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Long-term analysis of the Störmer–Verlet method for Hamiltonian systems with a solution-dependent high frequency

Ernst Hairer · Christian Lubich

Abstract The long-time behaviour of the Störmer–Verlet–leapfrog method is studied when this method is applied to highly oscillatory Hamiltonian systems with a slowly varying, solution-dependent high frequency. Using the technique of modulated Fourier expansions with state-dependent frequencies, which is newly developed here, the following results are proved: The considered Hamiltonian systems have the action as an adiabatic invariant over long times that cover arbitrary negative powers of the small parameter. The Störmer–Verlet method approximately conserves a modified action and a modified total energy over a long time interval that covers a negative integer power of the small parameter. This power depends on the size of the product of the stepsize with the high frequency.

Keywords Oscillatory Hamiltonian system · Modulated Fourier expansion · Störmer-Verlet scheme · Leapfrog integrator · Long-time energy conservation · Adiabatic invariant

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1 Introduction

In the last decade much insight into the properties of numerical integrators for highly oscillatory Hamiltonian systems has been gained, starting by thoroughly

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Ernst Hairer
Section de mathématiques, 2-4 rue du Lièvre, Université de Genève, CH-1211 Genève 4, Switzerland.
E-mail: Ernst.Hairer@unige.ch

Christian Lubich
Mathematisches Institut, Universität Tübingen, Auf der Morgenstelle, D-72076 Tübingen, Germany.
E-mail: Lubich@na.uni-tuebingen.de

studying the numerical methods on a nonlinear model problem with a single constant high frequency; see [14, Chap. XIII] and the original papers [10,9]. As an important tool, the technique of modulated Fourier expansions was first developed in this single-frequency context and later extended to several and infinitely many frequencies, which made it possible to explain remarkable analytical and numerical long-time properties in multi-frequency Hamiltonian systems [3,4] and classes of Hamiltonian partial differential equations; see, e.g., [5,7,8] for long-time analyses of numerical methods for such equations. We further refer to the review articles [11,12] and numerous references therein.

A key aspect for the numerical integration of oscillatory problems is that the product of the stepsize with the highest frequency in the system (the CFL number in the case of partial differential equations) is not required to be exceedingly small. Numerical long-time results for oscillatory problems under realistic stepsize conditions can be proved with modulated Fourier expansions, but are not accessible by standard backward error analysis; cf. [14, Chapters IX and XIII].

In this paper we consider a model problem with a single solution-dependent high frequency that was first studied analytically by Rubin & Ungar [19]. It describes motion under a strong constraining force and is given by the Hamiltonian

$$H(q_0,q_1,p_0,p_1) = \frac{1}{2}\Big(|p_0|^2 + |p_1|^2\Big) + \frac{\omega(q_0)^2}{2\,\varepsilon^2}\,|q_1|^2 + U(q_0,q_1) \tag{1.1}$$

with a small parameter $0 < \varepsilon \ll 1$. The variables $q = (q_0,q_1) \in \mathbb{R}^{d_0} \times \mathbb{R}^{d_1}$ and $p = (p_0,p_1) \in \mathbb{R}^{d_0} \times \mathbb{R}^{d_1}$ represent the positions and momenta, respectively, and $|\cdot|$ denotes the Euclidean norm. The frequency function ω and the potential U may depend on ε, but are assumed to be smooth in the sense that all their derivatives are bounded independently of ε. We assume that $\omega(q_0)$ has a fixed positive lower bound independently of q_0, say $\omega(q_0) \geq 1$.

The rescaled variant $H = \frac{1}{2}\big(p_0^2 + p_1^2\big) + \frac{1}{2}\omega(\varepsilon q_0)^2 q_1^2$ is a standard example in the theory of adiabatic invariants as described in [1, Chap. 5.4]. The fundamental role of such an Hamiltonian for magnetic traps and mirrors is discussed there and in [2, Chap. III.1]. In [6] the Hamiltonian (1.1) was considered as a model problem for adiabatic invariance in molecular dynamics and numerical weather prediction. For the constant-frequency case $\omega(q_0) \equiv 1$ the Hamiltonian (1.1) reduces to that of the model problem of [10] and [14, Chap. XIII].

The equations of motion are given by $p_0 = \dot q_0$, $p_1 = \dot q_1$ and the system of second-order differential equations

$$\begin{aligned} \ddot q_0 &= -\frac{\omega(q_0)|q_1|^2}{\varepsilon^2}\,\nabla_{q_0}\omega(q_0) - \nabla_{q_0}U(q_0,q_1) \\ \ddot q_1 &= -\frac{\omega(q_0)^2}{\varepsilon^2}\,q_1 - \nabla_{q_1}U(q_0,q_1). \end{aligned} \tag{1.2}$$

Initial values are assumed such that

$$q_1(0) = \mathcal{O}(\varepsilon), \quad q_0(0) = \mathcal{O}(1), \quad p_0(0) = \mathcal{O}(1), \quad p_1(0) = \mathcal{O}(1). \tag{1.3}$$

This implies that the total energy is bounded by a constant independent of ε. In this system, the components $q_1(t)$ oscillate fast with small amplitude $\mathcal{O}(\varepsilon)$ and with the slowly changing frequency $\omega(q_0(t))/\varepsilon$.

We consider the *action* (oscillatory energy divided by the frequency, rescaled with the factor ε^{-1})

$$I(q_0, q_1, p_0, p_1) = \frac{1}{2} \frac{|p_1|^2}{\omega(q_0)} + \frac{\omega(q_0)}{2\,\varepsilon^2}\,|q_1|^2, \tag{1.4}$$

which is $\mathcal{O}(1)$ at the initial values. The action is nearly conserved, up to deviations of size $\mathcal{O}(\varepsilon)$, over very long times; in the case of a single fast degree of freedom ($d_1 = 1$) see [18] for the Hamiltonian (1.1) and [1, Chap. 5.4] for the (rescaled) Hamiltonian without the potential U; for general $d_1 \geq 1$ we refer to Theorem 3.2 below. The action I is therefore called an *adiabatic invariant*; see also [15] for this notion.

In Section 2 we show that the exact solution admits an asymptotic expansion into products of slowly varying functions with integral powers of $e^{i\phi(t)/\varepsilon}$ for a suitable smooth phase function $\phi(t)$, whose time derivative is close to $\omega(q_0(t))$. This expansion is called a *varying-frequency modulated Fourier expansion*, a notion that extends the constant-frequency modulated Fourier expansion of [14, Chap. XIII]. Even if the truncated expansion is a valid solution approximation only over short time $t = \mathcal{O}(1)$, it is the key tool to proving the near-conservation of the action along the solution over long times $t = \mathcal{O}(\varepsilon^{-N})$ for arbitrary integer N, which is done in Section 3. This long-time adiabatic invariance result for (1.1) has previously been proved in the case of a single fast degree of freedom ($d_1 = 1$). For this case it was obtained using canonical coordinate transformations of Hamiltonian perturbation theory; see [18] and compare also [1, Chap. 5.4] for a closely related class of Hamiltonians. The proof via modulated Fourier expansions, which allows for arbitrarily many fast degrees of freedom without further ado (but still for a single high frequency), does not use any such nonlinear coordinate transforms. Not least because of this property, this proof can be extended to numerical methods, as we will show in this paper.

In Sections 4 to 6 we study the widely used Störmer–Verlet–leapfrog integrator applied to (1.2), for stepsizes $h = \mathcal{O}(\varepsilon)$ below the linear stability threshold. It has been shown in [17] that the adiabatic invariant is nearly preserved over long times by the Störmer–Verlet method with very small stepsizes $h = \mathcal{O}(\varepsilon^2)$, using standard backward error analysis. Here we show that both the adiabatic invariant and the total energy are well preserved over long times for larger stepsizes $h = \mathcal{O}(\varepsilon)$. We show in Section 4 that the numerical solution admits a modulated Fourier expansion with a modified phase function. This is used in Section 5 to show that the method nearly conserves a modified action over times $t = \mathcal{O}(\varepsilon^{-N})$ with a positive integer N that depends on an upper bound of the product of the stepsize with the frequencies. In Section 6 we show similarly that the method nearly conserves a modified energy over such long times. The expressions for the modified action and energy are the same as in the constant-frequency case, since derivatives of the frequency do not enter these expressions in leading order.

With the techniques developed and used in this paper, it is also feasible to extend known long-time results for trigonometric integrators [14, Chap. XIII] and the implicit-explicit symplectic method considered in [16,22,21,3] from the case of a constant high frequency to a solution-dependent high frequency. To present this paper as a concise proof of concept, we do not work out these interesting extensions here, but limit ourselves to the exemplary case of the Störmer–Verlet method.

With hindsight, it is remarkable to which extent results and techniques originally developed for constant-frequency systems generalise to a varying frequency — pitfalls and new technical difficulties notwithstanding.

2 Modulated Fourier expansion of the exact solution

We show that the solution $q(t) = \big(q_0(t), q_1(t)\big)$ of (1.2) admits a *modulated Fourier expansion*

$$q(t) \approx \sum_{k\in\mathbb{Z}} z^k(t)\, \mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon} = \sum_{k\in\mathbb{Z}} y^k(t), \tag{2.1}$$

where $y^k(t) = z^k(t)\, \mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$. The modulation functions $z^k(t) = \big(z_0^k(t), z_1^k(t)\big)$ and the phase function $\phi(t)$ are ε-dependent functions that are required to be smooth in the sense that all derivatives are bounded independently of ε. The following result extends Theorem XIII.5.1 of [14] to state-dependent frequencies.

Theorem 2.1 *Consider a solution $q(t)$ of (1.2) that satisfies the bounded energy condition (1.3) and stays in a compact set K for $0 \le t \le T$. Then the solution admits an expansion*

$$q(t) = \sum_{|k|\le N+1} z^k(t)\, \mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon} + R_N(t) \tag{2.2}$$

for arbitrary $N \ge 1$, where the phase function satisfies

$$\phi(t) = \int_0^t \omega\big(z_0^0(s)\big)\, \mathrm{d}s, \qquad \text{so that} \qquad \dot\phi(t) = \omega\big(z_0^0(t)\big). \tag{2.3}$$

The functions $z^k(t) = \big(z_0^k(t), z_1^k(t)\big)$ together with their derivatives (up to arbitrary order M) are bounded by

$$z_0^k = \begin{cases} \mathcal{O}(\varepsilon^k) & \text{for } k \text{ even} \\ \mathcal{O}(\varepsilon^{k+2}) & \text{for } k \text{ odd} \end{cases} \qquad z_1^k = \begin{cases} \mathcal{O}(\varepsilon^{k+2}) & \text{for } k \text{ even} \\ \mathcal{O}(\varepsilon^k) & \text{for } k \text{ odd} \end{cases} \tag{2.4}$$

for $k = 0, \dots, N+1$. Moreover, $z^{-k} = \overline{z^k}$ for all k. The remainder term and its derivative are bounded by

$$R_N(t) = \mathcal{O}(t^2\varepsilon^N) \quad \text{and} \quad \dot R_N(t) = \mathcal{O}(t\varepsilon^N) \quad \text{for} \quad 0 \le t \le T. \tag{2.5}$$

With this bound, the functions z_j^k are unique up to terms of size $\mathcal{O}(\varepsilon^{N+2})$. The constants symbolised by the $\mathcal{O}$-notation are independent of ε and t with $0 \le t \le T$, but they depend on N, T, the constants in (1.3), on bounds of derivatives of $\omega(q_0)$ and $U(q_0, q_1)$ on K, and on the maximum order M of considered derivatives of $z^k(t)$.

Proof The proof follows closely that of Theorem XIII.5.1 of [14]. We briefly sketch the main steps and highlight the main differences to the constant-frequency case. Inserting the finite sum of (2.2) and

$$\ddot{q}(t) \approx \sum_{|k|\le N+1} \Big(\ddot{z}^k(t) + 2\mathrm{i}k\dot{z}^k(t)\frac{\dot{\phi}(t)}{\varepsilon} + z^k(t)\Big(\mathrm{i}k\frac{\ddot{\phi}(t)}{\varepsilon} - k^2\frac{\dot{\phi}(t)^2}{\varepsilon^2}\Big)\Big)\,\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$$

into the differential equation, expanding the nonlinearities around the non oscillating part $z^0(t)$, and comparing the coefficients of $\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ yields, for $W(q_0, q_1) = \frac{1}{2}\varepsilon^{-2}\omega(q_0)^2|q_1|^2 + U(q_0, q_1)$,

$$\begin{aligned} \ddot{z}^k(t) + 2\mathrm{i}k\dot{z}^k(t)\frac{\dot{\phi}(t)}{\varepsilon} + z^k(t)\Big(\mathrm{i}k\frac{\ddot{\phi}(t)}{\varepsilon} - k^2\frac{\dot{\phi}(t)^2}{\varepsilon^2}\Big) \\ = -\sum_{m=1}^{N+1}\sum_{s(\alpha)=k}\frac{1}{m!}(\nabla W)^{(m)}(z^0)\,\mathbf{z}^\alpha, \end{aligned} \tag{2.6}$$

where the sum is over multi-indices $\alpha = (\alpha_1, \ldots, \alpha_m)$, $0 < |\alpha_j| \le N+1$, such that $s(\alpha) = \alpha_1 + \ldots + \alpha_m = k$, and $\mathbf{z}^\alpha = (z^{\alpha_1}, \ldots, z^{\alpha_m})$. For $k = 0$ there is an additional term $-\nabla W(z^0)$ on the right-hand side. The construction will be such that the bounds (2.4) hold. Therefore we have truncated the Taylor series expansion after the $(N+1)$th term in order to get a defect of size $\mathcal{O}(\varepsilon^N)$.

Assuming that the bounds (2.4) hold, the only ε^{-1}-terms in equations (2.6) appear for $|k| = 1$, for $z_1^{\pm1}$. They are $-z_1^{\pm1}\dot{\phi}(t)^2/\varepsilon^2$ on the left-hand side and $-z_1^{\pm1}\omega(z_0^0)^2/\varepsilon^2$ on the right-hand side. Taking these terms equal yields the relation (2.3). We then get a coupled system of differential equations for z_0^0 and $z_1^{\pm1}$ of the form

$$\begin{aligned} \ddot{z}_0^0 &= -\omega(z_0^0)\frac{2(z_1^1)^{\mathsf{T}} z_1^{-1}}{\varepsilon^2}\nabla_{q_0}\omega(z_0^0) - \nabla_{q_0}U(z_0^0, 0) + \mathcal{O}(\varepsilon) \\ \frac{\dot{z}_1^{\pm1}}{\varepsilon} &= -\frac{\nabla_{q_0}\omega(z_0^0)^{\mathsf{T}}\dot{z}_0^0}{2\omega(z_0^0)}\,\frac{z_1^{\pm1}}{\varepsilon} + \mathcal{O}(\varepsilon), \end{aligned}$$

where the $\mathcal{O}(\varepsilon)$-terms contain higher derivatives that have to be eliminated recursively. The first equation is obtained by equating the non oscillating terms, and the second equation is obtained by equating the coefficients of $\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ with $|k| = 1$ and using the relation (2.3) for substituting $\dot{\phi}(t)$ and $\ddot{\phi}(t)$. For all other coefficient functions z_j^k we get algebraic relations. Since $\phi(0) = 0$, initial values for the differential equations are obtained from

$$\sum_{|k|\le N+1} z^k(0) = q(0), \qquad \sum_{|k|\le N+1}\Big(\dot{z}^k(0) + \mathrm{i}kz^k(0)\frac{\dot{\phi}(0)}{\varepsilon}\Big) = \dot{q}(0). \tag{2.7}$$

From our assumption (1.3) on the initial values we get $z_0^0(0) = \mathcal{O}(1)$, $\dot z_0^0(0) = \mathcal{O}(1)$, and $z_1^{\pm 1}(0) = \mathcal{O}(\varepsilon)$. This implies the bounds (2.4) for z_0^0 and $z_1^{\pm 1}$.

Compared with the case of a constant high frequency, we now have additional terms with a factor ε^{-2} appearing on the right-hand side of (2.6). These terms change the bounds that we get for the functions z_j^k. With the arguments used for the constant frequency case we get $z_1^0 = \mathcal{O}(\varepsilon^2)$ and $z_0^1 = \mathcal{O}(\varepsilon^3)$, but for $|k| \geq 2$ we only obtain $z^k = \mathcal{O}(\varepsilon^k)$ instead of $\mathcal{O}(\varepsilon^{k+2})$. The fact that z_0^2 does not have a better bound than $\mathcal{O}(\varepsilon^2)$ is seen from the equation

$$-4\,\frac{\omega(z_0^0)^2}{\varepsilon^2}\,z_0^2 = -\omega(z_0^0)\nabla_{q_0}\omega(z_0^0)\,\frac{(z_1^1)^\mathsf{T} z_1^1}{\varepsilon^2} + \mathcal{O}(\varepsilon).$$

It remains to explain the improved bounds of (2.4). For z_1^2 we obtain

$$-3\,\frac{\omega(z_0^0)^2}{\varepsilon^2}\,z_1^2 = -\frac{2\omega(z_0^0)(\nabla_{q_0}\omega(z_0^0)^\mathsf{T} z_0^1)\,z_1^1}{\varepsilon^2} + \mathcal{O}(\varepsilon^3).$$

which yields $z_1^2 = \mathcal{O}(\varepsilon^4)$. For z_0^3 the right-hand side has two dominant terms which are products with factors (z_1^1, z_1^1, z_0^1) and (z_1^0, z_1^1, z_0^2). They are both of size $\mathcal{O}(\varepsilon^5)$.

The proof of (2.4) now continues by induction on k. For z_0^k the right-hand side consists of a sum of products with factors $(z_1^{\alpha_1}, z_1^{\alpha_2}, z_0^{\alpha_3}, \dots, z_0^{\alpha_m})$ with $m \geq 2$ and $\alpha_1 + \ldots + \alpha_m = k$. If k is odd, then either one among α_1 and α_2 is even or one of the remaining α_i is odd. In each case we get the improved estimate $z_0^k = \mathcal{O}(\varepsilon^{k+2})$.

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This construction yields a small defect of size $\mathcal{O}(\varepsilon^N)$ when the expansion is inserted into the differential equation (1.2). On a finite time interval $0 \leq t \leq T$ this implies the stated error bounds (2.5) by the same arguments as in the constant-frequency case. □

The construction of the previous proof implies that the functions $y^k(t) = z^k(t)\,\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ satisfy the second order differential equation

$$\ddot y^k = -\frac{1}{\varepsilon^2}\,\nabla_{-k}\mathcal{V}(\mathbf{y}) - \nabla_{-k}\mathcal{U}(\mathbf{y}) + \mathcal{O}(\varepsilon^N), \tag{2.8}$$

where $\mathbf{y} = (y^k)_{|k|\leq N+1}$ is the vector of coefficient functions and

$$\mathcal{U}(\mathbf{y}) = U(y^0) + \sum_{m=2}^{N+1} \sum_{s(\alpha)=0} \frac{1}{m!}\,U^{(m)}(y^0)\,\mathbf{y}^\alpha, \tag{2.9}$$

where the sum is over multi-indices $\alpha = (\alpha_1, \dots, \alpha_m)$, $0 < |\alpha_j| \leq N+1$, such that $s(\alpha) = \alpha_1 + \ldots + \alpha_m = 0$, and $\mathbf{y}^\alpha = (y^{\alpha_1}, \dots, y^{\alpha_m})$. The notation $\nabla_{-k}\mathcal{U}(\mathbf{y})$ indicates the partial derivative of $\mathcal{U}(\mathbf{y})$ with respect to y^{-k}. The function $\mathcal{V}(\mathbf{y})$ is defined like $\mathcal{U}(\mathbf{y})$ with $U(q)$ replaced by $V(q) = \frac{1}{2}\omega(q_0)^2|q_1|^2$.

3 Adiabatic invariant of the Hamiltonian system

The key to the existence of an adiabatic invariant is an invariance property of the extended potentials $\mathcal{U}$ and $\mathcal{V}$: with $S(\lambda)\mathbf{y} = (\mathrm{e}^{\mathrm{i}k\lambda} y^k)_{|k|\le N+1}$ we have

$$\mathcal{U}\big(S(\lambda)\mathbf{y}\big) = \mathcal{U}(\mathbf{y}) \quad \text{for all} \quad \lambda \in \mathbb{R}.$$

This implies

$$0 = \frac{\mathrm{d}}{\mathrm{d}\lambda}\Big|_{\lambda=0} \mathcal{U}\big(S(\lambda)\mathbf{y}\big) = -\sum_{|k|\le N+1} \mathrm{i}k (y^{-k})^{\mathsf{T}} \nabla_{-k} \mathcal{U}(\mathbf{y}), \tag{3.1}$$

and we have the same property for $\mathcal{V}(\mathbf{y})$. We multiply (2.8) with $-(\mathrm{i}k/\varepsilon)y^{-k}$, which is $\mathcal{O}(1)$ by (2.4), and sum over k. Hence, the expression

$$\mathcal{I}(\mathbf{y}, \dot{\mathbf{y}}) = -\frac{\mathrm{i}}{\varepsilon} \sum_{|k|\le N+1} k (y^{-k})^{\mathsf{T}} \dot{y}^k \tag{3.2}$$

satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big) = \mathcal{O}(\varepsilon^N). \tag{3.3}$$

We then obtain the following extension of Theorem XIII.6.2 of [14] to a state-dependent high frequency.

Theorem 3.1 *Under the assumptions of Theorem 2.1,*

$$\begin{aligned} \mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big) &= \mathcal{I}\big(\mathbf{y}(0), \dot{\mathbf{y}}(0)\big) + \mathcal{O}(\varepsilon^N) \\ \mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big) &= I\big(q(t), \dot{q}(t)\big) + \mathcal{O}(\varepsilon). \end{aligned}$$

The constants symbolised by $\mathcal{O}$ are independent of ε and t with $0 \le t \le T$, but depend on N and T.

Proof The first statement follows from (3.3). Differentiating $y^k = z^k \mathrm{e}^{\mathrm{i}k\phi/\varepsilon}$ with respect to t and using (2.4) yields

$$\dot{y}^k = \Big(\dot{z}^k + \mathrm{i}\frac{k\dot{\phi}}{\varepsilon} z^k\Big)\mathrm{e}^{\mathrm{i}k\phi/\varepsilon} = \mathrm{i}\frac{k\omega(z_0^0)}{\varepsilon} y^k + \mathcal{O}(\varepsilon^k),$$

which inserted into the definition of $\mathcal{I}$ gives

$$\mathcal{I}(\mathbf{y}, \dot{\mathbf{y}}) = \sum_{|k|\le N+1} k^2 \Big(\frac{\omega(z_0^0)}{\varepsilon^2} |y^k|^2 + \mathcal{O}(\varepsilon^k)\Big) = 2\frac{\omega(z_0^0)}{\varepsilon^2} |y^1|^2 + \mathcal{O}(\varepsilon).$$

Inserting the modulated Fourier expansion into $I(q, \dot{q})$ shows that the dominant term is the same as for $\mathcal{I}(\mathbf{y}, \dot{\mathbf{y}})$. □

Patching together many short intervals of length $\mathcal{O}(1)$, Theorems 2.1 and 3.1 yield the following long-time result in the same way as in the proof of Theorem XIII.6.3 of [14].

Theorem 3.2 *If the solution $q(t)$ of (1.2) stays in a compact set for $0 \le t \le \varepsilon^{-N}$, then*

$$I\big(q(t),\dot q(t)\big) = I\big(q(0),\dot q(0)\big) + \mathcal{O}(\varepsilon) + \mathcal{O}(t\varepsilon^N).$$

The constants symbolised by $\mathcal{O}$ are independent of ε and t with $0 \le t \le \varepsilon^{-N}$, but depend on N. □

The long-time adiabatic invariance of the actions (even over times exponentially long in $1/\varepsilon$) was previously proved by Reich [18] in the case of a single fast degree of freedom ($d_1 = 1$) using results from Hamiltonian perturbation theory. For the case of time-dependent frequencies $\omega(t)/\varepsilon$ a proof via modulated Fourier expansions is given in [20].

4 Modulated Fourier expansion for the Störmer–Verlet method

The Störmer–Verlet or leapfrog method (see, e.g., [13,14]) for a second-order differential equation $\ddot q = f(q)$, when used with stepsize h, determines position approximations $q_n \approx q(nh)$ via the two-step formula

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n). \tag{4.1}$$

The velocity (or momentum) approximation $p_n \approx \dot q(nh)$ is obtained from

$$p_n = \frac{1}{2h}\big(q_{n+1} - q_{n-1}\big). \tag{4.2}$$

As is well-known, the method admits a one-step formulation, which makes it a symplectic method in the Hamiltonian case where $f(q)$ is the negative gradient of a potential, as in (1.2).

In analogy to the exact solution of (1.2), we consider a *modulated Fourier expansion*

$$q_n \approx \sum_{k\in\mathbb{Z}} z^k(t)\,\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon} = \sum_{k\in\mathbb{Z}} y^k(t), \qquad t = nh, \tag{4.3}$$

for the numerical solution of the Störmer–Verlet method (4.1). We use the same symbols $z^k(t)$ and $\phi(t)$ for the numerical coefficient functions and phase function, respectively, which now depend on h and $\eta = h/\varepsilon$.

Theorem 4.1 *Consider the numerical solution q_n of the Störmer–Verlet method applied to (1.2) with initial values satisfying the bounded energy condition (1.3). Suppose that, for $0 \le nh \le T$, $q_n = (q_{n,0}, q_{n,1})$ stays in a compact set K and*

$$\frac{h}{\varepsilon}\omega(q_{n,0}) \le 2\sin\Big(\frac{\pi}{N+2}\Big) \tag{4.4}$$

for some odd integer $N \ge 1$. Then the numerical solution admits an expansion

$$q_n = \sum_{|k|\le N+1} z^k(t)\,\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon} + R_N(t), \qquad t = nh, \tag{4.5}$$

where $z_1^{\pm(N+1)}(t) = 0$*, and the phase function satisfies*

$$\sin\Big(\frac{h}{2\,\varepsilon}\dot\phi(t)\Big) = \frac{h}{2\,\varepsilon}\omega\big(z_0^0(t)\big) \qquad \textit{and} \qquad \phi(0) = 0. \tag{4.6}$$

The functions $z^k(t) = \big(z_0^k(t), z_1^k(t)\big)$ *together with their derivatives (up to arbitrary order* M*) are bounded by*

$$z_0^k = \begin{cases} \mathcal{O}(\varepsilon^k) & \textit{for } k \textit{ even} \\ \mathcal{O}(\varepsilon^{k+2}) & \textit{for } k \textit{ odd} \end{cases} \qquad z_1^k = \begin{cases} \mathcal{O}(\varepsilon^{k+2}) & \textit{for } k \textit{ even} \\ \mathcal{O}(\varepsilon^k) & \textit{for } k \textit{ odd} \end{cases} \tag{4.7}$$

for $k = 0, \ldots, N+1$*. Moreover,* $z^{-k} = \overline{z^k}$ *for all* k*. The remainder term is bounded by*

$$R_N(t) = \mathcal{O}(t^2\varepsilon^N) \qquad \textit{for} \quad 0 \le t = nh \le T. \tag{4.8}$$

With this bound, the functions z_j^k *are unique up to terms of size* $\mathcal{O}(\varepsilon^{N+2})$*. The constants symbolised by the* $\mathcal{O}$*-notation are independent of* ε*,* h *and* t *with* $0 \le t \le T$*, but they depend on* N*,* T*, the constants in (1.3), on bounds of derivatives of* $\omega(q_0)$ *and* $U(q_0, q_1)$ *on* K*, and on the maximum order* M *of considered derivatives of* $z^k(t)$*.*

Proof We aim to approximate

$$q_{n+1} - 2q_n + q_{n-1} \approx \sum_{|k|\le N+1}\Big(y^k(t+h) - 2y^k(t) + y^k(t-h)\Big),$$

where $y^k(t) = z^k(t)\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ with smooth functions $z^k(t)$ and $\phi(t)$. We expand $y^k(t+h)$ as (using $\eta = h/\varepsilon$)

$$y^k(t+h) = \Big(z^k(t) + h\dot z^k(t) + \frac{h^2}{2}\ddot z^k(t) + \ldots\Big)\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}\mathrm{e}^{\mathrm{i}k\eta\dot\phi(t)}\Big(1 + \mathrm{i}k\eta\frac{h}{2}\ddot\phi(t) + \ldots\Big).$$

With the notation $\delta_h^2 y^k(t) = \big(y^k(t+h) - 2y^k(t) + y^k(t-h)\big)/h^2$ we have $\delta_h^2 y^0(t) = \delta_h^2 z^0(t) = \ddot z^0(t) + \mathcal{O}(h^2)$ for $k = 0$. Using the identity $\mathrm{e}^{\mathrm{i}x} + \mathrm{e}^{-\mathrm{i}x} - 2 = 4\sin^2(x/2)$ we obtain for $k \ne 0$, omitting the argument t,

$$\delta_h^2 y^k = \frac{1}{h^2}\Big(4\sin^2\Big(\frac{k\eta\dot\phi}{2}\Big)z^k + 2\mathrm{i}h\sin\big(k\eta\dot\phi\big)\dot z^k + \mathrm{i}k\eta h\cos\big(k\eta\dot\phi\big)\ddot\phi z^k + \ldots\Big)\mathrm{e}^{\mathrm{i}k\phi/\varepsilon}.$$

Similar to our procedure for the exact solution, we insert this expression into the numerical scheme, we expand the nonlinearities around the non-oscillatory part $z^0(t)$, and we compare the coefficients of $\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$. As in the proof of Theorem 2.1 this yields differential and algebraic relations for the coefficient functions $z^k(t) = \big(z_0^k(t), z_1^k(t)\big)$ and for $\phi(t)$.

Replacing in the expression for $\delta_h^2 y^1$ the factor h^{-2} by $\eta^{-2}\varepsilon^{-2}$ and then equating the ε^{-2} terms in the part of the Störmer–Verlet scheme corresponding to the second equation of (1.2), yields the relation (4.6). For z_0^0 and $z_1^{\pm 1}$ we get the coupled system of differential equations

$$\ddot{z}_0^0 = -\omega(z_0^0)\frac{2(z_1^1)^\mathsf{T} z_1^{-1}}{\varepsilon^2}\nabla_{q_0}\omega(z_0^0) - \nabla_{q_0}U(z_0^0,0) + \mathcal{O}(\varepsilon)$$

$$\frac{\dot{z}_1^{\pm 1}}{\varepsilon} = -\frac{\nabla_{q_0}\omega(z_0^0)^\mathsf{T}\dot{z}_0^0}{2\omega(z_0^0)}\,\frac{z_1^{\pm 1}}{\varepsilon}\left(\frac{1-\frac{\eta^2}{2}\omega(z_0^0)^2}{1-\frac{\eta^2}{4}\omega(z_0^0)^2}\right) + \mathcal{O}(\varepsilon),$$

which up to the $\mathcal{O}(\varepsilon)$ terms and the factor in big brackets are identical to those for the exact solution. The initial values for the differential equations of z_0^0 and $z_1^{\pm 1}$ are determined from the condition that the equation (4.5) is satisfied without remainder term for $t = 0$ and $t = h$.

For $k \neq 0$ the coefficient of z_0^k in $\delta_h^2 y_0^k$ is $4h^{-2}\sin^2(k\eta\dot{\phi}/2)$. The coefficient of z_1^k in $\delta_h^2 y_1^k - \varepsilon^{-2}\omega(z_0^0)^2 y_1^k$ equals, using (4.6),

$$\begin{aligned}\frac{4}{h^2}\sin^2\Big(\frac{k\eta\dot{\phi}}{2}\Big) - \frac{\omega(z_0^0)^2}{\varepsilon^2} &= \frac{4}{h^2}\sin^2\Big(\frac{k\eta\dot{\phi}}{2}\Big) - \frac{4}{h^2}\sin^2\Big(\frac{\eta\dot{\phi}}{2}\Big)\\ &= \frac{4}{h^2}\sin\Big(\frac{(k-1)}{2}\eta\dot{\phi}\Big)\sin\Big(\frac{(k+1)}{2}\eta\dot{\phi}\Big).\end{aligned}$$

After the division by $4/h^2$, the coefficients of z_0^k (with $k \neq 0$) and z_1^k (with $k \neq \pm 1$) are therefore

$$\sin^2\Big(\frac{k}{2}\eta\dot{\phi}\Big) \qquad \text{and} \qquad \sin\Big(\frac{(k-1)}{2}\eta\dot{\phi}\Big)\sin\Big(\frac{(k+1)}{2}\eta\dot{\phi}\Big), \tag{4.9}$$

respectively. Since, by (4.4),

$$\sin\Big(\frac{\eta}{2}\dot{\phi}(t)\Big) = \frac{\eta}{2}\omega\big(z_0^0(t)\big) = \frac{\eta}{2}\omega(q_{n,0}) + \mathcal{O}(\varepsilon) \leq \sin\Big(\frac{\pi}{N+2}\Big) + \mathcal{O}(\varepsilon)$$

for $t = nh$, we have $\frac{\eta}{2}\dot{\phi}(t) \leq \frac{\pi}{N+2} + \mathcal{O}(\varepsilon)$, so that the first factor of (4.9) is bounded away from 0 for $|k| \leq N+1$, and the second factor is bounded away from 0 for $|k| \leq N$. Since we assumed $z_1^{\pm(N+1)} = 0$, this allows us to construct the functions z^k for $|k| \leq N+1$ in the same way as in the proof of Theorem 2.1, with the same bounds.

We next consider the defect in (4.1) on inserting the sum of (4.5). Up to terms of size $\mathcal{O}(\varepsilon^{N+1})$ the defect consists of smooth functions multiplied by $\mathrm{e}^{\mathrm{i}k\dot{\phi}/\varepsilon}$ with $|k| \geq N+1$. By construction, the coefficient of $\mathrm{e}^{\pm\mathrm{i}(N+1)\dot{\phi}/\varepsilon}$ vanishes in the 0-component of the defect. The coefficient of $\mathrm{e}^{\pm\mathrm{i}(N+1)\dot{\phi}/\varepsilon}$ in the 1-component of the defect consists of a sum of products with factors $(z_1^{\alpha_1}, z_0^{\alpha_2}, \ldots, z_0^{\alpha_m})$ with $m \geq 2$ and $\alpha_1 + \ldots + \alpha_m = \pm(N+1)$, divided by ε^2. If N is odd (i.e., $N+1$ even), then either α_1 is even or one of the remaining α_i is odd. In each case we get a $\mathcal{O}(\varepsilon^{N+1})$ bound for the coefficient of $\mathrm{e}^{\pm\mathrm{i}(N+1)\dot{\phi}/\varepsilon}$ in the 1-component of the defect. The coefficients of $\mathrm{e}^{\mathrm{i}k\dot{\phi}/\varepsilon}$ with $|k| \geq N+2$ are bounded by $\mathcal{O}(\varepsilon^N)$.

We thus obtain a small defect of size $\mathcal{O}(\varepsilon^N)$ when the expansion is inserted into the Störmer–Verlet scheme (4.1). On a finite time interval $0 \le t \le T$ this implies the stated error bounds (4.8) by the same arguments as in the constant-frequency case. □

The construction of the previous proof implies that the functions $y^k(t) = z^k(t)\,\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ satisfy the second order difference equation, with the notation $\delta_h^2 y^k(t) = \big(y^k(t+h) - 2y^k(t) + y^k(t-h)\big)/h^2$,

$$\delta_h^2 y^k(t) = -\frac{1}{\varepsilon^2}\,\nabla_{-k}\mathcal{V}\big(\mathbf{y}(t)\big) - \nabla_{-k}\mathcal{U}\big(\mathbf{y}(t)\big) + \mathcal{O}(\varepsilon^N), \tag{4.10}$$

where $\mathbf{y} = (y^k)_{|k|\le N+1}$ is the vector of coefficient functions and the extended potentials $\mathcal{U}(\mathbf{y})$ and $\mathcal{V}(\mathbf{y})$ are the same as in Section 2.

5 Adiabatic invariant of the Störmer–Verlet method

We consider the modulated Fourier expansion on an interval of length $\mathcal{O}(h)$, where we can replace the coefficient functions $z^k(t)$ and the phase function $\phi(t)$ of (4.6) by Taylor polynomials of degree $M \ge N+3$. Because of $h = \mathcal{O}(\varepsilon)$, this keeps the defect in (4.10) of size $\mathcal{O}(\varepsilon^N)$, and the remainder $R_N(t)$ in (4.5) of size $\mathcal{O}(t^2\varepsilon^N)$. We will show that the modulated Fourier expansion has two almost-invariants $\mathcal{I}_h[\mathbf{z}](t)$ and $\mathcal{H}_h[\mathbf{z}](t)$, where this notation indicates that the expression depends on $z^k(t), \dot z^k(t), \dots, (z^k)^{(M)}(t)$ for $|k| \le N+1$.

We introduce the modified frequency

$$\omega_h(q_0) = \omega(q_0)\sqrt{1 - \Big(\frac{h\omega(q_0)}{2\varepsilon}\Big)^2}$$

and the corresponding modified action

$$I_h(q,p) = \frac{1}{2}\frac{|p_1|^2}{\omega_h(q_0)} + \frac{\omega_h(q_0)}{2\,\varepsilon^2}\,|q_1|^2. \tag{5.1}$$

Theorem 5.1 *Under the assumptions of Theorem 4.1, there exists an almost-invariant $\mathcal{I}_h[\mathbf{z}](t)$ of the modulated Fourier expansion, such that*

$$\begin{aligned} \mathcal{I}_h[\mathbf{z}](t) &= \mathcal{I}_h[\mathbf{z}](0) + \mathcal{O}(t\varepsilon^N) \qquad \textit{for} \quad 0 \le t \le h \\ \mathcal{I}_h[\mathbf{z}](nh) &= I_h(q_n,p_n) + \mathcal{O}(\varepsilon) \qquad \textit{for} \quad n = 0,1. \end{aligned}$$

The constants symbolised by $\mathcal{O}$ are independent of ε and h, but depend on N and M.

In the proof we will use the following auxiliary result.

Lemma 5.1 *Let $\varphi(\tau)$ be a polynomial in τ of degree $d \geq 2$ with real coefficients bounded by B, let $0 < \varepsilon \leq 1$ and set*

$$f(\tau) = \mathrm{e}^{\mathrm{i}\varphi(\tau)/\varepsilon}.$$

Let $m \geq 2$ be an integer. Then,

$$\frac{1}{m!}\, f^{(m)}(0) = \frac{1}{m!}\Big(\frac{\mathrm{i}\dot\varphi(0)}{\varepsilon}\Big)^m \mathrm{e}^{\mathrm{i}\varphi(0)/\varepsilon} + \frac{r_m}{\varepsilon^m}$$

with

$$|r_m| \leq C c^m \Big(\frac{\varepsilon}{m!} + \frac{\varepsilon^{m(d-1)/d}}{(m/d)!}\Big),$$

where C and c depend only on B and d (and are, in particular, independent of ε and m).

Proof We consider the first terms in the Taylor expansion of $\varphi(\tau)$ and write

$$\varphi(\tau) = \varphi(0) + \tau\dot\varphi(0) + \tau^2\psi(\tau).$$

With the entire complex function

$$g(\tau) = \mathrm{e}^{\mathrm{i}(\varphi(0)+\tau\dot\varphi(0))/\varepsilon}\, \frac{\mathrm{e}^{\mathrm{i}\tau^2\psi(\tau)/\varepsilon} - 1}{\tau^2/\varepsilon}$$

we then have

$$f(\tau) = \mathrm{e}^{\mathrm{i}(\varphi(0)+\tau\dot\varphi(0))/\varepsilon} + \frac{\tau^2}{\varepsilon} g(\tau)$$

and hence

$$\frac{r_m}{\varepsilon^m} = \frac{1}{m!}\,\frac{\mathrm{d}^m}{\mathrm{d}\tau^m}\Big|_{\tau=0}\Big(\frac{\tau^2}{\varepsilon}\, g(\tau)\Big).$$

By Cauchy's estimates, the derivatives of g are bounded, for arbitrary radius $R > 0$, by

$$\frac{|g^{(m}(0)|}{m!} \leq \frac{M_g(R)}{R^m} \qquad \text{with} \qquad M_g(R) = \max_{|\tau|=R} |g(\tau)|,$$

and we note that

$$M_g(R) = \begin{cases} \mathcal{O}(\varepsilon \mathrm{e}^{cR^d/\varepsilon}) & \text{for } \ R \geq 1 \\ \mathcal{O}(\mathrm{e}^{cR/\varepsilon}) & \text{for } \ R \leq \text{Const.} \end{cases}$$

We optimise R in dependence of m, which leads us to choose

$$R^d = \frac{m\varepsilon}{cd} \quad \text{if} \quad \frac{m\varepsilon}{cd} \geq 1, \qquad \text{and} \qquad R = \frac{m\varepsilon}{c} \quad \text{else.}$$

This choice yields the bound

$$\frac{|g^{(m)}(0)|}{m!} \leq C\mathrm{e}^m \Big(\frac{c}{m\varepsilon}\Big)^m + C\varepsilon \mathrm{e}^{m/d}\Big(\frac{cd}{m\varepsilon}\Big)^{m/d},$$

which together with the Stirling formula for factorials and the Leibniz formula for the higher derivatives of products of functions yields the stated result. □

Proof (of Theorem 5.1). As explained before, we can assume that the coefficient functions $z^k(t)$ and the phase function $\phi(t)$ are polynomials of degree at most M. Hence, $y^k(t) = z^k(t)\mathrm{e}^{\mathrm{i}k\phi(t)}$ is an entire analytic function of t.

We multiply (4.10) with $-\mathrm{i}ky^{-k}/\varepsilon$, and sum over k. Using the invariance property (3.1) of $\mathcal{U}$ and $\mathcal{V}$, we obtain

$$-\frac{\mathrm{i}}{\varepsilon}\sum_{|k|\le N+1} k\, y^{-k}(t)^{\mathsf{T}}\, \delta_h^2 y^k(t) = \mathcal{O}(\varepsilon^N).$$

Since y^k is an entire function, it has a *convergent* Taylor expansion

$$\delta_h^2 y^k(t) = \sum_{\ell\ge 0} \frac{2h^{2\ell}}{(2\ell+2)!}\,\frac{d^{2\ell+2}}{dt^{2\ell+2}} y^k(t).$$

With the fourth of the "magic formulas" on p. 508 of [14] we therefore have (omitting the superscript k on y^k)

$$\begin{aligned}
\operatorname{Im}\big(\overline{y}^{\mathsf{T}}\,\delta_h^2 y\big) &= \sum_{\ell\ge 0}\frac{2h^{2\ell}}{(2\ell+2)!}\operatorname{Im}\big(\overline{y}^{\mathsf{T}} y^{(2\ell+2)}\big)\\
&= \sum_{\ell\ge 0}\frac{2h^{2\ell}}{(2\ell+2)!}\operatorname{Im}\frac{\mathrm{d}}{\mathrm{d}t}\big(\overline{y}^{\mathsf{T}} y^{(2\ell+1)} - \dot{\overline{y}}^{\mathsf{T}} y^{(2\ell)} + \cdots \pm \overline{y}^{(\ell)\mathsf{T}} y^{(\ell+1)}\big)\\
&= \frac{\mathrm{d}}{\mathrm{d}t}\sum_{\ell\ge 0}\frac{2h^{2\ell}}{(2\ell+2)!}\operatorname{Im}\big(\overline{y}^{\mathsf{T}} y^{(2\ell+1)} - \dot{\overline{y}}^{\mathsf{T}} y^{(2\ell)} + \cdots \pm \overline{y}^{(\ell)\mathsf{T}} y^{(\ell+1)}\big),
\end{aligned}$$

where interchanging the derivative with the infinite sum is justified by the analyticity of the functions. Each of the products $\frac{\mathrm{d}^r}{\mathrm{d}t^r}(y^{-k})^{\mathsf{T}}\frac{\mathrm{d}^s}{\mathrm{d}t^s}y^k$ can be written as a smooth function of z^k and its derivatives and of the derivatives of ϕ, which are expressed as functions of z_0^0 and its derivatives by (4.6). Note that $\phi(t)$ does not appear, since it cancels in the products. We then obtain that there is a smooth function $\mathcal{I}_h[\mathbf{z}](t)$ such that

$$\frac{d}{dt}\mathcal{I}_h[\mathbf{z}](t) = -\frac{\mathrm{i}}{\varepsilon}\sum_{|k|<N} k\, y^{-k}(t)^{\mathsf{T}}\,\delta_h^2 y^k(t) = \mathcal{O}(\varepsilon^N).$$

Integrating this equation yields the first statement of the theorem.

For the proof of the second statement we elaborate the dominant term of $\mathcal{I}_h[\mathbf{z}](t)$. We fix t and consider $y^k(t+\tau) = z^k(t+\tau)\mathrm{e}^{\mathrm{i}k\phi(t+\tau)/\varepsilon}$. For $k\ne 0$, Lemma 5.1 and the bounds (4.7) give us

$$\frac{1}{m!}\frac{\mathrm{d}^m}{\mathrm{d}t^m}y^k(t) = \frac{1}{m!}z^k(t)\Big(\frac{\mathrm{i}k}{\varepsilon}\dot\phi(t)\Big)^m \mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon} + \mathcal{O}\Big(\frac{1}{(m/M)!}\Big(\frac{c}{\varepsilon}\Big)^{m-1-|k|}\Big), \quad (5.2)$$

where c and the constant symbolised by $\mathcal{O}$ are independent of $m\ge 1$ and ε.

Inserting (5.2) into $(-1)^r \frac{\mathrm{d}^r}{\mathrm{d}t^r}(y^{-k})^\mathsf{T} \frac{\mathrm{d}^s}{\mathrm{d}t^s} y^k$, the dominant term is seen to be the same whenever $r+s = 2\ell+1$ and hence, omitting the superscript k in y^k, we obtain

$$\frac{2}{(2\ell+2)!}\Big(\overline{y(t)}^\mathsf{T} y^{(2\ell+1)}(t) - \overline{\dot y(t)}^\mathsf{T} y^{(2\ell)}(t) + \cdots \pm \overline{y^{(\ell)}(t)}^\mathsf{T} y^{(\ell+1)}(t)\Big)$$
$$= \frac{2}{(2\ell+2)!}(\ell+1)\Big(\frac{\mathrm{i}k}{\varepsilon}\dot\phi(t)\Big)^{2\ell+1}|z^k(t)|^2 + \mathcal{O}\Big(\frac{1}{(\ell/M)!}\Big(\frac{c}{\varepsilon}\Big)^{2\ell-2|k|}\Big).$$

This gives us

$$\begin{aligned}
\mathcal{I}_h[\mathbf{z}](t) &= -\frac{\mathrm{i}}{\varepsilon}\sum_{0<|k|\le N+1}\Big(\frac{\mathrm{i}k}{h}|z^k(t)|^2 \sum_{\ell\ge 0}\frac{(-1)^\ell}{(2\ell+1)!}\Big(\frac{kh}{\varepsilon}\dot\phi(t)\Big)^{2\ell+1} + \mathcal{O}(\varepsilon^{2|k|})\Big)\\
&= \frac{1}{\varepsilon h}\sum_{0<|k|\le N+1}\Big(k|z^k(t)|^2\sin\Big(\frac{kh}{\varepsilon}\dot\phi(t)\Big) + \mathcal{O}(h\varepsilon^{2|k|})\Big)\\
&= \frac{2}{\varepsilon h}|z^1(t)|^2\sin\Big(\frac{h}{\varepsilon}\dot\phi(t)\Big) + \mathcal{O}(\varepsilon).
\end{aligned}$$

Using (4.6) and the definition of the modified frequency to obtain

$$\sin\Big(\frac{h}{\varepsilon}\dot\phi(t)\Big) = 2\sin\Big(\frac{h}{2\varepsilon}\dot\phi(t)\Big)\cos\Big(\frac{h}{2\varepsilon}\dot\phi(t)\Big) = \frac{h}{\varepsilon}\omega_h\big(z_0^0(t)\big),$$

this finally becomes

$$\mathcal{I}_h[\mathbf{z}](t) = 2\omega_h(z_0^0(t))\frac{|z^1(t)|^2}{\varepsilon^2} + \mathcal{O}(\varepsilon). \tag{5.3}$$

To complete the proof of the second statement we also have to elaborate the dominant term of $I_h(q_n,p_n)$. From Theorem 4.1 we get for the velocity approximation p_n of (4.2) the modulated Fourier expansion at $t=t_n$,

$$p_n = \frac{1}{2h}\sum_{|k|\le N+1}\Big(y^k(t+h) - y^k(t-h)\Big) + \mathcal{O}(h\varepsilon^N),$$

where $y^k(t) = z^k(t)\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ are the coefficient functions of Theorem 4.1 corresponding to starting approximations q_{n-1} and q_n. Expanding the expression into a (convergent) Taylor series around $h=0$ and using (5.2), we obtain for the second component of $p_n = (p_{n,0}, p_{n,1})$ that

$$\begin{aligned}
p_{n,1} &= \frac{1}{2h}\sum_{|k|\le N+1}\sum_{\ell\ge 0}\frac{2h^{2\ell+1}}{(2\ell+1)!}\frac{\mathrm{d}^{2\ell+1}}{\mathrm{d}t^{2\ell+1}}y_1^k(t) + \mathcal{O}(h\varepsilon^N)\\
&= \frac{\mathrm{i}}{h}\sum_{|k|\le N+1}\Big(z_1^k(t)\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}\sum_{\ell\ge 0}\frac{(-1)^\ell}{(2\ell+1)!}\Big(\frac{kh}{\varepsilon}\dot\phi(t)\Big)^{2\ell+1} + \mathcal{O}(h\varepsilon^{|k|})\Big)\\
&= \frac{\mathrm{i}}{h}\Big(z_1^1(t)\mathrm{e}^{\mathrm{i}\phi(t)/\varepsilon} - z_1^{-1}(t)\mathrm{e}^{-\mathrm{i}\phi(t)/\varepsilon}\Big)\sin\Big(\frac{h}{\varepsilon}\dot\phi(t)\Big) + \mathcal{O}(\varepsilon)\\
&= \frac{\mathrm{i}}{\varepsilon}\Big(z_1^1(t)\mathrm{e}^{\mathrm{i}\phi(t)/\varepsilon} - z_1^{-1}(t)\mathrm{e}^{-\mathrm{i}\phi(t)/\varepsilon}\Big)\,\omega_h(z_0^0(t)) + \mathcal{O}(\varepsilon).
\end{aligned}$$

This yields

$$|p_{n,1}|^2 = \frac{1}{\varepsilon^2}\Big|z_1^1(t)\mathrm{e}^{\mathrm{i}\phi(t)/\varepsilon} - z_1^{-1}(t)\mathrm{e}^{-\mathrm{i}\phi(t)/\varepsilon}\Big|^2 \omega_h(z_0^0(t))^2 + \mathcal{O}(\varepsilon). \tag{5.4}$$

From Theorem 4.1 we have

$$|q_{n,1}|^2 = \Big|z_1^1(t)\mathrm{e}^{\mathrm{i}\phi(t)/\varepsilon} + z_1^{-1}(t)\mathrm{e}^{-\mathrm{i}\phi(t)/\varepsilon}\Big|^2 + \mathcal{O}(\varepsilon^3). \tag{5.5}$$

Using $q_{n,0} = z_0^0(t) + \mathcal{O}(\varepsilon^3)$ this yields, with $y_1^k(t) = z_1^k(t)\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$ at $t = t_n$,

$$\begin{aligned}
I_h(q_n,p_n) &= \frac{1}{2}\frac{|p_{n,1}|^2}{\omega_h(q_{n,0})} + \frac{\omega_h(q_{n,0})}{2\varepsilon^2}|q_{n,1}|^2 \\
&= \frac{\omega_h\big(z_0^0(t)\big)}{2\varepsilon^2}\Big(\big|y_1^1(t) - y_1^{-1}(t)\big|^2 + \big|y_1^1(t) + y_1^{-1}(t)\big|^2\Big) + \mathcal{O}(\varepsilon) \\
&= \frac{\omega_h\big(z_0^0(t)\big)}{\varepsilon^2}\cdot 2\big|y_1^1(t)\big|^2 + \mathcal{O}(\varepsilon) \\
&= \mathcal{I}_h[\mathbf{z}](t) + \mathcal{O}(\varepsilon),
\end{aligned}$$

which completes the proof. □

By patching together many short intervals, in the same way as in [14, Sect. XIII.7], we obtain from Theorem 5.1 the following long-time near-conservation result.

Theorem 5.2 *Under the conditions of Theorem 4.1,*

$$I_h(q_n,p_n) = I_h(q_0,p_0) + \mathcal{O}(\varepsilon) \qquad \text{for} \quad 0 \le nh \le \varepsilon^{-N+1},$$

where the constant symbolised by $\mathcal{O}$ is independent of n, h, ε, but depends on N.

Remark 5.1 The numerical experiments of [3] show that with

$$\frac{h\omega}{2\varepsilon} = \sin\Big(\frac{\pi}{N+1}\Big), \qquad \text{i.e.,} \qquad \sin\Big(\frac{h\dot\phi}{2\varepsilon}\Big) = \sin\Big(\frac{\pi}{N+1}\Big)$$

the error in the adiabatic invariant in the constant-frequency case does not behave more favourably than $\mathcal{O}(\varepsilon) + \mathcal{O}(t\varepsilon^N)$, as is illustrated for $N = 2, 3$. Condition (4.4), which appears in Theorem 4.1, shows that in Theorem 5.2 little is lost in comparison with the constant-frequency case.

6 Energy conservation of the Störmer–Verlet method

We show that the Störmer–Verlet method nearly conserves a modified energy over long times. We note that the total energy can be written as

$$H(q,p) = \omega(q_0) I(q,p) + \tfrac{1}{2}|p_0|^2 + U(q),$$

and with another modified frequency

$$\widetilde{\omega}_h(q_0) = \frac{2\varepsilon}{h}\,\arcsin\Big(\frac{h}{2\varepsilon}\omega(q_0)\Big)$$

we consider the modified energy

$$H_h(q,p) = \widetilde{\omega}_h(q_0) I_h(q,p) + \tfrac{1}{2}|p_0|^2 + U(q). \tag{6.1}$$

Theorem 6.1 *Under the assumptions of Theorem 4.1, there exists an almost-invariant* $\mathcal{H}_h[\mathbf{z}](t)$ *of the modulated Fourier expansion, such that*

$$\begin{aligned} \mathcal{H}_h[\mathbf{z}](t) &= \mathcal{H}_h[\mathbf{z}](0) + \mathcal{O}(t\varepsilon^N) \qquad \text{for} \quad 0 \le t \le h \\ \mathcal{H}_h[\mathbf{z}](nh) &= H_h(q_n,p_n) + \mathcal{O}(\varepsilon) \qquad \text{for} \quad n = 0,1. \end{aligned}$$

The constants symbolised by $\mathcal{O}$ *are independent of* ε *and* h*, but depend on* N *and* M*.*

Proof The proof proceeds similarly to that of Theorem 5.1. We can again assume that the coefficient functions $z^k(t)$ and the phase function $\phi(t)$ are polynomials, so that $y^k(t) = z^k(t)\mathrm{e}^{\mathrm{i}k\phi(t)}$ is an entire analytic function of t.

We multiply (4.10) with $\dot y^{-k}$ and sum over k to obtain

$$\sum_{|k|\le N+1} \dot y^{-k}(t)^{\mathsf T}\,\delta_h^2 y^k(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{\varepsilon^2}\mathcal{V}(\mathbf{y}) + \mathcal{U}(\mathbf{y})\Big) + \mathcal{O}(\varepsilon^N).$$

With the first of the "magic formulas" on p. 508 of [14] we have (omitting the superscript k on y^k)

$$\begin{aligned} &\mathrm{Re}\,\big(\bar{\dot y}^{\mathsf T}\,\delta_h^2 y\big) = \sum_{\ell\ge 0}\frac{2h^{2\ell}}{(2\ell+2)!}\,\mathrm{Re}\,\big(\bar{\dot y}^{\mathsf T} y^{(2\ell+2)}\big) \\ &= \sum_{\ell\ge 0}\frac{2h^{2\ell}}{(2\ell+2)!}\,\mathrm{Re}\,\frac{\mathrm{d}}{\mathrm{d}t}\big(\bar{\dot y}^{\mathsf T} y^{(2\ell+1)} - \bar{\ddot y}^{\mathsf T} y^{(2\ell)} + \cdots \mp \overline{y^{(\ell)}}^{\mathsf T} y^{(\ell+2)} \pm \tfrac{1}{2}\overline{y^{(\ell+1)}}^{\mathsf T} y^{(\ell+1)}\big) \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\sum_{\ell\ge 0}\frac{2h^{2\ell}}{(2\ell+2)!}\,\mathrm{Re}\,\big(\bar{\dot y}^{\mathsf T} y^{(2\ell+1)} - \bar{\ddot y}^{\mathsf T} y^{(2\ell)} + \cdots \mp \overline{y^{(\ell)}}^{\mathsf T} y^{(\ell+2)} \pm \tfrac{1}{2}\overline{y^{(\ell+1)}}^{\mathsf T} y^{(\ell+1)}\big). \end{aligned}$$

Each of the products $\frac{\mathrm{d}^r}{\mathrm{d}t^r}(y^{-k})^{\mathsf T}\frac{\mathrm{d}^s}{\mathrm{d}t^s}y^k$ can be written as a smooth function of z^k and its derivatives and of the derivatives of ϕ, which are expressed as functions of z_0^0 and its derivatives by (4.6). We then obtain that there is a smooth function $\mathcal{K}_h[\mathbf{z}](t)$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}_h[\mathbf{z}](t) = -\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{\varepsilon^2}\mathcal{V}(\mathbf{z}) + \mathcal{U}(\mathbf{z})\Big) + \mathcal{O}(\varepsilon^N).$$

Integrating this equation yields the first statement of the theorem for

$$\mathcal{H}_h[\mathbf{z}] = \mathcal{K}_h[\mathbf{z}] + \frac{1}{\varepsilon^2}\mathcal{V}(\mathbf{z}) + \mathcal{U}(\mathbf{z}).$$

Inserting (5.2) into $(-1)^{r-1}\frac{\mathrm{d}^r}{\mathrm{d}t^r}(y^{-k})^{\mathsf{T}}\frac{\mathrm{d}^s}{\mathrm{d}t^s}y^k$ for $k \neq 0$, the dominant term is seen to be the same whenever $r+s = 2\ell+2$ and hence, omitting the superscript k in y^k and omitting henceforth the argument t, we have

$$\begin{aligned}&\frac{2}{(2\ell+2)!}\Big(\bar{\dot y}^{\mathsf{T}} y^{(2\ell+1)} - \bar{\ddot y}^{\mathsf{T}} y^{(2\ell)} + \cdots \pm \tfrac12 \overline{y^{(\ell+1)}}^{\mathsf{T}} y^{(\ell+1)}\Big)\\ &\qquad = -\frac{2}{(2\ell+2)!}(\ell+\tfrac12)\Big(\frac{\mathrm{i}k}{\varepsilon}\dot\phi\Big)^{2\ell+2}|z^k|^2 + \mathcal{O}\Big(\frac{1}{(\ell/M)!}\Big(\frac{c}{\varepsilon}\Big)^{2\ell+1-2|k|}\Big).\end{aligned}$$

This gives

$$\begin{aligned}\mathcal{K}_h[\mathbf{z}] &= \tfrac12|\dot z^0|^2 - \sum_{0<|k|\le N+1}\Big(\sum_{\ell\ge0}\frac{2h^{2\ell}}{(2\ell+2)!}(\ell+\tfrac12)\Big(\frac{\mathrm{i}k}{\varepsilon}\dot\phi\Big)^{2\ell+2}|z^k|^2 + \mathcal{O}(\varepsilon^{2|k|-1})\Big)\\
&= \tfrac12|\dot z^0|^2 + \sum_{0<|k|\le N+1}\frac{k}{\varepsilon}\dot\phi\,\frac{|z^k|^2}{h}\sum_{\ell\ge0}\frac{(-1)^\ell}{(2\ell+1)!}\Big(\frac{kh}{\varepsilon}\dot\phi\Big)^{2\ell+1}\\
&\qquad\qquad + \sum_{0<|k|\le N+1}\frac{|z^k|^2}{h^2}\sum_{\ell\ge0}\frac{(-1)^{\ell+1}}{(2\ell+2)!}\Big(\frac{kh}{\varepsilon}\dot\phi\Big)^{2\ell+2} + \mathcal{O}(\varepsilon)\\
&= \tfrac12|\dot z^0|^2 + \frac{2|z^1|^2}{\varepsilon h}\,\dot\phi\,\sin\Big(\frac{h}{\varepsilon}\dot\phi\Big) - \frac{2|z^1|^2}{h^2}\Big(1-\cos\Big(\frac{h}{\varepsilon}\dot\phi\Big)\Big) + \mathcal{O}(\varepsilon)\\
&= \tfrac12|\dot z^0|^2 + \frac{2|z^1|^2}{\varepsilon^2}\,\widetilde\omega_h(z_0^0)\,\omega_h(z_0^0) - \frac{|z^1|^2}{\varepsilon^2}\omega(z_0^0)^2 + \mathcal{O}(\varepsilon)\\
&= \tfrac12|\dot z_0^0|^2 + \widetilde\omega_h(z_0^0)\,\mathcal{I}_h[\mathbf{z}] - \frac{1}{\varepsilon^2}\mathcal{V}(\mathbf{z}) + \mathcal{O}(\varepsilon),\end{aligned}$$

where in the second line we split $(\ell+\frac12) = (\ell+1)-\frac12$, in the last-but-one line we use the definitions of the modified frequencies ω_h, $\widetilde\omega_h$, and (4.6) in

$$1-\cos\Big(\frac{h}{\varepsilon}\dot\phi\Big) = 2\sin\Big(\frac{h}{2\varepsilon}\dot\phi\Big)^2 = 2\Big(\frac{h}{2\varepsilon}\Big)^2\omega(z_0^0)^2,$$

and in the last line we use (5.3) and the definition of $\mathcal{V}$ together with the bounds (4.7), which give

$$\mathcal{V}(\mathbf{z}) = \omega(z_0^0)^2|z_1^1|^2 + \mathcal{O}(\varepsilon^3).$$

We thus obtain

$$\mathcal{H}_h[\mathbf{z}] = \widetilde\omega_h(z_0^0)\,\mathcal{I}_h[\mathbf{z}] + \tfrac12|\dot z_0^0|^2 + U(z^0) + \mathcal{O}(\varepsilon),$$

and with Theorem 5.1 this yields the second statement of the theorem. □

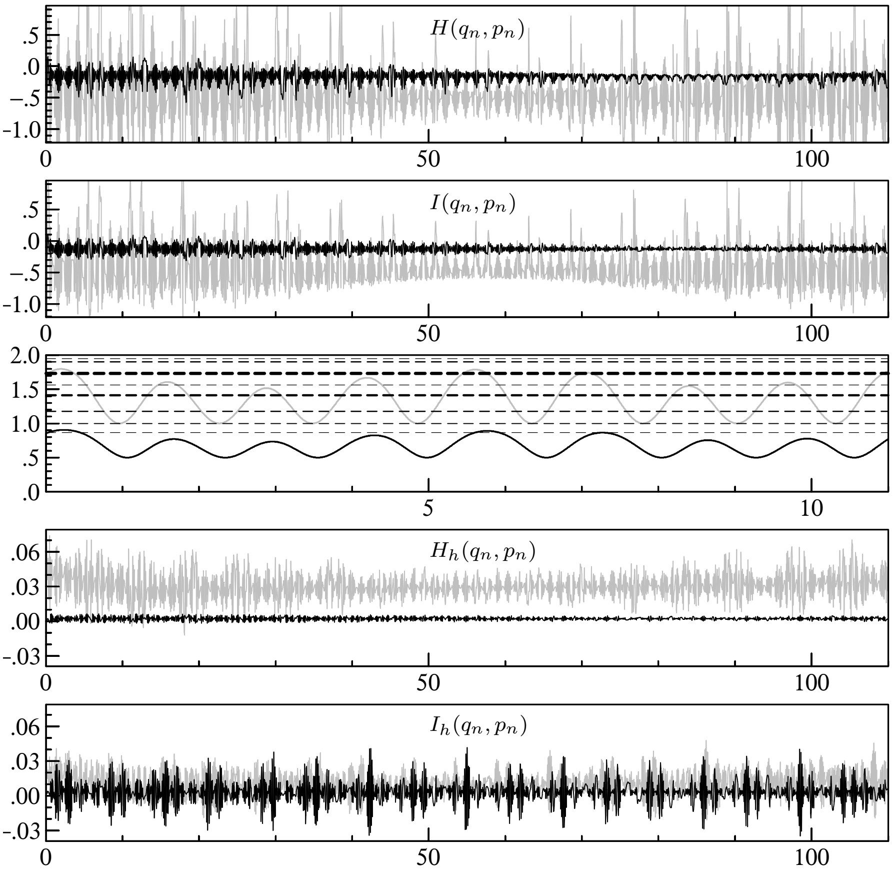

Fig. 7.1 Numerical experiment of Section 7. The pictures show the Hamiltonian H, the action I, as well as the modified Hamiltonian H_h and the modified action I_h along the numerical solution obtained with stepsizes $h = \varepsilon = 0.01$ (grey) and $h = \varepsilon/2$ (black). The picture in the middle shows the scaled frequency $h\omega(q_0)/\varepsilon$ as a function of time for both stepsizes. The horizontal lines indicate positions of numerical resonance.

As before, this leads to a long-time near-conservation result along the lines of [14, Sect. XIII.7].

Theorem 6.2 *Under the conditions of Theorem 4.1,*

$$H_h(q_n, p_n) = H_h(q_0, p_0) + \mathcal{O}(\varepsilon) \qquad \textit{for} \quad 0 \le nh \le \varepsilon^{-N+1},$$

where the constant symbolised by $\mathcal{O}$ *is independent of* n, h, ε*, but depends on* N*.*

7 Numerical experiment

We consider the problem of [14, Section I.5.1], where we replace the constant frequency ω by $\omega(q_0)/\varepsilon = \big(1 + \sin^2(q_{01})\big)/\varepsilon$ (q_{01} denotes the first component of the vector q_0). We put $\varepsilon = 0.01$ and we apply the Störmer–Verlet method (4.1) once with stepsize $h = \varepsilon$, and once with stepsize $h = \varepsilon/2$.

The upper two pictures of Figure 7.1 show the deviation of the Hamiltonian H and that of the action I along the numerical solution. For the larger stepsize $h = \varepsilon$ the result is drawn in grey, whereas that for $h = \varepsilon/2$ is in black. The lower two pictures present the analogous results for the modified Hamiltonian H_h of (6.1) and the modified action I_h of (5.1). Notice the different scale on the vertical axes. We see that the modified quantities are much better conserved than the original ones. For the modified Hamiltonian we see a huge improvement when passing from the larger to the smaller stepsize. No such improvement is observed for the modified action. This indicates that oscillations of this size are already in the action along the analytical solution.

For completeness, we have drawn in the middle picture of Figure 7.1 the function $h\omega(q_0)/\varepsilon$ along the numerical solution (again for both stepsizes). For the larger stepsize $h = \varepsilon$ this value is at certain time instances very close to 2 (for constant frequency the condition $h\omega/\varepsilon < 2$ is necessary for stability). The horizontal broken lines indicate the positions where $h\omega$ takes the values $2\sin(\pi r/k)$ for $k = 3, \ldots, 7$ and $r = 1, \ldots, (k-1)/2$ (numerical resonance). The smaller k, the thicker is the dashed line. We see that for the stepsize $h = \varepsilon/2$ the restriction (4.4) is satisfied with $N = 5$.

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