

Long-term analysis of numerical integrators for oscillatory Hamiltonian systems under minimal non-resonance conditions

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Abstract For trigonometric and modified trigonometric integrators applied to oscillatory Hamiltonian differential equations with one or several constant high frequencies, near-conservation of the total and oscillatory energies are shown over time scales that cover arbitrary negative powers of the step size. This requires non-resonance conditions between the step size and the frequencies, but in contrast to previous results the results do not require any non-resonance conditions among the frequencies. The proof uses modulated Fourier expansions with appropriately modified frequencies.

Keywords Oscillatory Hamiltonian systems · Modulated Fourier expansions · Trigonometric integrators · Störmer-Verlet scheme · IMEX scheme · Long-time energy conservation · Numerical resonances · Non-resonance condition

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1 Introduction

This paper is concerned with the energy behaviour over long times of numerical methods for oscillatory differential equations with one or several constant high frequencies:

$$\ddot{q}_j + \omega_j^2 q_j = -\nabla_j U(\mathbf{q}), \quad j = 0, \dots, \ell, \quad (1.1)$$

where $\mathbf{q} = (q_0, q_1, \dots, q_\ell)$ and the frequencies are $\omega_0 = 0$ and

$$\omega_j \geq \frac{1}{\varepsilon}, \quad 0 < \varepsilon \ll 1, \quad j = 1, \dots, \ell. \quad (1.2)$$

The coupling potential U is smooth with derivatives bounded independently of ε .

The numerical long-time near-conservation of energy for such equations has already been studied before for various numerical integrators, which will be considered also here: for trigonometric integrators in [6, 2] and [7, Chapter XIII], for the Störmer–Verlet method in [5], for an implicit-explicit (IMEX) method in [11, 10]. Most of these results concern the single-frequency case ($\ell = 1$). A nontrivial extension to the multi-frequency case ($\ell > 1$) is given in [2].

The proofs in those papers require numerical non-resonance conditions: first, it is needed that the product $h\omega_j$ of the step size h with the high frequencies (or $h\tilde{\omega}_j$ for methods that effectively work with different numerical frequencies $\tilde{\omega}_j$, such as the Störmer–Verlet and IMEX methods) is bounded away from integral multiples of π by a distance substantially larger than h , e.g., by $\sqrt{h}$. Numerical experiments, e.g., in [7, Chapter XIII], show clearly that this numerical non-resonance condition is necessary for a satisfactory numerical energy behaviour.

In this paper we show that without any further non-resonance condition, the *slow energy*, i.e., the total energy minus the oscillatory energy, remains well conserved over long times $t \leq h^{-N}$ for an arbitrary integer N , in the numerically interesting range $h \geq c_0\varepsilon$, provided the total energy remains bounded over such an interval.

To obtain also near-conservation of the *total and oscillatory energies* over times $t \leq h^{-N}$, it is required in [2] and [7, Chapter XIII] that sums of $\pm h\omega_j$ with at most $N+1$ terms must stay away from integral multiples of 2π . Here we will show that it suffices that they are away from *non-zero* integral multiples of 2π , and we present numerical results that illustrate the necessity of such a non-resonance condition between the step size and the frequencies.

Away from numerical near-resonances between the step size and the frequencies, our results will be uniform in the frequencies, without imposing any non-resonance condition among the frequencies.

What enables us to obtain long-time near-conservation of the total, slow and oscillatory energies under much less restrictive conditions than in the existing literature, is that we adopt ideas and techniques from [4] for the exact solution and combine them with those of [6] and [2] for the numerical solution.

In [4] and more recently also in [1] it is shown that the oscillatory energy, i.e., the sum of the harmonic energies $\frac{1}{2}|\dot{q}_j|^2 + \frac{1}{2}\omega_j^2|q_j|^2$ over $j = 1, \dots, \ell$, is nearly conserved over times ε^{-N} for arbitrary integers N , with estimates that are uniform in the frequencies ω_j satisfying (1.2). In the proof of this result, integral linear combinations of the frequencies are regrouped into non-resonant and near-resonant ones, with a gap appearing between them whose size depends only on ℓ and N , and then the frequencies are modified such that the near-resonances become exact resonances. With these modified frequencies, one then uses a modulated Fourier expansion and its almost-invariants as done previously in the literature. We will proceed in a similar way in this paper for the numerical problem and prove a numerical counterpart to the analytical result of [4] and [1].

After the preparatory Section 2 we state, in Section 3, our main results on the long-time near-conservation of the slow and oscillatory energies along numerical solutions of (1.1). After some illustrative numerical experiments in Section 4, the theoretical results are proved in the remaining sections. We introduce appropriately modified frequencies in Section 5 and use them in the modulated Fourier expansion constructed in Section 6. The result on bounds and approximation properties of the modulated Fourier expansion, which is stated in Section 6, is proved in Section 7. Two almost-invariants of the modulation system, which are close to the slow and oscillatory energies, are studied in Section 8. We are then in the position to prove the main results in Section 9.

2 Preparation

2.1 Oscillatory, slow and total energies and equations of motion

For momenta $\mathbf{p} = (p_0, p_1, \dots, p_\ell)$ and positions $\mathbf{q} = (q_0, q_1, \dots, q_\ell)$ with $p_j, q_j \in \mathbb{R}^{d_j}$ we consider the Hamiltonian

$$H(\mathbf{p}, \mathbf{q}) = H_\omega(\mathbf{p}, \mathbf{q}) + H_{\text{slow}}(\mathbf{p}, \mathbf{q}),$$

where the oscillatory and slow-motion energies are given by

$$H_\omega(\mathbf{p}, \mathbf{q}) = \sum_{j=1}^{\ell} \frac{1}{2} \left(|p_j|^2 + \omega_j^2 |q_j|^2 \right), \quad H_{\text{slow}}(\mathbf{p}, \mathbf{q}) = \frac{1}{2} |p_0|^2 + U(\mathbf{q}).$$

We assume high frequencies satisfying (1.2). If the oscillatory energy is bounded by a constant independent of ε , then $q_j = \mathcal{O}(\varepsilon)$ for $j = 1, \dots, \ell$, and we have that the slow energy $H_{\text{slow}}(\mathbf{p}, \mathbf{q})$ is $\mathcal{O}(\varepsilon)$ close to the energy of the isolated slow system $H_0(p_0, q_0) = \frac{1}{2} |p_0|^2 + U(q_0, 0, \dots, 0)$.

The equations of motion are (1.1) or, in vector notation,

$$\ddot{\mathbf{q}} + \mathbf{\Omega}^2 \mathbf{q} = \mathbf{g}(\mathbf{q}) \tag{2.1}$$

with the nonlinearity $\mathbf{g}(\mathbf{q}) = -\nabla U(\mathbf{q})$, and where $\mathbf{\Omega}$ is the diagonal matrix with entries ω_j .

2.2 Trigonometric integrators

For the numerical solution of (2.1) we consider trigonometric methods as studied in [7, Chapter XIII]. With the step size h , they are given in two-step form by

$$\begin{aligned} \mathbf{q}_{n+1} - 2\cos(h\mathbf{\Omega})\mathbf{q}_n + \mathbf{q}_{n-1} &= h^2\mathbf{\Psi}\mathbf{g}(\mathbf{\Phi}\mathbf{q}_n) \\ 2h\operatorname{sinc}(h\mathbf{\Omega})\mathbf{p}_n &= \mathbf{q}_{n+1} - \mathbf{q}_{n-1}, \end{aligned} \quad (2.2)$$

where $\mathbf{\Psi} = \psi(h\mathbf{\Omega})$ and $\mathbf{\Phi} = \phi(h\mathbf{\Omega})$ with real-valued bounded functions ψ and ϕ satisfying $\psi(0) = \phi(0) = 1$, and $\operatorname{sinc}(\xi) = \sin(\xi)/\xi$. For starting the computation we put $\mathbf{q}_0 = \mathbf{q}(0)$, $\mathbf{p}_0 = \mathbf{p}(0)$ and we compute the approximation $\mathbf{q}_1$ by putting $n = 0$ in (2.2) and by eliminating $\mathbf{q}_{-1}$. This yields

$$\mathbf{q}_1 = \cos(h\mathbf{\Omega})\mathbf{q}_0 + h\operatorname{sinc}(h\mathbf{\Omega})\mathbf{p}_0 + \frac{1}{2}h^2\mathbf{\Psi}\mathbf{g}(\mathbf{\Phi}\mathbf{q}_0). \quad (2.3)$$

It is known from [7, Section XIII.2.2] that the method is symplectic if and only if

$$\psi(h\omega_j) = \operatorname{sinc}(h\omega_j)\phi(h\omega_j) \quad \text{for } j = 1, \dots, \ell. \quad (2.4)$$

2.3 Modified trigonometric integrators

We further consider methods defined by

$$\begin{aligned} \mathbf{q}_{n+1} - 2\cos(h\tilde{\mathbf{\Omega}})\mathbf{q}_n + \mathbf{q}_{n-1} &= h^2\tilde{\mathbf{\Psi}}\mathbf{g}(\tilde{\mathbf{\Phi}}\mathbf{q}_n) \\ 2h\tilde{\chi}\mathbf{p}_n &= \mathbf{q}_{n+1} - \mathbf{q}_{n-1}, \end{aligned} \quad (2.5)$$

where $\tilde{\mathbf{\Omega}}$ is a diagonal matrix with entries $\tilde{\omega}_j$ such that $\tilde{\omega}_0 = 0$, $\tilde{\mathbf{\Psi}} = \psi(h\tilde{\mathbf{\Omega}})$, $\tilde{\mathbf{\Phi}} = \phi(h\tilde{\mathbf{\Omega}})$, and $\tilde{\chi} = \chi(h\tilde{\mathbf{\Omega}})$ with $\chi(0) = 1$. The choice $\tilde{\chi} = \mathbf{\Omega}^{-1}\tilde{\mathbf{\Omega}}\operatorname{sinc}(h\tilde{\mathbf{\Omega}})$ is proposed in [10]. The method is symplectic if and only if

$$\psi(h\tilde{\omega}_j) = \chi(h\tilde{\omega}_j)\phi(h\tilde{\omega}_j) \quad \text{for } j = 1, \dots, \ell.$$

An important class of such symplectic methods is given by

$$\begin{aligned} \mathbf{q}_{n+1} - 2\mathbf{q}_n + \mathbf{q}_{n-1} + h^2\mathbf{\Omega}^2\mathbf{q}_n + \alpha h^2\mathbf{\Omega}^2(\mathbf{q}_{n+1} - 2\mathbf{q}_n + \mathbf{q}_{n-1}) &= h^2\mathbf{g}(\mathbf{q}_n) \\ 2h\mathbf{p}_n &= (I + \alpha h^2\mathbf{\Omega}^2)(\mathbf{q}_{n+1} - \mathbf{q}_{n-1}). \end{aligned} \quad (2.6)$$

This can be written as a method (2.5) by defining $h\tilde{\omega}_j \in [0, \pi]$ through (see [5]; we omit the subscript j)

$$\cos(h\tilde{\omega}) = \frac{1 + (\alpha - \frac{1}{2})h^2\omega^2}{1 + \alpha h^2\omega^2} \quad \text{or equivalently} \quad \sin(\frac{1}{2}h\tilde{\omega}) = \frac{\frac{1}{2}h\omega}{\sqrt{1 + \alpha h^2\omega^2}},$$

provided that $h\omega < 2/\sqrt{1 - 4\alpha}$ if $\alpha < 1/4$, and without any restriction on $h\omega$ if $\alpha \geq 1/4$. With these modified frequencies, the method (2.6) becomes (2.5) with

$$\phi(\xi) = 1, \quad \psi(\xi) = \chi(\xi) = 1 - 4\alpha \sin^2(\frac{1}{2}\xi).$$

The Störmer–Verlet method is the special case $\alpha = 0$ of (2.6), and the implicit-explicit (or IMEX) integrator of [12] and [11] is the special case $\alpha = 1/4$.

3 Main results on energy conservation

We prove results on numerical energy conservation for trigonometric and modified trigonometric integrators. The technique of proof is related to that of [4] where a gap condition is created by suitably modifying the frequencies.

We collect assumptions that are relevant for all theorems to be presented in this work.

Assumption A. In addition to (1.2) we assume the following:

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

$$H(\mathbf{p}(0), \mathbf{q}(0)) \leq E. \quad (3.1)$$

- There is a radius $\rho > 0$ and a set $K \subset \mathbb{R}^{d_0}$ such that the potential $U(\mathbf{q})$ is bounded and has bounded derivatives of all orders in a ρ -neighbourhood of $K \times 0 \times \dots \times 0$. We denote this ρ -neighbourhood by K_ρ .
- The numerical solution values $\Phi \mathbf{q}_n$ (or $\tilde{\Phi} \mathbf{q}_n$) stay in $K_{\rho/2}$.
- The step size h satisfies $h/\varepsilon \geq c_0 > 0$.
- The frequencies ω_j are such that

$$|\sin(h\omega_j)| \geq \kappa = \kappa(h) \geq \sqrt{h} \quad \text{for } j = 1, \dots, \ell. \quad (3.2)$$

For modified trigonometric integrators this is assumed for the frequencies $\tilde{\omega}_j$ instead of ω_j .

Assumption B. The filter functions ϕ and ψ of the method (2.2) are such that the function

$$\sigma(\xi) = \text{sinc}(\xi) \frac{\phi(\xi)}{\psi(\xi)} \quad (3.3)$$

is bounded from below and above:

$$0 < c_1 \leq \sigma(h\omega_j) \leq C_1 \quad \text{for } j = 1, \dots, \ell,$$

or the same estimate holds for $-\sigma$ instead of σ .

Remark 3.1 The first three items of Assumption A are necessary for the following results. The last two items can be relaxed to the conditions $h/\varepsilon \geq c_0 h^\beta$ and $\kappa(h) \geq h^\gamma$ with positive β and γ smaller than 1, which lead to weaker estimates.

Assumption B is needed in our proofs. Numerical experiments indicate, however, that different signs among the $\sigma(h\omega_j)$ do not necessarily lead to a different energy behaviour.

3.1 Energy conservation for trigonometric integrators

As in [2] we consider the modified oscillatory energy, with $\sigma(\xi)$ from (3.3),

$$H_{\omega}^*(\mathbf{p}, \mathbf{q}) = \sum_{j=1}^{\ell} \sigma(h\omega_j) \frac{1}{2} \left(|p_j|^2 + \omega_j^2 |q_j|^2 \right). \quad (3.4)$$

If $\sigma(h\omega_j) = 1$ for $j = 1, \dots, \ell$, this expression is identical to the oscillatory energy H_{ω} . This condition on σ is equivalent to the symplecticity of the numerical flow defined by (2.2), see (2.4).

Theorem 3.1 *We fix an arbitrary integer $N \geq 1$ and $0 < \delta \leq 1/4$. Then there exists $h_0 > 0$ such that under Assumptions A and B, the numerical solution obtained by method (2.2) satisfies, for $h \leq h_0$,*

$$H_{\text{slow}}(\mathbf{p}_n, \mathbf{q}_n) = H_{\text{slow}}(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(h^{1-\delta}) \quad \text{for } 0 \leq nh \leq h^{-N},$$

as long as $H(\mathbf{p}_n, \mathbf{q}_n) \leq \text{Const}$. If, in addition, the step size and the frequencies satisfy the following numerical non-resonance condition:

$$\begin{aligned} &\text{Sums of } \pm h\omega_j \text{ with at most } N+1 \text{ terms are bounded away from} \\ &\text{nonzero integral multiples of } 2\pi \text{ with a distance of at least } \sqrt{h}, \end{aligned} \quad (3.5)$$

then we further have, with κ from (3.2),

$$H_{\omega}^*(\mathbf{p}_n, \mathbf{q}_n) = H_{\omega}^*(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(h^{1-\delta}/\kappa) \quad \text{for } 0 \leq nh \leq h^{-N}.$$

The constants symbolized by $\mathcal{O}$ are independent of n, h, ε , and ω_j , but depend on ℓ, N, δ , and the constants in Assumptions A and B. The maximal step size h_0 is independent of the frequencies ω_j .

For vectors $\mathbf{k} = (k_1, \dots, k_{\ell}) \in \mathbb{Z}^{\ell}$ of integers and the vector $\omega = (\omega_1, \dots, \omega_{\ell})$ of frequencies we write

$$\mathbf{k} \cdot \omega = \sum_{j=1}^{\ell} k_j \omega_j \quad \text{and} \quad \|\mathbf{k}\| = \sum_{j=1}^{\ell} |k_j|.$$

Condition (3.5) can then be rewritten as

$$|h(\mathbf{k} \cdot \omega) - r 2\pi| \geq \sqrt{h} \quad \text{for all } r \in \mathbb{Z}, r \neq 0, \text{ for all } \mathbf{k} \in \mathbb{Z}^{\ell} \text{ with } \|\mathbf{k}\| \leq N+1. \quad (3.6)$$

Theorem 3.1 is related to the results of [2]. A substantial difference is that here we do not require the numerical non-resonance condition from [2], which reads

$$\left| \sin\left(\frac{h}{2} \mathbf{k} \cdot \omega\right) \right| \geq \sqrt{h} \quad \text{for all } \mathbf{k} \in \mathbb{Z}^{\ell} \setminus \mathcal{M} \text{ with } \|\mathbf{k}\| \leq N+1 \quad (3.7)$$

with the resonance module $\mathcal{M} = \{\mathbf{k} \in \mathbb{Z}^{\ell} : \mathbf{k} \cdot \omega = 0\}$. This condition is more restrictive than the numerical non-resonance condition of Assumption A and

of (3.5), in particular in that the case $r = 0$ is not required in (3.6). In contrast to [2], where near-resonances among the frequencies are excluded, Theorem 3.1 is uniform in the choice of the frequencies $\omega_1, \dots, \omega_\ell$. On the other hand, under the non-resonance condition (3.7) and under further assumptions on the filter functions, the article [2] gives improved near-conservation estimates.

We note the following direct corollary on the conservation of the total and oscillatory energies.

Corollary 3.1 *If, in addition to the assumptions of Theorem 3.1 including (3.5), the method (2.2) is symplectic, then*

$$\begin{aligned} H(\mathbf{p}_n, \mathbf{q}_n) &= H(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(h^{1-\delta}/\kappa) \\ H_\omega(\mathbf{p}_n, \mathbf{q}_n) &= H_\omega(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(h^{1-\delta}/\kappa) \end{aligned} \quad \text{for } 0 \leq nh \leq h^{-N}.$$

Remark 3.2 If $\sigma(h\omega_j) > 0$ for $j = 1, \dots, \ell$, the modified oscillatory energy H_ω^* is the oscillatory energy H_ω in transformed variables $\hat{q}_j = \sigma(h\omega_j)^{1/2} q_j$ and $\hat{p}_j = \sigma(h\omega_j)^{1/2} p_j$. The method (2.2) in these variables is still of the form (2.2) with modified filter functions $\hat{\psi}(h\omega_j) = \sigma(h\omega_j)^{1/2} \psi(h\omega_j)$ and $\hat{\phi}(h\omega_j) = \sigma(h\omega_j)^{-1/2} \phi(h\omega_j)$. The method is thus symplectic in the transformed variables. This indicates why the modified oscillatory energy instead of the oscillatory energy shows up in Theorem 3.1.

3.2 Energy conservation for modified trigonometric integrators

We have the following result for the symplectic class of methods (2.6), which contains the Störmer–Verlet scheme and the IMEX integrator of [12] and [11] as special cases. Here we introduce

$$H_\omega^*(\mathbf{p}, \mathbf{q}) = \sum_{j=1}^{\ell} \sigma(h\tilde{\omega}_j) \frac{1}{2} \left(\left(\frac{\chi(h\tilde{\omega}_j)}{\text{sinc}(h\tilde{\omega}_j)} \right)^2 |p_j|^2 + \tilde{\omega}_j^2 |q_j|^2 \right).$$

For this class of methods, the non-resonance condition (3.2) as well as the condition on σ of Assumption B are satisfied under a step size restriction.

Theorem 3.2 *We consider the method (2.6). If $\alpha \geq 1/4$, we assume that the step size is restricted by $h\omega_j \leq \text{const}$ for $j = 1, \dots, \ell$, and if $\alpha < 1/4$, we assume that $h\omega_j \leq 2\theta/\sqrt{1-4\alpha}$ for $j = 1, \dots, \ell$ with $\theta < 1$. We fix an arbitrary integer $N \geq 1$ and $0 < \delta \leq 1/4$. Then there exists $h_0 > 0$ such that, under Assumption A without condition (3.2), the numerical solution obtained by method (2.6) satisfies, for $h \leq h_0$ under the above step size restriction,*

$$H_{\text{slow}}(\mathbf{p}_n, \mathbf{q}_n) = H_{\text{slow}}(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(h^{1-\delta}) \quad \text{for } 0 \leq nh \leq h^{-N},$$

as long as $H(\mathbf{p}_n, \mathbf{q}_n) \leq \text{Const}$. If, in addition, the step size h and the frequencies $\tilde{\omega}_j$ satisfy the numerical non-resonance condition (3.5), then we further have, with κ from (3.2),

$$H_\omega^*(\mathbf{p}_n, \mathbf{q}_n) = H_\omega^*(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(h^{1-\delta}/\kappa) \quad \text{for } 0 \leq nh \leq h^{-N}.$$

The constants symbolized by $\mathcal{O}$ are independent of n , h , ε , and ω_j , but depend on ℓ , N , δ , θ and the constants in Assumption A. The threshold h_0 is independent of the frequencies ω_j .

Theorem 3.2 follows from Theorem 3.1, using the frequencies $\tilde{\omega}_j$ instead of ω_j and the transformed momenta $\tilde{p}_j = (\chi(h\tilde{\omega}_j)/\text{sinc}(h\tilde{\omega}_j))p_j$: Since $h\tilde{\omega}_j \in [0, \pi]$, condition (3.2) of Assumption A is satisfied with some κ independent of h under the step size restriction of Theorem 3.2. Concerning Assumption B, the condition on σ is satisfied under the step size restriction of Theorem 3.2. This also implies that $|\chi(\xi)/\text{sinc}(\xi)| = |\psi(\xi)/\text{sinc}(\xi)| = |\phi(\xi)/\sigma(\xi)|$ is bounded for $\xi = h\tilde{\omega}_j$, $j = 1, \dots, \ell$. The step size restriction thus further ensures that the bounded energy condition (3.1) of Assumption A is also satisfied in the transformed variables and with the numerical frequencies $\tilde{\omega}_j$ instead of ω_j .

Remark 3.3 A result like Corollary 3.1 is not valid for the class of symplectic methods (2.6), because H_ω and H_ω^* differ by terms of size $\mathcal{O}(1)$; see also [5] and [7, Section XIII.8] for the Störmer–Verlet method. For the IMEX method ($\alpha = 1/4$) one obtains

$$H_\omega^*(\mathbf{p}, \mathbf{q}) = \sum_{j=1}^{\ell} \frac{\tilde{\omega}_j}{\omega_j} \frac{1}{2} \left(|p_j|^2 + \omega_j^2 |q_j|^2 \right).$$

Therefore, Corollary 3.1 is valid for the IMEX scheme for the special case of a single high frequency.

4 Numerical experiments under numerical resonances

The following experiments illustrate the numerical energy behaviour in situations, for which condition (3.5) in Theorem 3.1 is only fulfilled for small values of N , so that the time intervals $0 \leq nh \leq h^{-N}$ in Theorems 3.1 and 3.2 are *not* very long. It will be observed that *numerical resonances* then play a significant role in the preservation of the total oscillatory energy on longer time intervals.

Unless otherwise stated we use the symplectic trigonometric integrator (2.2) with filter functions [3]

$$\phi(\xi) = 1, \quad \psi(\xi) = \text{sinc}(\xi). \quad (4.1)$$

Experiment 1. Problem with one degree of freedom. We consider the scalar differential equation

$$\ddot{q} + \omega^2 q = -\nabla U(q), \quad U(q) = q^3 + q^4$$

with initial values $q(0) = 0.1 \omega^{-1}$ and $\dot{q}(0) = 1$. Figure 4.1 shows the deviation of the oscillatory energy as a function of time on the interval $[0, t_{\text{end}}]$. The two pictures correspond to the cases $h\omega = 2\pi/3$ and $h\omega = \pi/2$, each one for seven different values of $\omega = \varepsilon^{-1}$ (large deviations correspond to smaller values of ω).

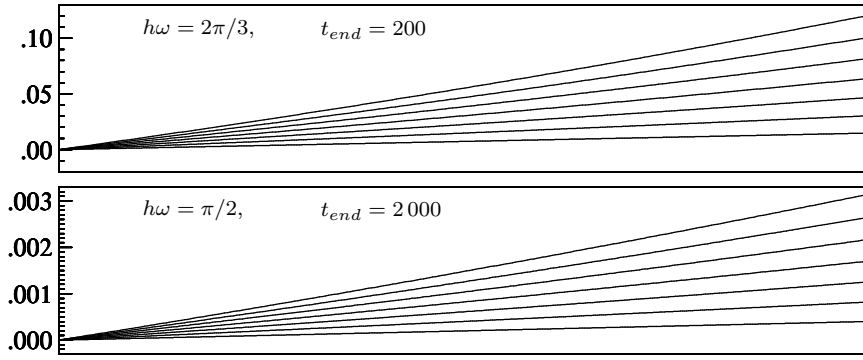


Fig. 4.1 Problem with one degree of freedom: deviation of the numerical oscillatory energy as a function of time t . In the upper picture the curves correspond to $\omega = 100 \cdot \ell^{-1/2}$, in the lower picture to $\omega = 100 \cdot \ell^{-1/3}$, in each case for $\ell = 1, 2, \dots, 7$.

The different frequencies are chosen so that for fixed time t the difference of two consecutive deviations is nearly constant. This allows us to guess that the dominant term in the deviation behaves like $\mathcal{O}(t\varepsilon^2)$ for $h\omega = 2\pi/3$, and like $\mathcal{O}(t\varepsilon^3)$ for $h\omega = \pi/2$. We note that condition (3.5) is satisfied with $N = 1$ for $h\omega = 2\pi/3$ and with $N = 2$ for $h\omega = \pi/2$. The near-preservation of the oscillatory energy on intervals of length $\mathcal{O}(h^{-N})$, stated in Corollary 3.1, can be observed in the numerical experiment.

Experiment 2. Alternating stiff and soft springs. We consider the motion of alternating stiff harmonic and soft nonlinear springs as discussed in [7, Section I.5 and Chapter XIII]. The corresponding differential equation is of the form treated in this article with only one high frequency $\omega = \varepsilon^{-1}$. Along the exact solution of the problem, the oscillatory energy satisfies $H_\omega(\mathbf{p}, \mathbf{q}) = H_\omega(\mathbf{p}_0, \mathbf{q}_0) + \mathcal{O}(\varepsilon)$ on exponentially long time intervals. We apply various trigonometric integrators to this problem, and we are mainly interested in using step sizes for which $h\omega \approx 2\pi r/k$ with integer values for r and k .

Figure 4.2 shows the deviation of the oscillatory energy for method (4.1), applied to the problem with $\omega = 50$ and step size according to $h\omega = 2\pi/3$. We observe that the deviation of the oscillatory energy is of size $\mathcal{O}(\varepsilon)$ on an interval of length $\mathcal{O}(\varepsilon^{-2})$. On longer time intervals the deviation behaves like a random walk. This is illustrated by computing trajectories with slightly perturbed initial values. Repeating the experiment with other values of ω , one finds that the deviation of the numerical oscillatory energy behaves like $\mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon^2\sqrt{t})$. Such a random walk behaviour has already been observed with computations by the simplified Takahashi–Imada method [8]. A similar experiment with $h\omega = \pi/2$ leads to a $\mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon^3\sqrt{t})$ behaviour. Figure 4.3 shows the maximum deviation of the numerical oscillatory energy until a fixed time $t = 100\,000$ as a function of $h\omega$.

For the modified trigonometric integrators (2.5) we expect similar results, because they can be interpreted as trigonometric integrators with modified

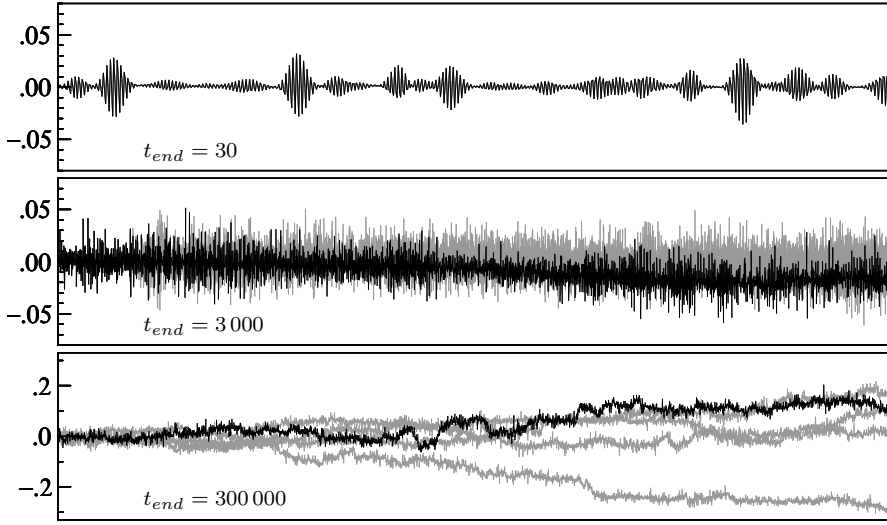


Fig. 4.2 Alternating stiff and soft springs: deviation of the numerical oscillatory energy as a function of time t . We consider the method (4.1) with $\omega = 50$, $h\omega = 2\pi/3$, and initial values from [7] (black curve). The gray curves are obtained when one of the initial values is perturbed to $1 \pm \delta$ with $|\delta| \leq 7 \cdot 10^{-16}$.

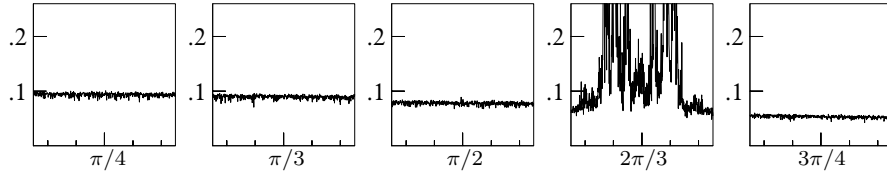


Fig. 4.3 Alternating stiff and soft springs: maximum deviation of the numerical oscillatory energy on a time interval of length 100 000 as a function of $h\omega$. The value of ω is fixed. Each picture shows this deviation on an equidistant grid (591 points) of an $h\omega$ -interval of length 0.1.

frequencies. We apply the IMEX integrator (2.6) with $\alpha = 0.25$ to the problem with alternating stiff and soft springs, where we take $\omega = 25$. In Figure 4.4 we present the results for two different step sizes: $h\omega = \sqrt{12}$ and $h\omega = 2$ which, by the relation of Section 2.3, correspond to $h\tilde{\omega} = 2\pi/3$ and $h\tilde{\omega} = \pi/2$, respectively. Similar as for the trigonometric method we observe a random walk behaviour: $\mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon^2\sqrt{t})$ for $h\omega = \sqrt{12}$, and $\mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon^3\sqrt{t})$ for $h\omega = 2$. The additional factor ε in the second experiment can be guessed from the figures, because a similar quantitative behaviour is observed on an interval that is ω^2 times longer.

Experiment 3. Multi-frequency example. We consider the oscillatory differential equation (1.1) with $\ell = 2$, $\omega_1 = \omega$, $\omega_2 = \sqrt{2}\omega$, and quadratic potential

$$U(\mathbf{q}) = 0.01 q_1 q_2.$$

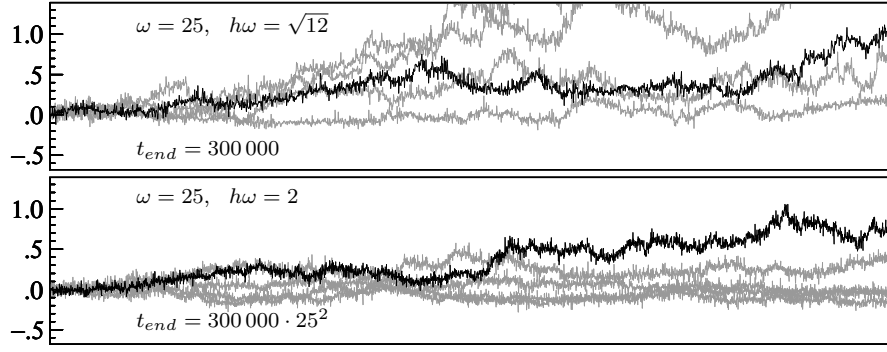


Fig. 4.4 Same experiment as for Figure 4.2, but with the IMEX method (2.6), $\alpha = 1/4$, and with $\omega = 25$. The upper picture corresponds to a step size such that $h\omega = \sqrt{12}$, i.e., $h\tilde{\omega} = 2\pi/3$, the lower picture such that $h\omega = 2$, i.e., $h\tilde{\omega} = \pi/2$.

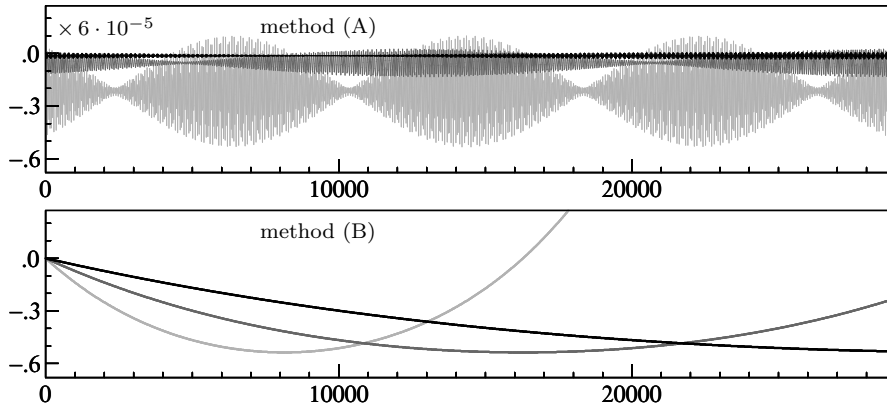


Fig. 4.5 Multi-frequency example: deviation of the oscillatory energy as a function of time t for two trigonometric methods, $\omega = 200$ (black), $\omega = 100$ and $\omega = 50$ in gray.

We apply two trigonometric methods with initial values $\mathbf{q}(0) = (0, 0.3\varepsilon, 0.8\varepsilon)$, $\dot{\mathbf{q}}(0) = (0, 0.6, 0.7)$ with $\varepsilon = \omega^{-1}$ and step size $h = 2\pi/(\omega_1 + \omega_2)$. The result can be seen in Figure 4.5. For the symplectic method (B), with filter functions given by (4.1), we observe a linear growth $\mathcal{O}(t\varepsilon)$ in the numerical oscillatory energy, which soon turns into a quadratic growth. For method (A) of [7, p. 481] (the non-symplectic Gautschi method), with filter functions $\phi(\xi) = 1$ and $\psi(\xi) = \text{sinc}^2(\xi/2)$, the deviation in the oscillatory energy is much smaller.

5 Numerical gap condition for modified frequencies

In order to decide whether a linear combination of frequencies is almost-resonant or non-resonant, we will use a gap in the linear combinations of frequencies. Similarly as in [4, Sect. 3.1] we construct new frequencies that satisfy a non-resonance condition outside a resonance module.

For finite ℓ we can detect a gap in the values of $\sin(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\omega})$ with small $\|\mathbf{k}\|$.

Lemma 5.1 *We fix an arbitrary integer $N \geq 1$ and $0 < \delta \leq 1/4$. There exists $0 < \mu \leq \delta/2$ depending on N, ℓ , and δ , such that for all $0 < h < 1$ there exists α with $\delta/2 \leq \alpha \leq \delta$ depending on the frequencies ω_j and the step size h such that the set*

$$\left\{ \left| \sin\left(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\omega}\right) \right| : \|\mathbf{k}\| \leq N + 1 \right\}$$

contains no element in the interval $[h^{1-\alpha+\mu}, h^{1-\alpha-\mu}]$.

Proof This set contains at most $M = \ell^{N+1}$ elements. Therefore, there exist α with $\delta/2 \leq \alpha \leq \delta$ depending on the frequencies and the time step size and $0 < \mu \leq \delta/2$ depending only on N, ℓ , and δ , such that this set contains no element in the interval $[h^{1-\alpha+\mu}, h^{1-\alpha-\mu}]$. $\square$

We use this gap to introduce modified frequencies $\varpi_1, \dots, \varpi_\ell$ for which near-resonant linear combinations, i.e., those taking a value below the gap, become exactly resonant. It is convenient to use the notation $\varpi_0 = \omega_0 = 0$.

Lemma 5.2 *Let N, δ , and μ be as in Lemma 5.1. Then there exists $h_0 < 1$ such that for fixed $0 < h \leq h_0$ satisfying condition (3.2) the following holds: there exist modified frequencies $\boldsymbol{\varpi} = (\varpi_1, \dots, \varpi_\ell)$ and a $\mathbb{Z}$ -module $\mathcal{M} \leq \mathbb{Z}^d$ such that, with α from Lemma 5.1,*

$$\sin\left(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\varpi}\right) = 0 \quad \text{for } \mathbf{k} \in \mathcal{M}, \quad (5.1)$$

$$\left| \sin\left(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\varpi}\right) \right| \geq \frac{1}{2} h^{1-\alpha-\mu} \quad \text{for } \mathbf{k} \notin \mathcal{M} \text{ with } \|\mathbf{k}\| \leq N + 1. \quad (5.2)$$

The module $\mathcal{M}$ does neither contain the unit vectors $\langle j \rangle = (0, \dots, 1, \dots, 0)$ nor their doubles $2\langle j \rangle$; if, in addition, the numerical non-resonance condition (3.5) holds, then the module contains only those $\mathbf{k} \in \mathbb{Z}^d$ with $\|\mathbf{k}\| \leq N + 1$ that satisfy $\mathbf{k} \cdot \boldsymbol{\varpi} = 0$. Moreover, there exists $\gamma > 0$ depending only on N and ℓ such that

$$|\varpi_j - \omega_j| \leq \gamma h^{-\alpha+\mu} \quad \text{for } j = 1, \dots, \ell. \quad (5.3)$$

Proof We denote by $\mathcal{M}$ the $\mathbb{Z}$ -module generated by

$$\left\{ \mathbf{k} \in \mathbb{Z}^\ell : \|\mathbf{k}\| \leq N + 1 \text{ and } \left| \sin\left(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\omega}\right) \right| \leq h^{1-\alpha+\mu} \right\}. \quad (5.4)$$

This module is spanned by $d \leq \ell$ integer-linearly independent elements $\mathbf{k}^1, \dots, \mathbf{k}^d$ (see, for instance, [9, Chap. III, Theorem 7.1]). Since the number of modules generated by some subset $\mathcal{R} \subseteq \{\mathbf{k} \in \mathbb{Z}^\ell : \|\mathbf{k}\| \leq N + 1\}$ depends only on N and ℓ , the matrix formed by the basis vectors as well its pseudo-inverse are bounded by a constant only depending on N and ℓ . The same is true for the coefficients, when the basis vectors are written as an integer-linear combination of linearly-independent elements of $\mathcal{R}$.

For the basis vectors we choose $m_i \in \mathbb{Z}$ such that $|\frac{h}{2}(\mathbf{k}^i \cdot \boldsymbol{\omega}) - \pi m_i|$ is minimal. Since $\mathbf{k}^i$ is a linear combination with integer coefficients of elements

in (5.4) and since $|\frac{h}{2}(\mathbf{k}^i \cdot \boldsymbol{\omega}) - \pi m_i| \leq (\pi/2) |\sin(\frac{h}{2}(\mathbf{k}^i \cdot \boldsymbol{\omega}))|$, it follows from the addition theorem for sine that $|\frac{h}{2}(\mathbf{k}^i \cdot \boldsymbol{\omega}) - \pi m_i| \leq \gamma_i h^{1-\alpha+\mu}$ with constants γ_i depending only on N and ℓ . We determine $\boldsymbol{\vartheta} = (\vartheta_1, \dots, \vartheta_\ell) \in \mathbb{R}^\ell$ as a solution of minimal norm of

$$\mathbf{k}^i \cdot \boldsymbol{\omega} + \mathbf{k}^i \cdot \boldsymbol{\vartheta} = \frac{2\pi m_i}{h}, \quad i = 1, \dots, \ell \quad (5.5)$$

and introduce new frequencies $\boldsymbol{\varpi} = (\varpi_1, \dots, \varpi_\ell)$ as

$$\varpi_j = \omega_j + \vartheta_j, \quad j = 1, \dots, \ell.$$

These new frequencies are constructed in such a way that (5.1) holds. In addition, the solution $\boldsymbol{\vartheta}$ of (5.5) is bounded as $\|\boldsymbol{\vartheta}\| \leq \gamma h^{-\alpha+\mu}$ with γ depending only on N and ℓ , so that (5.3) holds. Moreover, we have for $\mathbf{k} \notin \mathcal{M}$ with $\|\mathbf{k}\| \leq N+1$ by the choice of the module $\mathcal{M}$, Lemma 5.1 and (5.3)

$$h^{1-\alpha-\mu} < \left| \sin\left(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\omega}\right) \right| \leq \left| \sin\left(\frac{h}{2} \mathbf{k} \cdot \boldsymbol{\varpi}\right) \right| + \frac{\gamma}{2}(N+1)h^{1-\alpha+\mu},$$

and hence (5.2) holds if h satisfies $h^{2\mu}\gamma(N+1) \leq 1$.

The condition (3.2) is used to show that neither the unit vectors $\langle j \rangle$ nor their doubles $2\langle j \rangle$ are contained in $\mathcal{M}$. Indeed, if $\langle j \rangle \in \mathcal{M}$ or $2\langle j \rangle \in \mathcal{M}$, then by (5.3) and (5.1)

$$h^{1/2} \leq |\sin(h\omega_j)| \leq 2 \left| \sin\left(\frac{h}{2} \omega_j\right) \right| \leq h|\vartheta_j| \leq \gamma h^{1-\alpha+\mu}.$$

This gives a contradiction if $\gamma h^{1/2-\alpha+\mu} < 1$.

If, in addition, the numerical non-resonance condition (3.5) holds, then we have for $\mathbf{k} \in \mathcal{M}$ with $\|\mathbf{k}\| \leq N+1$ and $\mathbf{k} \cdot \boldsymbol{\varpi} \neq 0$ that, by (5.3) and (5.1),

$$h^{1/2} \leq \min_{0 \neq r \in \mathbb{Z}} \left| \frac{h}{2} \mathbf{k} \cdot \boldsymbol{\omega} - r\pi \right| \leq \left| \frac{h}{2} \mathbf{k} \cdot \boldsymbol{\vartheta} \right| + \min_{0 \neq r \in \mathbb{Z}} \left| \frac{h}{2} \mathbf{k} \cdot \boldsymbol{\varpi} - r\pi \right| \leq \frac{\gamma}{2}(N+1)\gamma h^{1-\alpha+\mu}.$$

This gives a contradiction if $(N+1)\gamma h^{1/2-\alpha+\mu} < 2$. $\square$

6 Modulated Fourier expansion

We fix an arbitrary integer $N \geq 1$ and $0 < \delta \leq 1/4$, and we denote by α and μ the constants of Lemma 5.1. For fixed step size $0 < h \leq h_0$ satisfying (3.2) and with h_0 from Lemma 5.2, we let $\boldsymbol{\varpi} = (\varpi_1, \dots, \varpi_\ell)$ be the modified frequencies and $\mathcal{M}$ the $\mathbb{Z}$ -module of Lemma 5.2. We denote by $\mathcal{N}$ a set of representatives of the equivalence classes in $\mathbb{Z}^\ell/\mathcal{M}$, which are chosen such that for each $\mathbf{k} \in \mathcal{N}$ the norm of $\mathbf{k}$ is minimal in the equivalence class $[\mathbf{k}] = \mathbf{k} + \mathcal{M}$, and with $\mathbf{k} \in \mathcal{N}$, also $-\mathbf{k} \in \mathcal{N}$. We further denote $\mathcal{K} = \{\mathbf{k} \in \mathcal{N} : \|\mathbf{k}\| \leq N+1\}$.

We make the approximation ansatz (modulated Fourier expansion)

$$\mathbf{q}_n \approx \sum_{\mathbf{k} \in \mathcal{K}} \mathbf{z}^{\mathbf{k}} (h^{-\alpha} t) e^{i(\mathbf{k} \cdot \boldsymbol{\varpi})t} \quad \text{for} \quad t = nh, \quad (6.1)$$

and denote the components of $\mathbf{q}_n$ by $q_{n,j}$ and those of $\mathbf{z}^{\mathbf{k}}$ by $z_j^{\mathbf{k}}$ for $j = 0, \dots, \ell$. We insert the ansatz (6.1) into (2.2), expand the right-hand side into a Taylor series around the smooth function $\Phi \mathbf{z}^0(h^{-\alpha}t)$ and compare the coefficients of $e^{i(\mathbf{k} \cdot \varpi)t}$. This yields

$$L_j^{\mathbf{k}} z_j^{\mathbf{k}} = 2(\cos(h\omega_j) - \cos(h\varpi_j)) z_j^{\mathbf{k}} - h^2 \psi(h\omega_j) \nabla_j^{-\mathbf{k}} \mathcal{U}(\Phi \mathbf{z}) + h^2 \delta_j^{\mathbf{k}}, \quad (6.2)$$

where we allow for a small defect $\delta_j^{\mathbf{k}}$. Here, $\nabla_j^{-\mathbf{k}} \mathcal{U}(\mathbf{x})$ denotes the derivative of

$$\mathcal{U}(\mathbf{x}) = U(\mathbf{x}^0) + \sum_{m=2}^N \sum_{j_1, \dots, j_m=0}^{\ell} \sum_{\mathbf{k}^1 + \dots + \mathbf{k}^m \in \mathcal{M}} \frac{1}{m!} \partial_{j_1} \dots \partial_{j_m} U(\mathbf{x}^0)(x_{j_1}^{\mathbf{k}^1}, \dots, x_{j_m}^{\mathbf{k}^m}) \quad (6.3)$$

with respect to $x_j^{-\mathbf{k}}$, where the last sum is over multi-indices $\mathbf{k}^l \in \mathcal{K}$ with $\mathbf{k}^l \neq \mathbf{0}$ and $\|\mathbf{k}^1\| + \dots + \|\mathbf{k}^m\| \leq N + 1$. The operator $L_j^{\mathbf{k}}$ in (6.2) is given by

$$\begin{aligned} (L_j^{\mathbf{k}} z_j^{\mathbf{k}})(\tau) &= e^{i(\mathbf{k} \cdot \varpi)h} z_j^{\mathbf{k}}(\tau + h^{1-\alpha}) - 2 \cos(h\varpi_j) z_j^{\mathbf{k}}(\tau) + e^{-i(\mathbf{k} \cdot \varpi)h} z_j^{\mathbf{k}}(\tau - h^{1-\alpha}) \\ &= 4s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}} z_j^{\mathbf{k}}(\tau) + 2is_{2\mathbf{k}} h^{1-\alpha} \dot{z}_j^{\mathbf{k}}(\tau) + c_{2\mathbf{k}} h^{2(1-\alpha)} \ddot{z}_j^{\mathbf{k}}(\tau) + \dots \end{aligned} \quad (6.4)$$

Here, $s_{\mathbf{k}} = \sin(\frac{h}{2} \mathbf{k} \cdot \varpi)$ and $c_{\mathbf{k}} = \cos(\frac{h}{2} \mathbf{k} \cdot \varpi)$, and the dots on $z_j^{\mathbf{k}}$ represent derivatives with respect to the scaled time $\tau = h^{-\alpha}t$. The higher order terms are linear combinations of the r th derivative of $z_j^{\mathbf{k}}$ (for $r \geq 3$) multiplied by $h^{r(1-\alpha)}$ and containing one of the factors $s_{2\mathbf{k}}$ or $c_{2\mathbf{k}}$.

To get initial values we insert the ansatz (6.1) into the relation $\mathbf{q}_0 = \mathbf{q}(0)$ and into the second formula of (2.2). This yields the equations (for $j = 0, \dots, \ell$)

$$\begin{aligned} q_{0,j} &= \sum_{\mathbf{k} \in \mathcal{K}} z_j^{\mathbf{k}}(0), \\ 2h \operatorname{sinc}(h\omega_j) p_{0,j} &= \sum_{\mathbf{k} \in \mathcal{K}} \left(z_j^{\mathbf{k}}(h^{1-\alpha}) e^{i(\mathbf{k} \cdot \varpi)h} - z_j^{\mathbf{k}}(-h^{1-\alpha}) e^{-i(\mathbf{k} \cdot \varpi)h} \right) \\ &= \sum_{\mathbf{k} \in \mathcal{K}} \left(2is_{2\mathbf{k}} z_j^{\mathbf{k}}(0) + 2c_{2\mathbf{k}} h^{1-\alpha} \dot{z}_j^{\mathbf{k}}(0) + is_{2\mathbf{k}} h^{2(1-\alpha)} \ddot{z}_j^{\mathbf{k}}(0) + \dots \right). \end{aligned} \quad (6.5)$$

The Taylor series expansions in the relations (6.4) and (6.5) are truncated after $L \geq (N+3)/(1-\alpha)$ terms, such that the remainder is of size $\mathcal{O}(h^{N+1})$. Since the following analysis requires estimates for the modulation functions $z_j^{\mathbf{k}}$ and their derivatives on the interval $\tau \in [0, 1]$ (which corresponds to $t \in [0, h^\alpha]$), we consider for functions $\mathbf{z} = (z_j^{\mathbf{k}})$ the norms

$$|z_j^{\mathbf{k}}|_{C^r} = \max_{0 \leq \tau \leq 1} \max_{0 \leq l \leq r} \left| \frac{d^l}{d\tau^l} z_j^{\mathbf{k}}(\tau) \right|, \quad \|\mathbf{z}\|_{C^r} = \sum_{j=0}^{\ell} \sum_{\mathbf{k} \in \mathcal{K}} |z_j^{\mathbf{k}}|_{C^r}. \quad (6.6)$$

Theorem 6.1 *For an arbitrarily fixed N and under Assumptions A and B the numerical solution $\mathbf{q}_n$ of (2.2) admits an expansion*

$$\mathbf{q}_n = \sum_{\mathbf{k} \in \mathcal{K}} \mathbf{z}^{\mathbf{k}}(h^{-\alpha}t) e^{i(\mathbf{k} \cdot \varpi)t} + \mathbf{r}_n \quad \text{for} \quad t = nh \leq h^\alpha, \quad (6.7)$$

where the coefficient functions $z_j^{\mathbf{k}}(\tau)$ satisfy $z_j^{-\mathbf{k}} = \overline{z_j^{\mathbf{k}}}$ and are bounded by

$$|z_0^{\mathbf{0}}|_{C^L} \leq C \quad (6.8)$$

$$|z_j^{\pm(j)}|_{C^L} \leq C\omega_j^{-1}, \quad j = 1, \dots, \ell \quad (6.9)$$

$$|z_j^{\mathbf{0}}|_{C^L} \leq Ch^2 |s_{(j)}|^{-2} |\psi(h\omega_j)| \varepsilon^2, \quad j = 1, \dots, \ell \quad (6.10)$$

and for all other $(j, \mathbf{k})$ by

$$|z_j^{\mathbf{k}}|_{C^L} \leq Ch^2 |s_{(j)+\mathbf{k}} s_{(j)-\mathbf{k}}|^{-1} |\psi(h\omega_j)| \varepsilon^{\|\mathbf{k}\|} \quad (6.11)$$

$$|z_j^{\mathbf{k}}|_{C^L} \leq Ch^2 |s_{(j)+\mathbf{k}} s_{(j)-\mathbf{k}}|^{-1} |\psi(h\omega_j)| (1 + |\mathbf{k} \cdot \boldsymbol{\varpi}|)^{-1} \quad (6.12)$$

with some $L \geq (N+3)/(1-\alpha)$. The functions $z_j^{\mathbf{k}}$ satisfy the equations (6.2) with a defect bounded for $0 \leq \tau \leq 1$ by

$$|\delta_0^{\mathbf{k}}(\tau)| \leq Ch^{N+1}, \quad |\delta_j^{\mathbf{k}}(\tau)| \leq C\omega_j^{-1} h^N \quad \text{for } j = 1, \dots, \ell. \quad (6.13)$$

For $0 \leq nh \leq h^\alpha$ the remainder term $\mathbf{r}_n = (r_{n,j})$ in (6.7) is bounded by

$$|r_{n,0}| \leq Ch^{N+1}, \quad |r_{n,j}| \leq C\omega_j^{-1} h^N \quad \text{for } j = 1, \dots, \ell. \quad (6.14)$$

The generic constant C is independent of ε and the frequencies $\omega_j \geq \varepsilon^{-1}$, but depends on ℓ , N , and the constants in Assumptions A and B.

Details of the proof of Theorem 6.1 will be given in Section 7 below. It combines the techniques of [4] for the analytic solution of (2.1) and those of [2] for the numerical solution.

The second formula of (2.2) requires a modulated Fourier expansion for the derivative approximation.

Corollary 6.1 *Under the assumptions of Theorem 6.1 the derivative approximation of (2.2) satisfies, for $\tau = h^{-\alpha}t$ and $t = nh \leq h^\alpha$,*

$$\mathbf{p}_n = \sum_{\mathbf{k} \in \mathcal{K}} \mathbf{w}^{\mathbf{k}}(\tau) e^{i(\mathbf{k} \cdot \boldsymbol{\varpi})t} + \dot{\mathbf{r}}_n,$$

where

$$\mathbf{w}^{\mathbf{k}}(\tau) = (2h \operatorname{sinc}(h\Omega))^{-1} \left(\mathbf{z}^{\mathbf{k}}(\tau + h^{1-\alpha}) e^{i(\mathbf{k} \cdot \boldsymbol{\varpi})h} - \mathbf{z}^{\mathbf{k}}(\tau - h^{1-\alpha}) e^{-i(\mathbf{k} \cdot \boldsymbol{\varpi})h} \right)$$

and

$$|\dot{r}_{n,0}| \leq Ch^N \quad \text{and} \quad |\dot{r}_{n,j}| \leq Ch^N / \kappa \quad \text{for } j = 1, \dots, \ell. \quad (6.15)$$

Proof The estimate for the remainder

$$\dot{\mathbf{r}}_n = (2h \operatorname{sinc}(h\Omega))^{-1} (\mathbf{r}_{n+1} - \mathbf{r}_{n-1}).$$

follows from (6.14) and Assumption A. $\square$

7 Proof of Theorem 6.1

Our aim is to construct functions $z_j^{\mathbf{k}}$ ($j = 0, \dots, \ell$ and $\mathbf{k} \in \mathcal{K}$) such that the defect in equations (6.2) is of size $\mathcal{O}(h^{N+1})$. For this we truncate the Taylor series expansions in (6.4) and (6.5) after $L \geq (N+3)/(1-\alpha)$ terms, and we consider a Picard iteration improving the approximation by a factor h^μ in every iteration. This requires $M \geq (N+1+\alpha)/\mu$ iterations.

7.1 Construction of the modulation functions

We denote by $\mathbf{z}^m = ([z_j^{\mathbf{k}}]^m)$ the m th iterate and distinguish between the following cases:

1. For $j = 0$ and $\mathbf{k} = \mathbf{0}$ the first two terms in the expansion (6.4) disappear and after division by $h^{2(1-\alpha)}$ we iterate with a second order differential equation (6.2) for $[z_0^{\mathbf{0}}]^{m+1}$:

$$\frac{d^2[z_0^{\mathbf{0}}]^{m+1}}{d\tau^2} + \left[\frac{2h^{2(1-\alpha)}}{4!} \frac{d^4 z_0^{\mathbf{0}}}{d\tau^4} + \frac{2h^{4(1-\alpha)}}{6!} \frac{d^6 z_0^{\mathbf{0}}}{d\tau^6} + \dots \right]^m = -h^{2\alpha} \nabla_0^{-\mathbf{0}} \mathcal{U}(\Phi \mathbf{z}^m). \quad (7.1)$$

Here and in the following equations the three dots indicate a truncation of the series after the term corresponding to the L th derivative. The notation $\nabla_j^{-\mathbf{k}} \mathcal{U}(\Phi \mathbf{z}^m)$ should be interpreted so that all appearing $z_j^{\mathbf{k}}$ (including $\mathbf{k} = \mathbf{0}$) are replaced by their m th iterate.

2. For $j \neq 0$ and $\mathbf{k} = \pm \langle j \rangle$ the first term in (6.4) disappears and we iterate using a first order differential equation for $[z_j^{\pm \langle j \rangle}]^{m+1}$:

$$\begin{aligned} & \pm 2i s_{2\langle j \rangle} \frac{d[z_j^{\pm \langle j \rangle}]^{m+1}}{d\tau} + \left[c_{2\langle j \rangle} h^{1-\alpha} \frac{d^2 z_j^{\pm \langle j \rangle}}{d\tau^2} \pm i \frac{s_{2\langle j \rangle}}{3} h^{2(1-\alpha)} \frac{d^3 z_j^{\pm \langle j \rangle}}{d\tau^3} + \dots \right]^m \\ & = 2h^{\alpha-1} (\cos(h\omega_j) - \cos(h\varpi_j)) [z_j^{\pm \langle j \rangle}]^m - h^{1+\alpha} \psi(h\omega_j) \nabla_j^{\mp \langle j \rangle} \mathcal{U}(\Phi \mathbf{z}^m). \end{aligned} \quad (7.2)$$

3. In all other cases we iterate with an explicit equation for $[z_j^{\mathbf{k}}]^{m+1}$:

$$\begin{aligned} & 4 s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}} [z_j^{\mathbf{k}}]^{m+1} + \left[2i s_{2\mathbf{k}} h^{1-\alpha} \dot{z}_j^{\mathbf{k}} + c_{2\mathbf{k}} h^{2(1-\alpha)} \ddot{z}_j^{\mathbf{k}} + \dots \right]^m \\ & = 2(\cos(h\omega_j) - \cos(h\varpi_j)) [z_j^{\mathbf{k}}]^m - h^2 \psi(h\omega_j) \nabla_j^{-\mathbf{k}} \mathcal{U}(\Phi \mathbf{z}^m). \end{aligned} \quad (7.3)$$

We need initial values $[z_0^{\mathbf{0}}]^{m+1}(0)$, $\frac{d}{d\tau}[z_0^{\mathbf{0}}]^{m+1}(0)$, and $[z_j^{\pm \langle j \rangle}]^{m+1}(0)$ for $j \neq 0$. Note that at the iteration m the values $\mathbf{z}^m(0) = ([z_j^{\mathbf{k}}]^m)(0)$ together with the derivatives of $[z_j^{\mathbf{k}}]^m$ at $\tau = 0$ are known. Extracting the dominant terms

in (6.5), the required initial values are determined by the equations

$$\begin{aligned} [z_0^{\mathbf{0}}]^{m+1}(0) &= q_{0,0} - \sum_{\mathbf{k} \neq \mathbf{0}} [z_0^{\mathbf{k}}]^m(0), \\ 2h^{1-\alpha} [z_0^{\mathbf{0}}]^{m+1}(0) &= 2hp_{0,0} - \sum_{\mathbf{k} \neq \mathbf{0}} \left[2i s_{2\mathbf{k}} z_0^{\mathbf{k}} + 2c_{2\mathbf{k}} h^{1-\alpha} \dot{z}_0^{\mathbf{k}} + \dots \right]^m(0) \\ &\quad - \left[\frac{2}{3!} h^{3(1-\alpha)} \frac{d^3 z_0^{\mathbf{0}}}{d\tau^3} + \frac{2}{5!} h^{5(1-\alpha)} \frac{d^5 z_0^{\mathbf{0}}}{d\tau^5} + \dots \right]^m(0) \end{aligned} \quad (7.4)$$

and for $j = 1, \dots, \ell$ by

$$\begin{aligned} [z_j^{\langle j \rangle} + z_j^{-\langle j \rangle}]^{m+1}(0) &= q_{0,j} - \sum_{\mathbf{k} \neq \pm \langle j \rangle} [z_j^{\mathbf{k}}]^m(0), \\ 2i s_{2\langle j \rangle} [z_j^{\langle j \rangle} - z_j^{-\langle j \rangle}]^{m+1}(0) &= 2h \operatorname{sinc}(h\omega_j) p_{0,j} - \sum_{\mathbf{k} \neq \pm \langle j \rangle} 2i s_{2\mathbf{k}} [z_j^{\mathbf{k}}]^m(0) \\ &\quad - \sum_{\mathbf{k} \in \mathcal{K}} \left[2c_{2\mathbf{k}} h^{1-\alpha} \dot{z}_j^{\mathbf{k}} + i s_{2\mathbf{k}} h^{2(1-\alpha)} \ddot{z}_j^{\mathbf{k}} + \dots \right]^m(0). \end{aligned} \quad (7.5)$$

The starting iterates are chosen for $(j, \mathbf{k}) = (0, \mathbf{0})$ as $[z_0^{\mathbf{0}}]^0(\tau) = q_{0,0}$, and $[z_j^{\mathbf{k}}]^0(\tau) = 0$ for all other indices $(j, \mathbf{k})$.

7.2 Bounds for the modulation functions

To get the desired bounds (6.8)–(6.12) of Theorem 6.1 for the coefficient functions of the modulated Fourier expansion, we first study the individual terms appearing in equations (7.1)–(7.3).

The coefficients of the terms in (7.1) corresponding to arguments of the m th iterate are all small because $0 < \alpha < 1$.

Next, we consider the coefficients of the terms in (7.2) corresponding to arguments of the m th iterate. Since $2\langle j \rangle \notin \mathcal{M}$ by Lemma 5.2, it follows from (5.2) that $|s_{2\langle j \rangle}| \geq \frac{1}{2} h^{1-\alpha-\mu}$. This implies that $|c_{2\langle j \rangle} h^{1-\alpha} / s_{2\langle j \rangle}| \leq 2h^\mu$ and $|h^{1+\alpha} \psi(h\omega_j) / s_{2\langle j \rangle}| \leq 2Ch^{2\alpha+\mu}$, which are small for positive α and μ . We have

$$\frac{h^{\alpha-1} (\cos(h\omega_j) - \cos(h\varpi_j))}{s_{2\langle j \rangle}} = \frac{2h^{\alpha-1} \sin(h \frac{\omega_j + \varpi_j}{2}) \sin(h \frac{\varpi_j - \omega_j}{2})}{\sin(h\varpi_j)},$$

which, by $|\sin(h \frac{\omega_j + \varpi_j}{2})| \leq |\sin(h\varpi_j)| + |\sin(h \frac{\omega_j - \varpi_j}{2})|$ and by (5.3) and (5.2), is seen to be bounded by $\mathcal{O}(h^\mu)$. This implies that, after division by $2i s_{2\langle j \rangle}$, the coefficients of the terms in (7.2) are small.

Finally, we consider the coefficients of the terms in (7.3). From the addition formula for sine we have

$$\left| \frac{s_{2\mathbf{k}}}{s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}}} \right| \leq \frac{|s_{\langle j \rangle + \mathbf{k}}| + |s_{\langle j \rangle - \mathbf{k}}|}{|s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}}|} \leq \frac{1}{|s_{\langle j \rangle - \mathbf{k}}|} + \frac{1}{|s_{\langle j \rangle + \mathbf{k}}|}. \quad (7.6)$$

For $\mathbf{k} \neq \pm \langle j \rangle$, we have $\langle j \rangle \pm \mathbf{k} \notin \mathcal{M}$ so that the estimate (5.2) can be applied. This implies that, after division by $s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}}$, the coefficient of $[\dot{z}_j^{\mathbf{k}}]^m$ in (7.3) is of size $\mathcal{O}(h^\mu)$, and that of the second derivative is $\mathcal{O}(h^{2\mu})$. Similar computations show that the last two terms have coefficients of size $\mathcal{O}(h^{2\mu})$ and $\mathcal{O}(h^{2\alpha+2\mu})$, respectively.

Another useful estimate for the following analysis is

$$|\psi(h\omega_j)| = \left| \frac{\text{sinc}(h\omega_j)\phi(h\omega_j)}{\sigma(h\omega_j)} \right| \leq \frac{C}{h\omega_j}, \quad (7.7)$$

which follows from Assumption B.

We now prove by induction on m , for $m = 0, 1, \dots, M$,

$$|[z_0^{\mathbf{0}}]^m|_{C^r} \leq C \quad (7.8)$$

$$|[z_j^{\pm \langle j \rangle}]^m|_{C^r} \leq C\omega_j^{-1}, \quad j = 1, \dots, \ell \quad (7.9)$$

$$|[z_j^{\mathbf{0}}]^m|_{C^r} \leq Ch^2 |s_{\langle j \rangle}|^{-2} |\psi(h\omega_j)| \varepsilon^2, \quad j = 1, \dots, \ell \quad (7.10)$$

and for all other $(j, \mathbf{k})$

$$|[z_j^{\mathbf{k}}]^m|_{C^r} \leq Ch^2 |s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}}|^{-1} |\psi(h\omega_j)| \varepsilon^{|\mathbf{k}|} \quad (7.11)$$

$$|[z_j^{\mathbf{k}}]^m|_{C^r} \leq Ch^2 |s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}}|^{-1} |\psi(h\omega_j)| (1 + |\mathbf{k} \cdot \varpi|)^{-1} \quad (7.12)$$

where $r = L(M - m + 1)$. By definition of the starting iterates, $[z_0^{\mathbf{0}}]^0(\tau) = q_{0,0}$ is constant and all other functions vanish, so that the statements hold for $m = 0$.

Assuming the bounds to be true at level m , (7.10) and (7.11) follow for the $(m + 1)$ th iterate from the previous bounds on the coefficients of the equation (7.3) and the fact that every summand in $\nabla_j^{-\mathbf{k}} \mathcal{U}(\Phi \mathbf{z})$ contains factors $z_{j_1}^{\mathbf{k}^1}, \dots, z_{j_m}^{\mathbf{k}^m}$ with $\mathbf{k}^1 + \dots + \mathbf{k}^m = \mathbf{k}$ modulo $\mathcal{M}$. The estimate (7.12) follows by applying the triangular inequality to $\mathbf{k} \cdot \varpi = \mathbf{k}^1 \cdot \varpi + \dots + \mathbf{k}^m \cdot \varpi$ and using

$$1 + |\mathbf{k} \cdot \varpi| \leq (1 + |\mathbf{k}^1 \cdot \varpi|) \cdot \dots \cdot (1 + |\mathbf{k}^m \cdot \varpi|).$$

The same argument applied to $\omega_j = \mathbf{k}^1 \cdot \varpi + \dots + \mathbf{k}^m \cdot \varpi$ yields the estimate $|\dot{z}_j^{\pm \langle j \rangle}|^{m+1}|_{C^r} \leq C\omega_j^{-1}$ from equation (7.2), and we get $|\dot{z}_0^{\mathbf{0}}|^{m+1}|_{C^r} \leq Ch^{2\alpha}$ from (7.1) using $\alpha \leq 1/2$.

In order to derive estimates of the initial values $[z_0^{\mathbf{0}}]^{m+1}(0)$, $[\dot{z}_0^{\mathbf{0}}]^{m+1}(0)$ and $[z_j^{\pm \langle j \rangle}]^{m+1}(0)$, we use that

$$q_{0,0} \leq C, \quad p_{0,0} \leq C, \quad \omega_j q_{0,j} \leq C, \quad p_{0,j} \leq C \quad \text{for } j = 1, \dots, \ell \quad (7.13)$$

by the bounded energy condition (3.1) and the bounds on the potential and the numerical solution of Assumption A. From the relations (7.4), still using the estimates at level m and in particular $|[z_0^{\mathbf{k}}]^m|_{C^r} \leq C\varepsilon h^{2\alpha}$ for $\mathbf{k} \neq \mathbf{0}$, we obtain the bounds $|[z_0^{\mathbf{0}}]^{m+1}(0)| \leq C$ and $|\dot{z}_0^{\mathbf{0}}|^{m+1}(0)| \leq Ch^\alpha$ from the condition $\varepsilon \leq h/c_0$. Using (7.7) and the condition $\varepsilon \leq h/c_0$ of Assumption A we get $|\dot{z}_j^{\mathbf{k}}|^m|_{C^r} \leq C\omega_j^{-1}$ and $h^{1-\alpha} |\dot{z}_j^{\mathbf{k}}|^m|_{C^r} / |s_{2\langle j \rangle}| \leq C\omega_j^{-1}$ for $j \neq 0$. Using

in addition (7.6) we get $|s_{2\mathbf{k}}[z_j^{\mathbf{k}}]^m|_{C^r}/|s_{2\langle j \rangle}| \leq C\omega_j^{-1}$ for $j \neq 0$. These estimates yield $|[z_j^{\pm\langle j \rangle}]^{m+1}(0)| \leq C\omega_j^{-1}$ from (7.5). The bounds (7.8) and (7.9) are finally obtained by integration of the relations (7.1) and (7.2), respectively.

7.3 Bounds for the defect

Here, we prove the estimate (6.13) for the defect $\delta_j^{\mathbf{k}}$ in Theorem 6.1. The defect $\delta_j^{\mathbf{k}}(\tau)$ of (6.2) for the M th iterate of Section 7.1 is equal to $[\delta_j^{\mathbf{k}}]^M(\tau)$, where $[\delta_j^{\mathbf{k}}]^m(\tau)$ is the defect in inserting the m th iterate $\mathbf{z}^m = ([z_j^{\mathbf{k}}]^m)$ into the modulation equations (6.2). It satisfies for $(j, \mathbf{k}) = (0, \mathbf{0})$

$$[\delta_0^{\mathbf{0}}]^m = -h^{-2\alpha} \left(\frac{d^2[z_0^{\mathbf{0}}]^{m+1}}{d\tau^2} - \frac{d^2[z_0^{\mathbf{0}}]^m}{d\tau^2} \right),$$

for $j = 1, \dots, \ell$ and $\mathbf{k} = \pm\langle j \rangle$

$$[\delta_j^{\pm\langle j \rangle}]^m = \mp 2i s_{2\langle j \rangle} h^{-1-\alpha} \left(\frac{d[z_j^{\pm\langle j \rangle}]^{m+1}}{d\tau} - \frac{d[z_j^{\pm\langle j \rangle}]^m}{d\tau} \right),$$

and for all other $(j, \mathbf{k})$

$$[\delta_j^{\mathbf{k}}]^m = -\frac{4}{h^2} s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}} \left([z_j^{\mathbf{k}}]^{m+1} - [z_j^{\mathbf{k}}]^m \right).$$

With the notation

$$\mathbf{A}\mathbf{z} = \mathbf{v} = (v_j^{\mathbf{k}}) \quad \text{with} \quad \begin{cases} v_0^{\mathbf{0}} = h^{-2\alpha} z_0^{\mathbf{0}} \\ v_0^{\mathbf{k}} = 4 s_{\mathbf{k}}^2 h^{-2} z_0^{\mathbf{k}} & \mathbf{k} \neq \mathbf{0} \\ v_j^{\pm\langle j \rangle} = 2 h \omega_j s_{2\langle j \rangle} h^{-1-\alpha} z_j^{\pm\langle j \rangle}, & j = 1, \dots, \ell \\ v_j^{\mathbf{k}} = 4 h \omega_j s_{\langle j \rangle + \mathbf{k}} s_{\langle j \rangle - \mathbf{k}} h^{-2} z_j^{\mathbf{k}} & \text{else,} \end{cases}$$

and the above formulas for the defect we have in the norm (6.6) that

$$|[\delta_0^{\mathbf{k}}]^m| \leq \|\mathbf{v}^{m+1} - \mathbf{v}^m\|_{C^2}, \quad |[\delta_j^{\mathbf{k}}]^m| \leq (h\omega_j)^{-1} \|\mathbf{v}^{m+1} - \mathbf{v}^m\|_{C^1}$$

for $j = 1, \dots, \ell$ and all $\mathbf{k} \in \mathcal{K}$. We therefore study $\mathbf{v}^{m+1} - \mathbf{v}^m$ and show by induction on m that for $m \leq M$ and $r = L(M - m + 1)$,

$$\|\mathbf{v}^{m+1} - \mathbf{v}^m\|_{C^r} = \mathcal{O}(h^{m\mu-\alpha}), \quad (7.14)$$

which implies the estimate (6.13) of the defect in Theorem 6.1 if we use $M \geq (N + 1 + \alpha)/\mu$ iterations for the construction of the modulation functions. In the following estimates we repeatedly use (7.7) to obtain the factor ω_j^{-1} where needed. For $m = 0$, the definition of $\mathbf{v}^0$ and the bounds of Section 7.2 yield $|[v_j^{\mathbf{k}}]^1 - [v_j^{\mathbf{k}}]^0|_{C^{LM+L}} = \mathcal{O}(h^{-\alpha})$.

For the induction proof we first consider the functions $[v_j^{\mathbf{k}}]^m$ defined in (7.3). The bounds of Section 7.2 yield

$$|[v_j^{\mathbf{k}}]^{m+1} - [v_j^{\mathbf{k}}]^m|_{C^r} \leq Ch^\mu \|\mathbf{v}^m - \mathbf{v}^{m-1}\|_{C^{r+L}}.$$

We next consider the diagonal elements $[v_j^{\pm(j)}]^m$. From (7.5) we obtain that

$$|[v_j^{\pm(j)}]^{m+1}(0) - [v_j^{\pm(j)}]^m(0)| \leq Ch^\mu \|\mathbf{v}^m - \mathbf{v}^{m-1}\|_{C^L}.$$

Integration of equation (7.2) then yields

$$|[v_j^{\pm(j)}]^{m+1}(\tau) - [v_j^{\pm(j)}]^m(\tau)| \leq Ch^\mu \|\mathbf{v}^m - \mathbf{v}^{m-1}\|_{C^L}, \quad 0 \leq \tau \leq 1.$$

Repeated differentiation in (7.2) further shows that

$$|[v_j^{\pm(j)}]^{m+1} - [v_j^{\pm(j)}]^m|_{C^r} \leq Ch^\mu \|\mathbf{v}^m - \mathbf{v}^{m-1}\|_{C^{r+L}}.$$

Using $2(1 - \alpha) \geq \mu$ and $2\alpha \geq \mu$ we also bound

$$|[v_0^{\mathbf{0}}]^{m+1} - [v_0^{\mathbf{0}}]^m|_{C^r} \leq Ch^\mu \|\mathbf{v}^m - \mathbf{v}^{m-1}\|_{C^{r+L}}.$$

Summarizing we get

$$\|\mathbf{v}^{m+1} - \mathbf{v}^m\|_{C^r} \leq Ch^\mu \|\mathbf{v}^m - \mathbf{v}^{m-1}\|_{C^{r+L}}.$$

This proves (7.14) and the estimate of the defect of Theorem 6.1.

7.4 Solution approximation

In this section we prove the bounds (6.14), which then completes the proof of Theorem 6.1. We consider the M th iterates of the modulation functions (with $M \geq (N+1+\alpha)/\mu$) and omit the superscript M on the modulation functions and their defects. The truncated modulated Fourier expansion

$$\tilde{\mathbf{q}}_n = \sum_{\mathbf{k} \in \mathcal{K}} \mathbf{z}^{\mathbf{k}}(h^{-\alpha}t) e^{i(\mathbf{k} \cdot \boldsymbol{\varpi})t}, \quad t = nh, \quad (7.15)$$

inserted into the method (2.2)

$$\tilde{\mathbf{q}}_{n+1} - 2\cos(h\boldsymbol{\Omega})\tilde{\mathbf{q}}_n + \tilde{\mathbf{q}}_{n-1} = -h^2\boldsymbol{\Psi}\nabla U(\boldsymbol{\Phi}\tilde{\mathbf{q}}_n) + h^2\mathbf{d}_n$$

has a defect $\mathbf{d}_n$. The j th component of the defect is given by

$$\begin{aligned} d_{n,j} = & \sum_{\mathbf{k} \in \mathcal{K}} (\delta_j^{\mathbf{k}}(h^{-\alpha}t) - \hat{\rho}_j^{\mathbf{k}}(h^{-\alpha}t)) e^{i(\mathbf{k} \cdot \boldsymbol{\varpi})t} \\ & - \psi(h\omega_j) \left(\sum_{\mathbf{k} \in \mathcal{N}} \nabla_j^{-\mathbf{k}} \hat{\mathcal{U}}(\boldsymbol{\Phi}\mathbf{z}(h^{-\alpha}t)) e^{i(\mathbf{k} \cdot \boldsymbol{\varpi})t} + \rho_{n,j} \right), \end{aligned} \quad (7.16)$$

where $\delta_j^{\mathbf{k}}$ is defined in (6.2), $\hat{\rho}_j^{\mathbf{k}}$ denotes the remainder term of the truncated Taylor series expansions in (6.4), and $(\rho_{n,j})$ denotes the remainder term in the truncated Taylor series expansion of the gradient of U around $\boldsymbol{\Phi}\mathbf{z}^{\mathbf{0}}(h^{-\alpha}t)$. The second (finite) sum collects those terms that were neglected in the definition of $\mathcal{U}$ in (6.3), i.e., $\hat{\mathcal{U}}$ is defined as $\mathcal{U}$ in (6.3) but with the last sum over $\mathbf{k}^l \in \mathcal{N}$

with $\mathbf{k}^l \neq \mathbf{0}$ and $\|\mathbf{k}^1\| + \dots + \|\mathbf{k}^m\| > N + 1$. Writing $\tilde{\mathbf{q}}_n = \mathbf{z}^0(h^{-\alpha}t) + \hat{\mathbf{q}}_n$, and omitting the index n and the argument $\tau = h^{-\alpha}t$ we have

$$\rho_{n,j} = \nabla_j U(\Phi \tilde{\mathbf{q}}) - \nabla_j U(\Phi \mathbf{z}^0) - \sum_{m=1}^N \sum_{j_1, \dots, j_m=0}^n \frac{1}{m!} \partial_{j_1} \dots \partial_{j_m} \nabla_j U(\Phi \mathbf{z}^0)(\hat{q}_{j_1}, \dots, \hat{q}_{j_m}).$$

In the following we work with the weighted norm

$$\|\mathbf{d}_n\|_{\omega} = |d_{n,0}| + \sum_{j=1}^{\ell} h\omega_j |d_{n,j}|.$$

On τ -intervals of length 1, which corresponds to $t = nh \leq h^{\alpha}$, the first term in (7.16) is $\mathcal{O}(h^{N+1})$ by definition of the modulation functions (see Section 7.3), and the j th component of the other two terms contains a factor $\psi(h\omega_j)\varepsilon^{N+1}$ as a consequence of the appearance of sufficiently many factors of $z_j^{\mathbf{k}}$. By Assumption A ($h/\varepsilon \geq c_0 > 0$) and (7.7) this implies that

$$\|\mathbf{d}_n\|_{\omega} = \mathcal{O}(h^{N+1}) \quad \text{for} \quad nh \leq h^{\alpha}.$$

As for the defect in Section 7.3 it follows from (7.4) and (7.5) that

$$\begin{aligned} \tilde{q}_{0,0} - q_{0,0} &= [z_0^0]^M(0) - [z_0^0]^{M+1}(0) \\ \tilde{q}_{0,j} - q_{0,j} &= [z_j^{\langle j \rangle} + z_j^{-\langle j \rangle}]^M(0) - [z_j^{\langle j \rangle} + z_j^{-\langle j \rangle}]^{M+1}(0). \end{aligned}$$

The estimate (7.14) for $m = M$ proves that $\|\tilde{\mathbf{q}}_0 - \mathbf{q}_0\|_{\omega} = \mathcal{O}(h^{N+1})$. Similarly, for the truncated derivative approximation

$$\tilde{\mathbf{p}}_n = \sum_{\mathbf{k} \in \mathcal{K}} \mathbf{w}^{\mathbf{k}}(\tau) e^{i(\mathbf{k} \cdot \boldsymbol{\omega})t}, \quad t = nh$$

with components $\tilde{p}_{n,j}$ (see Corollary 6.1), we have (up to an error of size $\mathcal{O}(h^{N+3})$)

$$\begin{aligned} h(\tilde{p}_{0,0} - p_{0,0}) &= h^{1-\alpha}([z_0^0]^M(0) - [z_0^0]^{M+1}(0)) \\ h \operatorname{sinc}(h\omega_j)(\tilde{p}_{0,j} - p_{0,j}) &= i s_{2\langle j \rangle}([z_j^{\langle j \rangle} - z_j^{-\langle j \rangle}]^M(0) - [z_j^{\langle j \rangle} - z_j^{-\langle j \rangle}]^{M+1}(0)). \end{aligned}$$

The estimate (7.14) and the relation (2.3) for $\mathbf{q}_1$ yield the bound $\|\tilde{\mathbf{q}}_1 - \mathbf{q}_1\|_{\omega} = \mathcal{O}(h^{N+1})$. We have used that the nonlinearity $\Psi \nabla U(\Phi \mathbf{q})$ is Lipschitz-continuous in the norm $\|\cdot\|_{\omega}$ with a constant that only depends on bounds of the derivatives of the potential U . Using a discrete Gronwall Lemma, a standard analysis of the propagation of errors in the method (2.2) (see [7, Section XIII.4.1]) then proves the bound of $\mathbf{r}_n = \mathbf{q}_n - \tilde{\mathbf{q}}_n$ for $0 \leq nh \leq h^{\alpha}$ as stated in Theorem 6.1.

8 Almost-invariants of the modulation system

In this section we show that the system for the modulation functions has two almost-invariants – one is related to the slow energy $H_{\text{slow}}(\mathbf{p}, \mathbf{q})$ and the other to the oscillatory energy $H_{\omega}(\mathbf{p}, \mathbf{q})$.

8.1 Almost-invariant related to the slow energy

We multiply the equation (6.2) by $\phi(h\omega_j)(\dot{z}_j^{-\mathbf{k}})^\top$ and sum over all $j \in \{0, \dots, \ell\}$ and $\mathbf{k} \in \mathcal{K}$ to obtain

$$\begin{aligned} \frac{h^{-\alpha}}{h^2} \sum_{j=0}^{\ell} \sum_{\mathbf{k} \in \mathcal{K}} \frac{\phi(h\omega_j)}{\psi(h\omega_j)} \left((\dot{z}_j^{-\mathbf{k}})^\top L_j^{\mathbf{k}} z_j^{\mathbf{k}} - 2(\cos(h\omega_j) - \cos(h\varpi_j)) (\dot{z}_j^{-\mathbf{k}})^\top z_j^{\mathbf{k}} \right) \\ = -h^{-\alpha} \frac{d}{d\tau} \mathcal{U}(\Phi \mathbf{z}) + h^{-\alpha} \sum_{j=0}^{\ell} \sum_{\mathbf{k} \in \mathcal{K}} \frac{\phi(h\omega_j)}{\psi(h\omega_j)} (\dot{z}_j^{-\mathbf{k}})^\top \delta_j^{\mathbf{k}}. \end{aligned} \quad (8.1)$$

As in [7, page 508] the left-hand side of this equation is seen to be a total differential. Therefore, there exists a function $\mathcal{E}[\mathbf{z}](t)$, which depends on the values at $\tau = h^{-\alpha}t$ of the function $\mathbf{z}$ and of its first L derivatives, such that

$$\frac{d}{dt} \mathcal{E}[\mathbf{z}](t) = \mathcal{O}(h^{N+2-\alpha}/\kappa) = \mathcal{O}(h^{N+1}). \quad (8.2)$$

Here, we have used the bounds of Theorem 6.1 for the defect $\delta_j^{\mathbf{k}}$ and for the $z_j^{\mathbf{k}}$, and the estimate

$$\left| \frac{\phi(h\omega_j)}{\psi(h\omega_j)} \right| = \left| \frac{\sigma(h\omega_j)}{\text{sinc}(h\omega_j)} \right| \leq \frac{C_1 h \omega_j}{\kappa}, \quad (8.3)$$

which follows from Assumptions A and B.

Theorem 8.1 *In the situation of Theorem 6.1 we have for $0 \leq t = nh \leq h^\alpha$*

$$\begin{aligned} \mathcal{E}[\mathbf{z}](t) &= \mathcal{E}[\mathbf{z}](0) + \mathcal{O}(th^{N+1}) \\ \mathcal{E}[\mathbf{z}](t) &= H_{\text{slow}}(\mathbf{p}_n, \mathbf{q}_n) + \mathcal{O}(\varepsilon h^{-\alpha}) + \mathcal{O}(h^{2(1-\alpha)}). \end{aligned}$$

Proof The first statement follows by integration of (8.2). We next show that

$$\mathcal{E}[\mathbf{z}](t) = \frac{1}{2} |h^{-\alpha} \dot{z}_0^{\mathbf{0}}(\tau)|^2 + U(\Phi \mathbf{z}^{\mathbf{0}}) + \mathcal{O}(\varepsilon h^{-\alpha}) + \mathcal{O}(h^{2(1-\alpha)}). \quad (8.4)$$

By definition (6.3) of $\mathcal{U}$ and the estimates (6.8)–(6.12) on the modulation functions we have $\mathcal{U}(\Phi \mathbf{z}) = U(\Phi \mathbf{z}^{\mathbf{0}}) + \mathcal{O}(\varepsilon^2)$. The term with $j = 0$ and $\mathbf{k} = \mathbf{0}$ in (8.1) yields $\frac{1}{2} |h^{-\alpha} \dot{z}_0^{\mathbf{0}}|^2 + \mathcal{O}(h^{2(1-\alpha)})$. The term with $j = 0$ and $\mathbf{k} \neq \mathbf{0}$ gives $\mathcal{O}(\varepsilon^2)$ because of the estimates (5.2) and (6.11). For $j > 0$ and $\mathbf{k} = \pm \langle j \rangle$ the dominant term is

$$\begin{aligned} \frac{1}{h^2} \frac{\phi(h\omega_j)}{\psi(h\omega_j)} \left(\cos(h\omega_j) - \cos(h\varpi_j) \right) |z_j^{\pm \langle j \rangle}|^2 \\ = \frac{1}{h^2} \frac{\sigma(h\omega_j) h \omega_j}{\sin(h\omega_j)} 2 \sin\left(\frac{h(\omega_j + \varpi_j)}{2}\right) \sin\left(\frac{h(\omega_j - \varpi_j)}{2}\right) |z_j^{\pm \langle j \rangle}|^2 \\ = \mathcal{O}(h^{-2} h \omega_j h^{1-\alpha+\mu} \omega_j^{-2}) = \mathcal{O}(\omega_j^{-1} h^{-\alpha+\mu}) = \mathcal{O}(\varepsilon h^{-\alpha}), \end{aligned}$$

where we have used the bounds (5.3) and (6.9). All further terms are smaller. This proves (8.4).

To relate the right-hand side of (8.4) to the slow energy $H_{\text{slow}}(\mathbf{p}_n, \mathbf{q}_n)$ we use the modulated Fourier expansions from Theorem 6.1 and Corollary 6.1, and the first estimate of Lemma 8.1 below. We note the bound $\Phi \mathbf{z}^0 - \mathbf{z}^0 = \mathcal{O}(\varepsilon^2)$, which gives us $U(\Phi \mathbf{z}^0) - U(\mathbf{q}_n) = \mathcal{O}(\varepsilon)$. This yields

$$H_{\text{slow}}(\mathbf{p}_n, \mathbf{q}_n) = \frac{1}{2} |h^{-\alpha} \dot{z}_0^0|^2 + U(\Phi \mathbf{z}^0) + \mathcal{O}(\varepsilon),$$

which together with (8.4) proves the result. $\square$

Lemma 8.1 *For $j = 0$ we have*

$$p_{n,0} = h^{-\alpha} \dot{z}_0^0(\tau) + \mathcal{O}(h^{2-3\alpha}) + \mathcal{O}(\varepsilon h^\alpha).$$

For $j = 1, \dots, \ell$ we have

$$p_{n,j} = i \frac{\sin(h\varpi_j)}{\sin(h\omega_j)} \omega_j \left(z_j^{(j)}(\tau) - z_j^{-(j)}(\tau) \right) + \mathcal{O}(h^{1-\alpha}/\kappa).$$

Proof The estimates follow from Corollary 6.1 and the bounds from Theorem 6.1. We use the estimate (7.6) of Section 7.2, and (5.2) to bound the factors $s_{(j)\pm\mathbf{k}}$ from below. $\square$

8.2 Almost-invariant related to the oscillatory energy

Since the sum in the definition of $\mathcal{U}(\mathbf{z})$ is over multi-indices $\mathbf{k}^1, \dots, \mathbf{k}^m$ with $\mathbf{k}^1 + \dots + \mathbf{k}^m \in \mathcal{M}$ and $\|\mathbf{k}^1\| + \dots + \|\mathbf{k}^m\| \leq N + 1$, we have under condition (3.5) by Lemma 5.2 that then $(\mathbf{k}^1 + \dots + \mathbf{k}^m) \cdot \varpi = 0$, and therefore

$$\mathcal{U}(S(\theta)\Phi\mathbf{z}) = \mathcal{U}(\Phi\mathbf{z}), \quad S(\theta)\mathbf{x} = (e^{i(\mathbf{k} \cdot \varpi)\theta} x_j^{\mathbf{k}}).$$

Differentiating this relation with respect to θ yields

$$0 = \frac{d}{d\theta} \Big|_{\theta=0} \mathcal{U}(S(\theta)\Phi\mathbf{z}) = \sum_{j=0}^{\ell} \sum_{\mathbf{k} \in \mathcal{K}} i(\mathbf{k} \cdot \varpi) \phi(h\omega_j) (z_j^{\mathbf{k}})^{\top} \nabla_j^{\mathbf{k}} \mathcal{U}(\Phi\mathbf{z}).$$

Similar as before we multiply the equation (6.2) by $\phi(h\omega_j)(-\mathbf{k} \cdot \varpi)(z_j^{-\mathbf{k}})^{\top}$ and sum over all $j \in \{0, \dots, \ell\}$ and $\mathbf{k} \in \mathcal{K}$ to obtain

$$\begin{aligned} -\frac{i}{h^2} \sum_{j=0}^{\ell} \sum_{\mathbf{k} \in \mathcal{K}} \frac{\phi(h\omega_j)}{\psi(h\omega_j)} (\mathbf{k} \cdot \varpi) & \left((z_j^{-\mathbf{k}})^{\top} L_j^{\mathbf{k}} z_j^{\mathbf{k}} - 2(\cos(h\omega_j) - \cos(h\varpi_j)) (z_j^{-\mathbf{k}})^{\top} z_j^{\mathbf{k}} \right) \\ & = -i \sum_{j=0}^{\ell} \sum_{\mathbf{k} \in \mathcal{K}} (\mathbf{k} \cdot \varpi) \frac{\phi(h\omega_j)}{\psi(h\omega_j)} (z_j^{-\mathbf{k}})^{\top} \delta_j^{\mathbf{k}}. \end{aligned}$$

The coefficients of the terms $(z_j^{-\mathbf{k}})^{\top} z_j^{\mathbf{k}}$ and $(z_j^{\mathbf{k}})^{\top} z_j^{-\mathbf{k}}$ in this expression have opposite sign and therefore cancel in the sum. Consequently, as in Section 8.1, the formulas of [7, page 508] show that the left-hand expression is a total

differential. Therefore, there exists a function $\mathcal{I}[\mathbf{z}](t)$, which depends on the values at $\tau = h^{-\alpha}t$ of the function $\mathbf{z}$ and of its first L derivatives, such that

$$\frac{d}{dt}\mathcal{I}[\mathbf{z}](t) = \mathcal{O}(h^{N+1}/\kappa) = \mathcal{O}(h^N). \quad (8.5)$$

For this estimate we use the bounds (6.9) and (6.12) for $(\mathbf{k} \cdot \boldsymbol{\varpi})z_j^{\mathbf{k}}$, the bound (6.13) for $\delta_j^{\mathbf{k}}$, and the estimate (8.3).

Theorem 8.2 *In the situation of Theorem 6.1 we have under condition (3.5) for $0 \leq t = nh \leq h^\alpha$*

$$\begin{aligned} \mathcal{I}[\mathbf{z}](t) &= \mathcal{I}[\mathbf{z}](0) + \mathcal{O}(th^N) \\ \mathcal{I}[\mathbf{z}](t) &= H_\omega^*(\mathbf{p}_n, \mathbf{q}_n) + \mathcal{O}(h^{1-\alpha}/\kappa), \end{aligned}$$

where H_ω^* is defined in (3.4).

Proof The first statement follows by integration of (8.5). The dominant term of $\mathcal{I}[\mathbf{z}](t)$ is that for $\mathbf{k} = \pm\langle j \rangle$ with the lowest derivative. With $\sigma(\xi)$ from (3.3) it is given by

$$\sum_{j=1}^{\ell} \sigma(h\omega_j) 2\omega_j^2 \left(\frac{\varpi_j \sin(h\varpi_j)}{\omega_j \sin(h\omega_j)} \right) |z_j^{\langle j \rangle}(h^{-\alpha}t)|^2.$$

Using (5.3), the expression in brackets is seen to be of the form $1 + \mathcal{O}(h^{1-\alpha}/\kappa)$. All other terms are at most of size $\mathcal{O}(h^{1-\alpha+\mu}/\kappa)$. $\square$

9 Proof of Theorem 3.1

9.1 Transition from one interval to the next

Theorems 8.1 and 8.2 are only valid on a short time interval of length $\nu h \leq h^\alpha$. Here, we consider the modulated Fourier expansion corresponding to starting values $(\mathbf{q}_\nu, \mathbf{p}_\nu)$ and compare the almost-invariants to those corresponding to $(\mathbf{q}_0, \mathbf{p}_0)$.

Lemma 9.1 *In the situation of Theorem 6.1, let $z_j^{\mathbf{k}}(\tau)$ be the coefficient functions of the modulated Fourier expansion for initial data $(\mathbf{q}_0, \mathbf{p}_0)$. We let $\tilde{z}_j^{\mathbf{k}}(\tau)$ be the coefficient functions corresponding to $(\mathbf{q}_\nu, \mathbf{p}_\nu)$ for ν with $\nu h \leq h^\alpha$. Then,*

$$\begin{aligned} \mathcal{E}[\mathbf{z}](\nu h) &= \mathcal{E}[\tilde{\mathbf{z}}](0) + \mathcal{O}(h^{N-1}) \\ \mathcal{I}[\mathbf{z}](\nu h) &= \mathcal{I}[\tilde{\mathbf{z}}](0) + \mathcal{O}(h^{N-1}). \end{aligned}$$

Proof Let $\mathbf{z}^M = ([z_j^{\mathbf{k}}]^M)$ be the last iterate in the construction of the modulation function $\mathbf{z}$ for initial data $(\mathbf{q}_0, \mathbf{p}_0)$, and let $\tilde{\mathbf{z}}^m = ([\tilde{z}_j^{\mathbf{k}}]^m)$ be the m th iterate of the modulation function $\tilde{\mathbf{z}}$ corresponding to initial data $(\mathbf{q}_\nu, \mathbf{p}_\nu)$. We aim in estimating the difference $\Delta \mathbf{z}^m(\tau) = \mathbf{z}^M(\nu h^{1-\alpha} + \tau) - \tilde{\mathbf{z}}^m(\tau)$. The functions $[\tilde{z}_j^{\mathbf{k}}]^m$ satisfy the relations of Section 7.1 with $(\mathbf{q}_0, \mathbf{p}_0)$ replaced by $(\mathbf{q}_\nu, \mathbf{p}_\nu)$. The functions $[z_j^{\mathbf{k}}]^M$ satisfy the same relations, where the superscripts m and $m+1$ are changed to M and the defect $\delta_j^{\mathbf{k}}$ is added (see the formulas of Section 7.3). For the rescaled differences $\Delta \mathbf{v}^m(\tau) = \Lambda \Delta \mathbf{z}^m(\tau)$ the same arguments as in Section 7.3 yield

$$\|\Delta \mathbf{v}^{m+1}\|_{C^r} \leq Ch^\mu \|\Delta \mathbf{v}^m\|_{C^{r+L}} + Dh^{N-\alpha}/\kappa \quad (9.1)$$

with $r = L(M - m)$. The bounds (6.13) for the defect introduce an inhomogeneity of size $\mathcal{O}(h^{N+1})$ in (9.1), whereas the bounds (6.14) for the difference between $\mathbf{q}_n$ and $\tilde{\mathbf{q}}_n$ of (7.15) and those of (6.15) for the derivative approximations introduce an inhomogeneity of size $\mathcal{O}(h^{N-\alpha}/\kappa)$. From (9.1) it follows by induction on m that

$$\|\Delta \mathbf{v}^m\|_{C^{L(M-m+1)}} \leq (Ch^\mu)^m \|\Delta \mathbf{v}^0\|_{C^{L(M+1)}} + mDh^{N-\alpha}/\kappa.$$

Since the bounds of Theorem 6.1 give $\|\Delta \mathbf{v}^0\|_{C^{L(M+1)}} = \mathcal{O}(h^{-\alpha})$, we obtain after $M \geq (N+\alpha)\mu$ iterations that $\|\Delta \mathbf{v}^M\|_{C^L} = \mathcal{O}(h^{N-\alpha}/\kappa)$ and consequently also

$$\|\Delta \mathbf{z}^M\|_{C^L} = \mathcal{O}(h^{N-1}).$$

Using Lipschitz estimates for $\mathcal{E}$ and $\mathcal{I}$ yields the result. $\square$

9.2 From short to long time intervals

We put the estimates for many short time intervals of length $\nu h \leq h^\alpha$ together to get the long-time result of Theorem 3.1. For $m = 0, 1, 2, \dots$, let $\mathbf{z}_m(\tau)$ collect the coefficient functions of the modulated Fourier expansion starting from $(\mathbf{q}_{m\nu}, \mathbf{p}_{m\nu})$. Since we aim at proving that the modified oscillatory energy H_ω^* remains nearly constant, we consider, instead of the bounded energy assumption (3.1), the condition

$$|H_\omega^*(\mathbf{p}(0), \mathbf{q}(0))| + |H_{\text{slow}}(\mathbf{p}(0), \mathbf{q}(0))| \leq E^*. \quad (9.2)$$

This condition follows with $E^* = (C_1 + 1)E + (C_1 + 2)\hat{K}$ from Assumptions A and B, where $\hat{K}$ denotes the bound of the potential U on the set K_ρ of Assumption A. Since $|\sigma(h\omega_j)| \geq c_1 > 0$ and all $\sigma(h\omega_j)$ have the same sign, we can use (9.2) instead of (3.1) in the proof of Theorem 6.1 (estimates (7.13)).

As long as (9.2) holds with $2E^*$ instead of E^* , Theorem 8.2 yields for $0 \leq nh \leq h^\alpha$

$$|\mathcal{I}[\mathbf{z}_m](nh) - \mathcal{I}[\mathbf{z}_m](0)| \leq Cnh^{N+1}.$$

By Lemma 9.1,

$$|\mathcal{I}[\mathbf{z}_m](\nu h) - \mathcal{I}[\mathbf{z}_{m+1}](0)| \leq Ch^{N-1}.$$

Summing up these estimates over m and applying the triangle inequality yields, for $0 \leq n \leq \nu$,

$$|\mathcal{I}[\mathbf{z}_m](nh) - \mathcal{I}[\mathbf{z}_0](0)| \leq (m + (m\nu + n)h^2)Ch^{N-1}.$$

By Theorem 8.2, we have

$$|\mathcal{I}[\mathbf{z}_m](nh) - H_{\omega}^*(\mathbf{p}_{m\nu+n}, \mathbf{q}_{m\nu+n})| \leq C'h^{1-\alpha}/\kappa.$$

Combining these bounds we obtain for $t = (m\nu + n)h$ (and $\nu h \approx h^\alpha$)

$$|H_{\omega}^*(\mathbf{p}_{m\nu+n}, \mathbf{q}_{m\nu+n}) - H_{\omega}^*(\mathbf{p}_0, \mathbf{q}_0)| \leq 2Cth^{N-1-\alpha} + 2C'h^{1-\alpha}/\kappa,$$

which is $\mathcal{O}(h^{1-\alpha}/\kappa)$ for $t \leq h^{-N+2}$. In the same way, we obtain for $t = (m\nu + n)h$ (and $\nu h \approx h^\alpha$), using the almost-invariant $\mathcal{E}$ and Theorem 8.1 instead of $\mathcal{I}$ and Theorem 8.2,

$$|H_{\text{slow}}(\mathbf{p}_{m\nu+n}, \mathbf{q}_{m\nu+n}) - H_{\text{slow}}(\mathbf{p}_0, \mathbf{q}_0)| \leq 2Cth^{N-1-\alpha} + 2C'(\varepsilon h^{-\alpha} + h^{2(1-\alpha)}),$$

which is $\mathcal{O}(\varepsilon h^{-\alpha}) + \mathcal{O}(h)$ for $t \leq \varepsilon h^{-N+1}$ and $\mathcal{O}(h^{1-\alpha})$ for $t \leq h^{-N+2}$. These estimates ensure that, for sufficiently small step size, (9.2) holds with $2E^*$ instead of E^* on such time intervals. Replacing the arbitrary integer N by $N + 2$ yields the statements of Theorem 3.1.

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