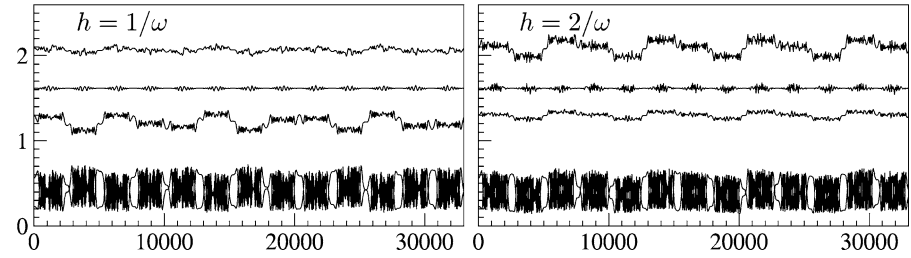

Figure 3.2: Oscillatory energies as in Figure 2.1 along the numerical solution of (3.2) with $\phi(\xi) = 1$ and $\psi(\xi) = \mathrm{sinc}^2(\xi/2)$.

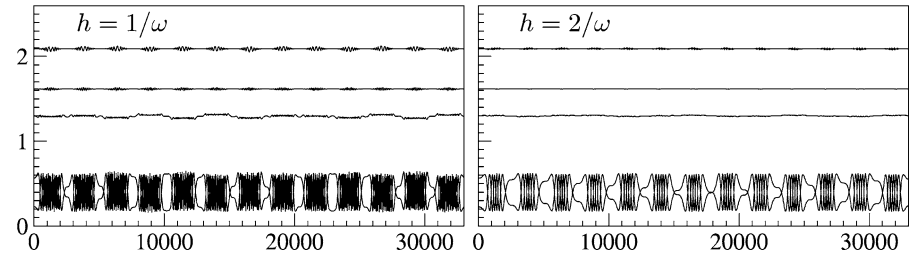

Figure 3.3: Oscillatory energies as in Figure 2.1 along the numerical solution of (3.2) with $\phi(\xi) = \mathrm{sinc}(\xi)$ and $\psi(\xi) = \mathrm{sinc}(\xi)\phi(\xi)$.

oscillatory energies along the numerical solution with those of the exact solution. In all cases, the conditions of Theorems 3.1 and 3.2 are satisfied.

In the first experiment we take the (symplectic) method (3.2) with $\phi(\xi) = 1$ and $\psi(\xi) = \mathrm{sinc}(\xi)$, which has $\sigma(\xi) = 1$, so that H and H^*, and I_μ and I_μ^*

coincide. We apply the method to the differential equation with large step sizes so that $h\omega = h/\varepsilon$ takes the values 1, 2, 4, and 8. Figure 3.1 shows the various oscillatory energies which can be compared with the exact values in Figure 2.1. For all step sizes, the oscillatory energy I_2 corresponding to the non-resonant frequency $\sqrt{2}\omega$ and the sum $I_1 + I_3$ are well conserved on long time intervals, in accordance with Theorem 3.2. Oscillations in these expressions increase with h. The individual energies I_1 and I_3 corresponding to the resonant frequencies $\omega = 1/\varepsilon$ and $2/\varepsilon$ are not preserved on the time scale considered here, cf. Fig. 2.1. In fact, Theorem 3.1 here yields only a time scale $\mathcal{O}(h\varepsilon^{-2})$. 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 (2.6). 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 $\psi(\xi) = \mathrm{sinc}^2(\xi/2)$ (Figure 3.2). For this method $\sigma(\xi)$ is not identical to 1, and hence H and H^*, and I_μ and I^*_μ do not coincide. The oscillatory energy $I_2 = \sigma_2^{-1} I^*_\mu$ with $\mu = (0, 1, 0) \perp \mathcal{M}$, which corresponds to the non-resonant frequency $\sqrt{2}\omega$, is approximately conserved over long times. Since Theorem 3.2 only states that the *modified* energies are well preserved, it is not surprising that neither $I_1 + I_3$ nor the original total energy H (not shown in the figure) are conserved. The modified energies H^* and $\sigma_1 I_1 + \sigma_3 I_3$ (not shown) are indeed well conserved, and so is the smooth energy K, in agreement with (3.12).

Figure 3.3 shows the result for the (symplectic) method with $\phi(\xi) = \mathrm{sinc}(\xi)$ and $\psi(\xi) = \mathrm{sinc}(\xi)\phi(\xi)$. Since $\sigma(\xi) = 1$, the oscillatory energy I_2 for $\sqrt{2}\omega$ and also $I_1 + I_3$ are well conserved, in agreement with Theorem 3.2. However, the energy exchange between the resonant frequencies is not correctly reproduced. This behaviour is not explained by Theorems 3.1 and 3.2, but it corresponds to the analysis in [11, Sect. XIII.4.2] which, for the single-frequency case, explains the incorrect energy exchange of methods that do not satisfy $\psi(\xi)\phi(\xi) = \mathrm{sinc}(\xi)$ (and thus, of all symplectic methods in the class considered, with the exception of the above method with $\phi(\xi) = 1$ and $\psi(\xi) = \mathrm{sinc}(\xi)$). That analysis could be extended to the multi-frequency case considered here.

4 Modulated Fourier expansions.

For a given vector $\lambda = (\lambda_1, \ldots, \lambda_\ell)$ and for the resonance module $\mathcal{M}$ defined by (2.2), 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 $|k| = |k_1| + \cdots + |k_\ell|$ 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 (3.5),

$$\mathcal{N} = \{k \in \mathcal{K} : |k| < N\}, \qquad \mathcal{N}^* = \mathcal{N} \setminus \{(0, \ldots, 0)\}. \tag{4.1}$$

The following result establishes a modulated Fourier expansion for the numerical solution. It is the multi-frequency version of Theorem XIII.5.2 of [11]. Its proof follows the lines of the proof of that theorem, with rather obvious adaptations.

THEOREM 4.1. *Consider the numerical solution of the system* (3.1) *by the method* (3.2) *with step size* h. *Under the conditions* (3.4)–(3.6), *the numerical solution admits an expansion*

$$x_n = y(t) + \sum_{k\in\mathcal{N}^*} \mathrm{e}^{\mathrm{i}k\cdot\omega t} z^k(t) + \Psi\cdot\mathcal{O}(t^2h^N) \tag{4.2}$$

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*

$$\begin{aligned} y_0 &= \mathcal{O}(1), \qquad y_j = \mathcal{O}\biggl(\frac{\varepsilon^2\psi(\xi_j)}{\operatorname{sinc}^2(\xi_j/2)}\biggr), \\ z_j^{\pm\langle j\rangle} &= \mathcal{O}(\varepsilon), \qquad \dot z_j^{\pm\langle j\rangle} = \mathcal{O}\biggl(\frac{\varepsilon^2\psi(\xi_j)}{\operatorname{sinc}(\xi_j)}\biggr), \\ z_j^k &= \mathcal{O}\bigl(h\varepsilon^{|k|}\psi(\xi_j)\bigr) \quad \text{for } k \ne \pm\langle j\rangle \end{aligned} \tag{4.3}$$

for $j = 1,\dots,\ell$. *Here,* $\langle j\rangle = (0,\dots,1,\dots,0)$ *is the* j*th 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* (3.5), *but they depend on* E, N, c, *and* T.

In terms of the difference operator of the method (3.2),

$$\begin{aligned} L(hD) &:= \mathrm{e}^{hD} - 2\cos h\Omega + \mathrm{e}^{-hD} = 2\bigl(\cos(\mathrm{i}hD) - \cos h\Omega\bigr) \\ &= 4\sin\biggl(\frac{1}{2}h\Omega + \frac{1}{2}\mathrm{i}hD\biggr)\sin\biggl(\frac{1}{2}h\Omega - \frac{1}{2}\mathrm{i}hD\biggr) \end{aligned} \tag{4.4}$$

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

$$\begin{aligned} L(hD)y &= h^2\Psi\biggl(g(\Phi y) + \sum_{s(\alpha)\sim 0} \frac{1}{m!} g^{(m)}(\Phi y)(\Phi z)^\alpha\biggr), \\ L(hD + \mathrm{i}hk\cdot\omega)z^k &= h^2\Psi \sum_{s(\alpha)\sim k} \frac{1}{m!} g^{(m)}(\Phi y)(\Phi z)^\alpha. \end{aligned} \tag{4.5}$$

Here, the sums on the right-hand side are over all $m \ge 1$ and over multi-indices $\alpha = (\alpha_1,\dots,\alpha_m)$ 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 $(\Phi z^{\alpha_1}, \dots, \Phi z^{\alpha_m})$. We remark that Equations (4.5) arise from the fact that for $y^k(t) = \mathrm{e}^{\mathrm{i}k\cdot\omega t} z^k(t)$ we have

$$L(hD)y^k(t) = \mathrm{e}^{\mathrm{i}k\cdot\omega t} L(hD + \mathrm{i}hk\cdot\omega) z^k(t), \tag{4.6}$$

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. [11, Theorem XIII.5.3].

THEOREM 4.2. *Under the conditions of Theorem* 4.1*, the velocity approximation admits an expansion*

$$\dot{x}_n = v(t) + \sum_{k\in\mathcal{N}^*} \mathrm{e}^{\mathrm{i}k\cdot\omega t} w^k(t) + \mathcal{O}(t^2 h^{N-1}) \tag{4.7}$$

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

$$\begin{aligned} v_0 &= \dot{y}_0 + \mathcal{O}(h^2), \qquad v_j = \mathcal{O}\Big(\frac{\varepsilon^2\psi(\xi_j)}{\operatorname{sinc}^2(\xi_j/2)\operatorname{sinc}(\xi_j)}\Big), \\ w_j^{\pm\langle j\rangle} &= \pm\mathrm{i}\omega_j z_j^{\pm\langle j\rangle} + \mathcal{O}\Big(\frac{\varepsilon^2\psi(\xi_j)}{\operatorname{sinc}^2(\xi_j)}\Big), \\ w_j^k &= \mathcal{O}\Big(\frac{h\varepsilon^{|k|}\psi(\xi_j)}{\operatorname{sinc}(\xi_j)}\Big) \quad \text{for } k \ne \pm\langle j\rangle. \end{aligned} \tag{4.8}$$

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* (3.5)*, but they depend on* E*,* N*,* c*, and* T*.*

As a consequence of Theorems 4.1 and 4.2, the oscillatory energy (2.3) along the numerical solution takes the form

$$I_j(x_n, \dot{x}_n) = 2\omega_j^2 \|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}\Big(\frac{\varepsilon\psi(\xi_j)}{\operatorname{sinc}^2(\xi_j/2)}\Big) + \mathcal{O}\big(h\psi(\xi_j)\big) \tag{4.9}$$

for $t = nh \le T$. The assumptions (3.5) and (3.6) 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 (3.7), we get the sharper formula $I_j(x_n, \dot{x}_n) = 2\omega_j^2\|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}(\varepsilon)$.

5 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 (4.5) 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 4.1. We introduce the extended potential

$$\mathcal{U}(\mathbf{y}) = U(\Phi y^0) + \sum_{s(\alpha)\sim 0} \frac{1}{m!} U^{(m)}(\Phi y^0)(\Phi \mathbf{y})^\alpha, \tag{5.1}$$

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 (4.5) that the functions $y^k(t)$ satisfy

$$\Psi^{-1}\Phi h^{-2} L(hD) y^k = -\nabla_{-k}\mathcal{U}(\mathbf{y}) + \Phi \cdot \mathcal{O}(h^N), \tag{5.2}$$

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

5.1 The energy-type almost-invariant of the modulation system.

We multiply (5.2) by $(\dot{y}^{-k})^T$ and sum over $k \in \mathcal{N}$ to obtain

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

Since we know bounds of the modulation functions z^k and of their derivatives from Theorem 4.1, we switch to the quantities z^k and we get the equivalent relation

$$\sum_{k\in\mathcal{N}} (\dot{z}^{-k} - \mathrm{i}k\cdot\omega z^{-k})^T \Psi^{-1}\Phi h^{-2} L(hD + \mathrm{i}hk\cdot\omega) z^k + \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}(\mathbf{z}) = \mathcal{O}(h^N). \tag{5.3}$$

As in [11, p. 444] we obtain that the left-hand side of (5.3) 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 (5.3) thus becomes

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

Together with the estimates (4.3) and the decomposition (4.4), this construction of $\mathcal{H}^*$ yields the following multi-frequency extension of Lemma XIII.6.4 of [11].

LEMMA 5.1. *Under the assumptions of Theorem* 4.1, *the modulation functions* $\mathbf{z} = (z^k)_{k\in\mathcal{N}}$ *of the numerical solution satisfy*

$$\mathcal{H}^*[\mathbf{z}](t) = \mathcal{H}^*[\mathbf{z}](0) + \mathcal{O}(th^N) \tag{5.4}$$

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

$$\begin{aligned} \mathcal{H}^*[\mathbf{z}](t) \;=\; & \frac{1}{2}\|\dot{y}_0(t)\|^2 + \sum_{j=1}^{\ell} \sigma(h\omega_j) 2\omega_j^2 \|z_j^{\langle j\rangle}(t)\|^2 + U(\Phi y(t)) \;+ \\ & + \mathcal{O}(h^2) + \mathcal{O}(\varepsilon\sqrt{h}). \end{aligned} \tag{5.5}$$

By (4.9) and condition (3.11), 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 (5.5) yields

$$\mathcal{H}^*[\mathbf{z}](t) = H^*(x_n, \dot{x}_n) + \mathcal{O}(h) \tag{5.6}$$

at $t = nh \le T$, with $H^*(x, \dot{x})$ of (3.9). Without the condition (3.11) the error is of size $\mathcal{O}(\sqrt{h})$.

5.2 The momentum-type almost-invariants of the modulation system.

Equations (5.2) 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

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

so that, by the multi-linearity of the derivative, definition (5.1) yields

$$\mathcal{U}\big(S_\mu(\tau)\mathbf{y}\big) = U(\Phi y^0) + \sum_{s(\alpha)\sim 0} \frac{\mathrm{e}^{\mathrm{i}s(\alpha)\cdot\mu\tau}}{m!} U^{(m)}(\Phi y^0)(\Phi\mathbf{y})^\alpha. \tag{5.7}$$

If $\mu \perp \mathcal{M}$, then the relation $s(\alpha) \sim 0$ implies $s(\alpha)\cdot\mu = 0$, and hence the expression (5.7) is independent of τ. It therefore follows that

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

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 (5.7) depend on τ. However, for these terms with $s(\alpha) \in \mathcal{M}$ and $s(\alpha)\cdot\mu \ne 0$ we have $|s(\alpha)| \ge M = \min\{|k| : 0 \ne k \in \mathcal{M}\}$ and if $\mu \perp \mathcal{M}_N$, then $|s(\alpha)| \ge N+1$. The bounds (4.3) then yield

$$\sum_{k\in\mathcal{N}} \mathrm{i}(k\cdot\mu)(y^k)^T \nabla_k \mathcal{U}(\mathbf{y}) = \begin{cases} \mathcal{O}(\varepsilon^M) & \text{for arbitrary } \mu, \\ \mathcal{O}(\varepsilon^{N+1}) & \text{for } \mu \perp \mathcal{M}_N \end{cases} \tag{5.8}$$

for the vector $\mathbf{y} = \mathbf{y}(t)$ as given by Theorem 4.1. Multiplying relation (5.2) by $\frac{\mathrm{i}}{\varepsilon}(-k\cdot\mu)(y^{-k})^T$ and summing over $k \in \mathcal{N}$, we obtain with (5.8) 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

$$-\frac{\mathrm{i}}{\varepsilon} \sum_{k\in\mathcal{N}} (k\cdot\mu)(z^{-k})^T \Psi^{-1}\Phi h^{-2} L(hD + \mathrm{i}hk\cdot\omega) z^k = \mathcal{O}(h^N) + \mathcal{O}(\varepsilon^{M-1}). \tag{5.9}$$

As in (5.3), 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:

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

Together with the estimates of Theorem 4.1 this yields the following result.

LEMMA 5.2. *Under the assumptions of Theorem* 4.1*, the modulation functions* $\mathbf{z}$ *satisfy*

$$\mathcal{I}^*_\mu[\mathbf{z}](t) = \mathcal{I}^*_\mu[\mathbf{z}](0) + \mathcal{O}(th^N) + \mathcal{O}(t\varepsilon^{M-1}) \tag{5.10}$$

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

$$\mathcal{I}^*_\mu[\mathbf{z}](t) = \mathcal{I}^*_\mu[\mathbf{z}](0) + \mathcal{O}(th^N) \tag{5.11}$$

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

$$\mathcal{I}^*_\mu[\mathbf{z}](t) = \sum_{j=1}^{\ell} \sigma(h\omega_j)\frac{\mu_j}{\lambda_j} 2\omega_j^2 \|z_j^{\langle j\rangle}(t)\|^2 + \mathcal{O}(\varepsilon\sqrt{h}), \tag{5.12}$$

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

By (4.9) and (3.11), the relation (5.12) implies

$$I^*_\mu(x_n, \dot{x}_n) = \mathcal{I}^*_\mu[\mathbf{z}](t) + \mathcal{O}(\varepsilon) \tag{5.13}$$

at $t = nh \le T$, with $I^*_\mu(x, \dot{x})$ of (3.10). Without assumption (3.11) we have an error of size $\mathcal{O}(\sqrt{h})$.

For the choice $\mu = \langle j \rangle$, relations (4.9) and (5.12) together with the bounds (3.7) and $|\sigma_j| \ge c_1\,\varepsilon/\sqrt{h}$ for $\sigma_j = \sigma(h\omega_j)$ (which follows from (3.5) and (3.8)) yield, at $t = nh \le T$,

$$I_j(x_n, \dot{x}_n) = \frac{\lambda_j}{\sigma_j}\mathcal{I}^*_{\langle j\rangle}[\mathbf{z}](t) + \mathcal{O}(h). \tag{5.14}$$

Without condition (3.7) the error is $\mathcal{O}(\sqrt{h})$.

5.3 Proof of Theorems 3.1 and 3.2.

With the proof of Theorem XIII.7.1 of [11, p. 447], which patches many short time intervals together, the estimates (5.4) and (5.6) yield directly the result for $H^*(x_n, \dot{x}_n)$ in Theorem 3.2. In the same way, (5.11) and (5.13) yield the result for $I^*_\mu(x_n, \dot{x}_n)$ in Theorem 3.2. Subtracting (5.12) with $\mu = \lambda$ from (5.5) yields the statement (3.12) for the smooth energy $K(x_n, \dot{x}_n)$. In the same way, relation (5.14) yields the estimate for $I_j(x_n, \dot{x}_n)$ of Theorem 3.1. 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 3.1.

6 Energy conservation of the Störmer–Verlet method.

The Störmer–Verlet method applied to (3.1) reads

$$x_{n+1} - 2x_n + x_{n-1} = -h^2\Omega^2 x_n + h^2 g(x_n). \tag{6.1}$$

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 (3.2) with modified frequencies,

$$x_{n+1} - 2\cos(h\widetilde{\Omega})x_n + x_{n-1} = h^2 g(x_n), \tag{6.2}$$

where

$$\widetilde{\Omega} = \operatorname{diag}(\widetilde{\omega}_j) \quad \text{with } \sin\left(\frac{1}{2}h\widetilde{\omega}_j\right) = \frac{1}{2}h\omega_j. \tag{6.3}$$

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 $\widetilde{\omega}_j$,

$$\widetilde{\mathcal{M}} = \{k \in \mathbb{Z}^\ell : k_1\widetilde{\omega}_1 + \cdots + k_\ell\widetilde{\omega}_\ell = 0\}, \tag{6.4}$$

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

$$2h\dot{x}_n = x_{n+1} - x_{n-1} \tag{6.5}$$

does not correspond to (3.3) 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 4 and 5 with the arguments of [11, Theorem XIII.8.1], we obtain the long-time near-conservation of the modified energies

$$H^*(x, \dot{x}) \;=\; H(x, \dot{x}) + \frac{1}{2}\sum_{j=1}^{\ell} \gamma(\xi_j)\|\dot{x}_j\|^2, \tag{6.6}$$

$$I_j^*(x, \dot{x}) \;=\; I_j(x, \dot{x}) + \frac{1}{2}\gamma(\xi_j)\|\dot{x}_j\|^2 \tag{6.7}$$

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 (2.6),

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

Moreover, by the arguments of [11, 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,

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

Here we need the following assumptions in analogy to (3.4)–(3.6):

- 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:

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

- We assume the numerical non-resonance condition

$$\left|\sin\left(\frac{1}{2}hk\cdot\widetilde{\omega}\right)\right| \ge c\sqrt{h} \quad \text{for all } k\in\mathbb{Z}^\ell\setminus\widetilde{\mathcal{M}} \text{ with } |k|\le N, \tag{6.8}$$

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

THEOREM 6.1. *Under the above conditions, the smooth energy along the numerical solution $(x_n,\dot{x}_n)$ of the Störmer–Verlet method satisfies*

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

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

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

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 (6.1) to the problem of Example 2.1. The oscillatory energies along the numerical solution are shown in the upper two pictures of Figure 6.1 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 (6.7) can hardly be observed. In contrast to the exact solution (see Figure 2.1), 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 (6.3) take the values $(1,\sqrt{2},2)/\varepsilon$, we recover the energy exchange in the numerical solution, though now there is no exchange

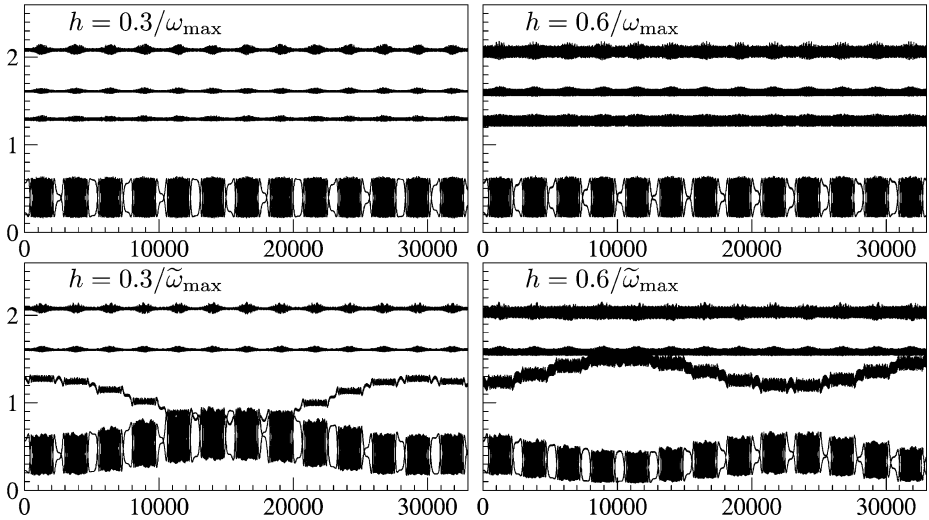

Figure 6.1: Oscillatory energies as in the figures of Section 3 for the Störmer–Verlet method; the two upper pictures correspond to $\omega_j = \lambda_j/\varepsilon$ with $\varepsilon = 1/70$ and $\lambda = (1, \sqrt{2}, 2)$; the two lower pictures correspond to $\omega_j = \sin(h\widetilde{\omega}_j/2) \cdot 2/h$ with $\widetilde{\omega}_j = \lambda_j/\varepsilon$ and the same λ_j and ε as before.

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 $h\omega_{\max}$.

7 Oscillatory energies along the exact solution.

The techniques of Sections 4 and 5 can also be applied to the exact solution of the Hamiltonian system (2.1). This then yields the following result.

THEOREM 7.1. *Assume the energy bound* (3.4) *and let* N *be such that the non-resonance condition* (2.7) *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*

$$I_j\big(x(t), \dot{x}(t)\big) = I_j\big(x(0), \dot{x}(0)\big) + \mathcal{O}(\varepsilon) \quad \text{for } 0 \le t \le \varepsilon \cdot \min(\varepsilon^{-M+1}, \varepsilon^{-N}) \tag{7.1}$$

for $j = 1, \dots, \ell$. *The integer* $M = \min\{|k| : 0 \neq k \in \mathcal{M}\}$ *is as in Theorem* 3.1. *We further have*

$$I_\mu\big(x(t), \dot{x}(t)\big) = I_\mu\big(x(0), \dot{x}(0)\big) + \mathcal{O}(\varepsilon) \quad \text{for } 0 \le t \le \varepsilon^{-N+1} \tag{7.2}$$

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 (7.2) is in complete agreement with the results of [2] where estimates on exponentially long time intervals are provided for $\mu \perp \mathcal{M}$. The formula (7.1) 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

$$x(t) = y(t) + \sum_{k \in \mathcal{N}^*} \mathrm{e}^{\mathrm{i}k\cdot\omega t} z^k(t) + \mathcal{O}(t^2\varepsilon^N). \tag{7.3}$$

In complete analogy to Theorem 4.1 the modulation functions $z^k(t)$ together with their derivatives are bounded on finite time intervals by

(7.4)
$$y_0 = \mathcal{O}(1), \quad y_j = \mathcal{O}(\varepsilon^2), \quad z_j^{\pm\langle j\rangle} = \mathcal{O}(\varepsilon), \quad \dot{z}_j^{\pm\langle j\rangle} = \mathcal{O}(\varepsilon^2), \quad z_j^k = \mathcal{O}(\varepsilon^{|k|+1}).$$

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

$$\ddot{y}^k + \Omega^2 y^k = -\nabla_{-k}\mathcal{U}(\mathbf{y}) + \mathcal{O}(\varepsilon^N), \tag{7.5}$$

which is the analogue of (5.2). Here, $\mathcal{U}(\mathbf{y})$ is defined as in (5.1) without the factors Φ. With (7.4) and (7.5) instead of (4.3) and (5.2), the analysis of Sections 4 and 5 proves the theorem.

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