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Oscillations over long times in numerical Hamiltonian systems

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1.1 Introduction

The numerical treatment of ordinary differential equations has continued to be a lively area of numerical analysis for more than a century, with interesting applications in various fields and rich theory. There are three main developments in the design of numerical techniques and in the analysis of the algorithms:

- *Non-stiff differential equations.* In the 19th century (Adams, Bashforth, and later Runge, Heun and Kutta), numerical integrators have been designed that are efficient (high order) and easy to apply (explicit) in practical situations.
- *Stiff differential equations.* In the middle of the 20*th* century one became aware that earlier developed methods are impractical for a certain class of differential equations (stiff problems) due to stability restrictions. New integrators (typically implicit) were needed as well as new theories for a better understanding of the algorithms.
- *Geometric numerical integration.* In long-time simulations of Hamiltonian systems (molecular dynamics, astronomy) neither classical explicit methods nor implicit integrators for stiff problems give satisfactory results. In the last few decades, special numerical methods have been designed that preserve the geometric structure of the exact flow and thus have an improved long-time behaviour.

The basic developments (algorithmic and theoretical) of these epochs are documented in the monographs [HNW93], [HW96], and [HLW06]. Within geometric numerical integration we can also distinguish between non-stiff and stiff situations. Since here the main emphasis is on con-

servative Hamiltonian systems, the term "stiff" has to be interpreted as "highly oscillatory".

The present survey is concerned with geometric numerical integration with emphasis on theoretical insight for the long-time behaviour of numerical solutions. There are several degrees of difficulty:

- *Non-stiff Hamiltonian systems — backward error analysis.* The main theoretical tool for a better understanding of the long-time behaviour of numerical methods for structured problems is backward error analysis (Sect. 1.2). Rigorous statements over exponentially long times have been obtained in [BG94, HL97, Rei99] for symplectic integrators. Unfortunately, the analysis is restricted to the non-stiff situation, and does not provide any information for problems with high oscillations.
- *Highly oscillatory problems — modulated Fourier expansion.* The main part of this survey treats Hamiltonian systems of the form

$$\ddot{q} + \Omega^2 q = -\nabla U(q), \tag{1.1}$$

  where Ω is a diagonal matrix with real entries between 0 and a large ω, and $U(q)$ is a smooth potential function. The additional difficulty is the presence of two time scales, and the crucial role of harmonic actions in the long-time analysis. Basic work for the analytic solution is in [BGG87]. Section 1.3 presents the technique of modulated Fourier expansions which permits to prove simultaneously the conservation of energy and actions for the analytic and the numerical solution (where the product of the time step size and ω is of size one or larger). This is developed in [HL01, CHL03] for one high frequency and in [CHL05] for several high frequencies.
- *Non-linear wave equations.* An extension to infinite dimension with arbitrarily large frequencies permits to treat the long-time behaviour of one-dimensional semi-linear wave equations. Long-time conservation of harmonic actions along the analytic solution is studied in [Bou96, Bam03]. The technique of modulated Fourier expansion yields new insight into the long-time behavior of the analytic solution [CHL07b], of pseudo-spectral semi-discretizations [HL08], and of full discretizations [CHL07a]. This is discussed in Sect. 1.4.

In Sect. 1.5, an interesting analogy between highly oscillatory differential equations and linear multistep methods for non-stiff problems $\ddot{q} = -\nabla U(q)$ is established (see [HL04]). The inverse of the step size plays the role of ω, and the parasitic solutions of the multistep method

correspond to high oscillations in the solution of (1.1). The near conservation of the harmonic actions thus yields the bounded-ness of the parasitic solutions over long times, and permits to prove that special linear multistep methods are suitable for the long-time integration of Hamiltonian systems (like those arising in the computation of planetary motion).

1.2 Backward error analysis

An important tool for a better understanding of the long-time behaviour of numerical methods for ordinary differential equations is backward error analysis. We present the main ideas, some important consequences, and also its limitations in the case of highly oscillatory problems.

1.2.1 General idea

The principle applies to general ordinary differential equations $\dot{y} = f(y)$ and to general (numerical) one-step methods $y_{n+1} = \Phi_h(y_n)$, such as Runge–Kutta, Taylor series, composition and splitting methods. It consists in searching for a modified differential equation

$$\dot{z} = f_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + \ldots, \qquad z(0) = y_0, \qquad (1.2)$$

where the vector field is written as a formal series in powers of the step size h, such that the numerical solution for the original problem is equal (in the sense of formal power series) to the exact solution of the modified differential equation (see Fig. 1.1).

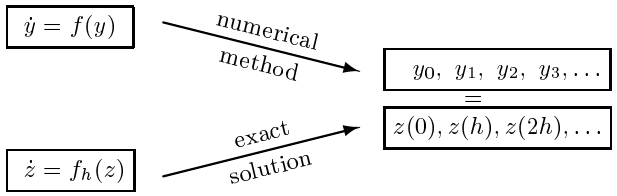


Fig. 1.1. Idea of backward error analysis

To obtain the coefficient functions $f_j(y)$, we note that we have the relation $z(t+h) = \Phi_h\big(z(t)\big)$ for the (formal) solution of (1.2). Expanding both sides of this relation into a power series of h and comparing equal powers of h, permits us to compute the functions $f_j(y)$ in a recursive manner.

The importance of backward error analysis resides in the fact that for differential equations with certain structures (Hamiltonian, reversible, divergence-free, etc.) solved with suitable geometric integrators (symplectic, symmetric, volume-preserving, etc.), the modified differential equation has the same structure as the original problem. The study of the modified differential equation then gives insight into the numerical solution. The rest of this section is devoted to make these statements more precise for the important special case of the Störmer–Verlet (leapfrog) discretisation.

1.2.2 Störmer–Verlet discretisation

For ease of presentation we restrict our considerations to the special Hamiltonian system

$$\ddot{q} = f(q) \quad \text{with} \quad f(y) = -\nabla U(q), \tag{1.3}$$

where $U(q)$ is a smooth potential function. Its most obvious discretisation (augmented with an approximation to the velocity $p = \dot{q}$) is

$$\begin{aligned} q^{n+1} - 2q^n + q^{n-1} &= h^2 f(q^n) \\ q^{n+1} - q^{n-1} &= 2h\, p^n. \end{aligned} \tag{1.4}$$

Due to pioneering work on higher order variants by Störmer, and due to its importance in molecular dynamics simulations recognised by Verlet, it is often called Störmer–Verlet method. In the literature on partial differential equations it is known as the leapfrog discretisation.

Introducing $p^{n+1/2} := (q^{n+1} - q^n)/h$ as an intermediate slope, this method can be written as

$$\begin{aligned} p^{n+1/2} &= p^n + \frac{h}{2} f(q^n) \\ q^{n+1} &= q^n + h\, p^{n+1/2} \\ p^{n+1} &= p^{n+1/2} + \frac{h}{2} f(q^{n+1}) \end{aligned} \tag{1.5}$$

which is clearly recognised as a symmetric one-step method for (1.3). It is a geometric integrator par excellence: the numerical flow $(q^n, p^n) \mapsto (q^{n+1}, p^{n+1})$ is symplectic when $f(q) = -\nabla U(q)$, it is volume preserving in the phase space, and it is time reversible (see [HLW03]). It is also the basic scheme for various extensions to higher order methods: composition and splitting methods, partitioned Runge–Kutta methods, and symmetric multistep methods.

1.2.3 Formal backward error analysis

We search for a modified differential equation such that its solution $\big(q(t), p(t)\big)$, which should not be confused with the solution of (1.3), formally interpolates the numerical solution of (1.4), i.e.,

$$\begin{aligned} q(t+h) - 2q(t) + q(t-h) &= h^2 f\big(q(t)\big) \\ q(t+h) - q(t-h) &= 2h\, p(t). \end{aligned} \tag{1.6}$$

Expanding the left hand sides into Taylor series around $h = 0$, eliminating higher derivatives by successive differentiation, and expressing the resulting differential equations in terms of q and p, yields

$$\begin{aligned} \dot p &= f(q) + \frac{h^2}{12}\Big(f''(q)(p,p) + f'(q)f(q)\Big) - \frac{h^4}{720}\Big(f''''(q)\big(p,p,p,p\big) \\ &\quad + 6\, f'''(q)\big(f(q),p,p\big) + 24\, f''(q)\big(f'(q)p,p\big) + 3\, f''(q)\big(f(q),f(q)\big) \\ &\quad + 6\, f'(q)f''(q)(p,p) + 6\, f'(q)f'(q)f(q)\Big) + \mathcal{O}(h^6) \\ \dot q &= p - \frac{h^2}{6}\, f'(q)p + \frac{h^4}{180}\Big(f'''(q)\big(p,p,p\big) + 3\, f''(q)\big(f(q),p\big) \\ &\quad + 6\, f'(q)f'(q)p\Big) + \mathcal{O}(h^6). \end{aligned} \tag{1.7}$$

Due to the symmetry of the method, the modified differential equation becomes a series in even powers of h.

For the case of a Hamiltonian system (1.3), i.e., $f(q) = -\nabla U(q)$, the modified differential equation (1.7) is also Hamiltonan

$$\dot p = -\nabla_q H_h(p,q), \qquad \dot q = \nabla_p H_h(p,q)$$

with modified Hamiltonian

$$\begin{aligned} H_h(p,q) &= \tfrac{1}{2}\|p\|^2 + U(q) + \frac{h^2}{24}\Big(2\, U''(q)\big(p,p\big) - \|U'(q)\|^2\Big) \\ &\quad - \frac{h^4}{720}\Big(U^{(4)}(q)\big(p,p,p,p\big) - 6\, U'''(q)\big(U'(q),p,p\big) \\ &\qquad + 3\, U''(q)\big(U'(q),U'(q)\big) - 12\, \|U''(q)p\|^2\Big) + \mathcal{O}(h^6). \end{aligned} \tag{1.8}$$

An important consequence of this observation is the following: since the numerical solution of the Störmer–Verlet discretisation is (at least formally) equal to the exact solution of the modified differential equation, we have that $H_h(p^n, q^n) = \mathit{const}$. As long as the numerical solution stays in a compact set, this implies that the energy $H(p,q) = \frac{1}{2}\|p\|^2 + U(q)$ remains close to a constant, i.e., $H(p^n, q^n) = \mathit{const} + \mathcal{O}(h^2)$ without any dirft.

The next section shows how this statement can be made rigorous.

1.2.4 Rigorous backward error analysis

For a rigorous analysis, the modified differential equation constructed in the previous sections has to be truncated suitably:

$$\dot{z} = f_{h,N}(z) = f(z) + hf_2(z) + \ldots + h^{N-1}f_N(z), \qquad z(0) = y_0. \quad (1.9)$$

Obviously, equality does not hold any more in Fig. 1.1 and an error of size $\mathcal{O}(h^{N+1})$ is introduced. More precisely, if $y_{n+1} = \Phi_h(y_n)$ denotes the one-step method, and $\varphi_{N,t}(y)$ the flow of the truncated differential equation (1.9), we have $\|\Phi_h(y_0) - \varphi_{N,h}(y_0\| \leq C_N h^{N+1}$ for arbitrary N. The freedom of choosing the truncation index N can be used to minimise this estimate. For analytic $f(y)$ and for standard numerical integrators (such as partitioned Runge–Kutta methods including the Störmer–Verlet discretisation), the choice $N \sim h^{-1}$ yields an estimate

$$\|\Phi_h(y_0) - \varphi_{N,h}(y_0\| \leq h\gamma M\, \mathrm{e}^{-\alpha/\omega h}, \quad (1.10)$$

where α and γ are constants that only depend on the numerical method, M is an upper bound of $f(y)$ on a disc of radius $2R$ around the initial value y_0, and $\omega = M/R$ is related to a Lipschitz constant of $f(y)$. A detailed proof can be found in [HLW06, Chap. IX].

Notice that (1.10) yields an estimate for one step only (local error). To get estimates for the global error and information on the long-time behaviour, knowledge on the propagation of perturbations is needed.

- *Conservation of energy.* In the case of a symplectic method applied to a Hamiltonian system, the modified equation is Hamiltonian (see Section 1.2.3). The truncated modified Hamiltonian $H_{N,h}(p, q)$ is exactly conserved along the solution of (1.9). Therefore, local deviations in $H_{N,h}(p^n, q^n)$ are just summed up, and one obtains from (1.10) that this modified Hamiltonian is conserved along the numerical solution up to exponentially small errors $\mathcal{O}(\mathrm{e}^{-\gamma/2\omega h})$ on exponentially long time intervals $0 \leq t \leq \mathcal{O}(\mathrm{e}^{\gamma/2\omega h})$. This implies the absence of any drift in the numerical Hamiltonian $H(p^n, q^n)$.
- *Integrable Hamiltonian systems.* Symplectic integrators applied to a nearly integrable Hamiltonian system give raise to a modified equation that is a perturbed Hamiltonian system. The celebrated KAM theory can be used get insight into the long-time behaviour of numerical integrators, e.g., linear growth of the global error.
- *Chaotic systems.* In the presence of positive Lyapunov exponents, the numerical solution remains close to the exact solution of the truncated

modified equation only on time intervals of length $\mathcal{O}(h^{-1})$. Energy is well conserved by symplectic integrators also in this situation.

1.2.5 Limitation in the presence of high oscillations

The estimate (1.10) does not give any useful information if the product ωh is of size one or larger. Recall that ω is a kind of Lipschitz constant of the vector field $f(y)$ which, in the case of a stable Hamiltonian system, can be interpreted as the highest frequency in the solution. This means that for highly oscillatory differential equations the step size is restricted to unrealistic small values.

From the example of the harmonic oscillator $H(p,q) = \frac{1}{2}(p^2 + \omega^2 q^2)$ it can be seen that the estimate (1.10) cannot qualitatively be improved. In fact, for all reasonable integrators, the scaled numerical solution $(\omega q^n, p^n)$ depends on the step size h only via the product ωh.

The aim of the next section is to present a theory that permits to analyse the long-time behaviour of numerical time integrators in the presence of high oscillations.

1.3 Modulated Fourier expansion

In this section we consider Hamiltonian systems

$$\ddot{q} + \Omega^2 q = g(q), \qquad g(q) = -\nabla U(q), \tag{1.11}$$

where, for ease of presentation, Ω is a diagonal matrix and $U(q)$ is a smooth potential function. Typically, Ω will contain diagonal entries ω with large modulus. We are interested in the long-time behaviour of numerical solutions when ω times the step size h is not small, so that classical backward error analysis cannot be applied.

1.3.1 Modulated Fourier expansion of the analytic solution

We start with the situation, where Ω contains only diagonal entries which are either 0 or ω, and we split the components of q accordingly, i.e., $q = (q_0, q_1)$ and $\Omega = \operatorname{diag}(0, \omega I)$. Both, q_0 and q_1 are allowed to be vectors. There are two time scales in the solution of equation (1.11):

- fast time ωt in oscillations of the form $\mathrm{e}^{\mathrm{i}\omega t}$;
- slow time t due to the zero eigenvalue and the non-linearity.

In the absence of the non-linearity $g(q)$, the solution of (1.11) is a linear combination of 1, t, and $\mathrm{e}^{\pm \mathrm{i}\omega t}$. For the general case we make the ansatz

$$q(t) = \sum_{k\in\mathbb{Z}} z^k(t)\, \mathrm{e}^{\mathrm{i}k\omega t}, \tag{1.12}$$

where $z^k(t)$ are smooth functions with derivatives bounded uniformly in ω. The function $z^0(t)$ is real-valued, and $z^{-k}(t)$ is the complex conjugate of $z^k(t)$. Inserting (1.12) into the differential equation (1.11), expanding the non-linearity into a Taylor series arount z^0, and comparing coefficients of $\mathrm{e}^{\mathrm{i}k\omega t}$ yields

$$\begin{pmatrix} \ddot z_0^k + 2\mathrm{i}k\omega \dot z_0^k - k^2\omega^2 z_0^k \\ \ddot z_1^k + 2\mathrm{i}k\omega \dot z_1^k + (1-k^2)\,\omega^2 z_1^k \end{pmatrix} = \sum_{m\ge 0} \frac{1}{m!} \sum_{s(\alpha)=k} g^{(m)}(z^0)\, z^\alpha, \tag{1.13}$$

where $\alpha = (\alpha_1, \dots, \alpha_m)$ is a multi-index, $s(\alpha) = \sum_{j=1}^m \alpha_j$, and $g^{(m)}(z^0)\, z^\alpha = g^{(m)}(z^0)\big(z^{\alpha_1}, \dots, z^{\alpha_m}\big)$. The second sum is over multi-indices $\alpha = (\alpha_1, \dots, \alpha_m)$ with $\alpha_j \neq 0$.

To obtain smooth functions $z_j^k(t)$ with derivatives bounded uniformly for large ω, we separate the dominating term in the left-hand side of (1.13), and eliminate higher derivatives by iteration. This gives a second order differential equation for z_0^0, first order differential equations for z_1^1 and z_1^{-1}, and algebraic relations for all other variables. Under the "bounded energy" assumption on the initial values

$$\|\dot q(0)\|^2 + \|\Omega\, q(0)\|^2 \le E, \tag{1.14}$$

it is possible to prove that the coefficient functions are bounded (on intervals of size one) as follows: $z_0^0(t) = \mathcal{O}(1)$, $z_1^{\pm 1}(t) = \mathcal{O}(\omega^{-1})$, $\dot z_1^{\pm 1}(t) = \mathcal{O}(\omega^{-2})$, and $z_j^k(t) = \mathcal{O}(\omega^{-|k|-2})$ for the remaining indices (j,k), see [HLW06, Sect. XIII.5].

The time average of the potential $U(q)$ along the analytic solution (1.12) only depends on the smooth coefficient functions $z^k(t)$ and is (formally) given by (with $\mathbf{z} = (\dots, z^{-1}, z^0, z^1, z^2, \dots)$)

$$\mathcal{U}(\mathbf{z}) = U(z^0) + \sum_{m\ge 1} \frac{1}{m!} \sum_{s(\alpha)=0} U^{(m)}(z^0) z^\alpha. \tag{1.15}$$

It is an interesting fact and crucial for the success of the expansion (1.12) that the functions $y^k(t) = z^k(t)\, \mathrm{e}^{\mathrm{i}k\omega t}$ are solution of the infinite dimensional Hamiltonian system

$$\ddot y^k + \Omega^2 y^k = -\nabla_{-k} \mathcal{U}(\mathbf{y}), \tag{1.16}$$

where ∇_{-k} indicates the derivative with respect to the component "$-k$" of the argument $\mathbf{y}$. Its Hamiltonian

$$\mathcal{H}(\mathbf{y},\dot{\mathbf{y}}) = \frac{1}{2}\sum_{k\in\mathbb{Z}}\Big((\dot{y}^{-k})^T\dot{y}^k + (y^{-k})^T\Omega^2 y^k\Big) + \mathcal{U}(\mathbf{y}) \tag{1.17}$$

is therefore a conserved quantity of the system (1.16), and hence also of (1.13). Since $q_0(t) = z_0^0(t) + \mathcal{O}(\omega^{-3})$, $\dot{q}_0(t) = \dot{z}_0^0(t) + \mathcal{O}(\omega^{-2})$, $q_1(t) = z_1^1(t)\,\mathrm{e}^{\mathrm{i}\omega t} + z_1^{-1}(t)\,\mathrm{e}^{-\mathrm{i}\omega t} + \mathcal{O}(\omega^{-2}) = y_1^1(t) + y_1^{-1}(t) + \mathcal{O}(\omega^{-2})$ and $\dot{q}_1(t) = \mathrm{i}\omega\big(y_1^1(t) - y_1^{-1}(t)\big) + \mathcal{O}(\omega^{-2})$ by the estimates for z_j^k, the quantity (1.17) is $\mathcal{O}(\omega^{-1})$ close to the total energy of the system

$$H\big(q(t),\dot{q}(t)\big) = \frac{1}{2}\big(\|\dot{q}(t)\|^2 + \|\Omega q(t)\|^2\big) + U\big(q(t)\big). \tag{1.18}$$

The averaged potential $\mathcal{U}(\mathbf{y})$ is invariant under the one-parameter group of transformations $y^k \to \mathrm{e}^{\mathrm{i}k\tau}y^k$. Therefore, Noether's theorem yields the additional conserved quantity

$$\mathcal{I}(\mathbf{y},\dot{\mathbf{y}}) = -\mathrm{i}\omega\sum_{k\in\mathbb{Z}} k\,(y^{-k})^T\dot{y}^k \tag{1.19}$$

for the system (1.16). It is $\mathcal{O}(\omega^{-1})$ close to the harmonic energy

$$I\big(q(t),\dot{q}(t)\big) = \frac{1}{2}\big(\|\dot{q}_1(t)\|^2 + \omega^2\|q_1(t)\|^2\big) \tag{1.20}$$

of the highly oscillatory part of the system.

The analysis of this section can be made rigorous by truncating the arising series and by patching together estimates on short intervals to get information on intervals of length ω^{-N} (with arbitrary N). In this way one can prove that the harmonic energy (1.20) remains constant up to oscillations of size $\mathcal{O}(\omega^{-1})$ on intervals of length ω^{-N}, a result first obtained by [BGG87].

1.3.2 Exponential integrators

Since $q^{n+1} - 2\cos(h\Omega)\,q^n + q^{n-1} = 0$ is an exact discretisation of the equation $\ddot{q} + \Omega^2 q = 0$, it is natural to consider the numerical scheme

$$q^{n+1} - 2\cos(h\Omega)\,q^n + q^{n-1} = h^2\Psi g(\Phi q^n) \tag{1.21}$$

as discretisation of (1.11). Here, $\Psi = \psi(h\Omega)$ and $\Phi = \phi(h\Omega)$, where the filter functions $\psi(\xi)$ and $\phi(\xi)$ are even, real-valued functions satisfying

$\psi(0) = \phi(0) = 1$. Special cases are the following:

(A)	$\psi(h\Omega) = \operatorname{sinc}^2(\frac{1}{2}h\Omega)$	$\phi(h\Omega) = 1$	[Gau61]
(B)	$\psi(h\Omega) = \operatorname{sinc}(h\Omega)$	$\phi(h\Omega) = 1$	[Deu79]
(C)	$\psi(h\Omega) = \operatorname{sinc}^2(h\Omega)$	$\phi(h\Omega) = \operatorname{sinc}(h\Omega)$	[GASSS99]

where $\operatorname{sinc}(\xi) = \sin\xi/\xi$. It is also natural to complete formula (1.21) with a derivative approximation p^n given by

$$q^{n+1} - q^{n-1} = 2h \operatorname{sinc}(h\Omega)\, p^n, \tag{1.22}$$

because, for $q(t) = \exp(\mathrm{i}\Omega t)\, q^0$, the derivative $p(t) = \dot{q}(t)$ satisfies this relation without error.

Written as a one-step method, we obtain

$$\begin{aligned} \widetilde{p}^n &= p^n + \frac{h}{2}\, \Psi_1 g(\Phi q^n) \\ q^{n+1} &= \cos(h\Omega)\, q^n + \Omega^{-1} \sin(h\Omega)\, \widetilde{p}^n \\ p^{n+1} &= \Omega \sin(h\Omega)\, q^n + \cos(h\Omega)\, \widetilde{p}^n + \frac{h}{2}\, \Psi_1 g(\Phi q^{n+1}), \end{aligned} \tag{1.23}$$

where $\Psi_1 = \psi_1(h\Omega)$ with $\psi_1(\xi) = \psi(\xi)/\operatorname{sinc}(\xi)$. Notice that, for $\Omega \to 0$, this integrator reduces to the Störmer–Verlet discretisation (1.5).

1.3.3 Modulated Fourier expansion of numerical solution

We are interested in the long-time behaviour of numerical approximations to the highly oscillatory Hamiltonian system (1.11). Our focus will be on the near conservation of the total energy (1.18) and of the harmonic energy (1.20) over long times.

In complete analogy to what we did in Sect. 1.3.1 for the analytic solution, we separate the fast and slow modes by the ansatz

$$q^n = \widetilde{q}(t_n) \qquad \text{with} \qquad \widetilde{q}(t) = \sum_{k\in\mathbb{Z}} z^k(t)\, \mathrm{e}^{\mathrm{i}k\omega t}, \tag{1.24}$$

where $t_n = nh$, and the coefficient functions are again assumed to be smooth with derivatives bounded uniformly in ω. Inserting this ansatz into the numerical scheme (1.21), expanding the functions $z^k(t \pm h)$ into Taylor series around $h = 0$ and the non-linearity into a Taylor series around z^0, and finally comparing coefficients of $\mathrm{e}^{\mathrm{i}k\omega t}$ yields

$$\mathcal{L}^k(hD)\, z^k = h^2 \sum_{m\geq 0} \frac{1}{m!} \sum_{s(\alpha)=k} \Psi\, g^{(m)}(z^0)\, (\Phi z)^\alpha, \tag{1.25}$$

where, with the abbreviations $s_k = \sin(\frac{1}{2}kh\omega)$ and $c_k = \cos(\frac{1}{2}kh\omega)$, the differential operator is given by

$$\mathcal{L}^k(hD)\, z^k = \begin{pmatrix} -s_k^2 z_0^k + 2\mathrm{i}hs_{2k}\dot{z}_0^k + h^2 c_{2k}\ddot{z}_0^k + \frac{1}{3}\mathrm{i}h^3 s_{2k}\dddot{z}_0^k + \dots \\ -s_{k-1}s_{k+1} z_1^k + 2\mathrm{i}hs_{2k}\dot{z}_1^k + h^2 c_{2k}\ddot{z}_1^k + \frac{1}{3}\mathrm{i}h^3 s_{2k}\dddot{z}_1^k + \dots \end{pmatrix}$$

As in (1.13) we separate the dominating term in the left-hand expression of (1.25). This gives a second order differential equation for z_0^0, first order differential equations for z_1^1 and z_1^{-1}, and algebraic relations for the other functions, provided that s_k^2 for $k \neq 0$ and $s_{k-1}s_{k+1}$ for $k \neq \pm 1$ are bounded away from zero. To achieve this, we assume the numerical non-resonance condition

$$|\sin(\tfrac{1}{2}kh\omega)| \geq c\sqrt{h} \qquad \text{for} \qquad k = 1, 2, \dots, N \tag{1.26}$$

with some fixed $N \geq 2$.

The functions $\psi_1(\xi)$ and $\phi(\xi)$ in the one-step formulation (1.23) of the exponential integrator have the role to suppress or weaken numerical resonance, when $h\omega$ is close to an integral multiple of π. For the product $h\omega$ we therefore suppose

$$|\psi_1(h\omega)| \leq C\,|\operatorname{sinc}(\tfrac{1}{2}h\omega)|, \qquad |\phi(h\omega)| \leq C\,|\operatorname{sinc}(\tfrac{1}{2}h\omega)| \tag{1.27}$$

with some moderate constant C. Moreover, in addition to the standard assumption of a small step size h, we restrict our considerations to large frequencies ω and, in particular, to

$$h\omega \geq c_0 \qquad \text{for some given} \quad c_0 > 0, \tag{1.28}$$

which is precisely the situation where standard backward error analysis (Sect. 1.2) is not applicable.

These assumptions permit us to carry over the analysis from the analytic solution to the numerical solution of the exponential integrator. The coefficient functions z_j^k can be bounded in a similar way and they decay rapidly with increasing k. With the averaged potential $\mathcal{U}(\mathbf{z})$ of (1.15), the system (1.25) can be written as

$$\mathcal{L}^k(hD)z^k = -h^2\,\Psi\,\nabla_{-k}\mathcal{U}(\Phi\mathbf{z}), \tag{1.29}$$

where $\Phi\mathbf{z}$ is the vector composed of Φz^k. We would like to extract from this relation a conserved quantity. Notice that the Hamiltonian (1.17) can be obtained from (1.16) by taking the scalar product of the Hamiltonian equation (1.16) with $\dot{z}^{-k}$, by summing up over all $k \in \mathbb{Z}$, and by writing the appearing expressions as total differentials. Here, we can try the same. Taking the scalar product of the equation (1.29)

with $\Psi^{-1}\Phi\,\dot z^{-k}$ and summing up over all $k \in \mathbb{Z}$, the right-hand side is recognised as the total derivative of $\mathcal{U}(\Phi\mathbf{z})$. On the left-hand side, this procedure yields linear combinations of expressions of the form

$$\Re\langle \dot z^{-k}, (z^k)^{(2\ell)}\rangle, \qquad \Im\langle \dot z^{-k}, (z^k)^{(2\ell+1)}\rangle$$

which all, by miracle, can be written as a total derivative, e.g.,

$$\begin{aligned}
\Re\langle \dot{\bar z}, \ddot z\rangle &= \frac{d}{dt}\Re\Big(\frac{1}{2}\,\langle \dot{\bar z}, \dot z\rangle\Big), \qquad \Re\langle \dot{\bar z}, \dddot z\rangle &= \frac{d}{dt}\Re\Big(\langle \dot{\bar z}, \ddot z\rangle - \frac{1}{2}\,\langle \ddot{\bar z}, \dot z\rangle\Big),\\
\Im\langle \dot{\bar z}, \ddot z\rangle &= \frac{d}{dt}\Im\Big(\langle \dot{\bar z}, \dot z\rangle\Big), \qquad \Im\langle \dot{\bar z}, z^{(5)}\rangle &= \frac{d}{dt}\Im\Big(\langle \dot{\bar z}, \dddot z\rangle - \langle \ddot{\bar z}, \ddot z\rangle\Big).
\end{aligned}$$

This yields a conserved quantity for the system (1.25) that is $\mathcal{O}(h)$ close to the Hamiltonian (1.18) of (1.11).

If we take the scalar product of (1.29) with $\mathrm{i}k\omega\, z^{-k}$, we get in a similar manner a second conserved quantity. This one turns out to be $\mathcal{O}(h)$ close the harmonic energy (1.20).

To make the analysis rigorous we truncate all appearing series after N terms, and we then patch together the estimates on small time intervals. Under the assumptions of this section this proves that the numerical solution of the exponential integrator satisfies

$$\begin{aligned}
H(q^n, p^n) &= H(q^0, p^0) + \mathcal{O}(h)\\
I(q^n, p^n) &= I(q^0, p^0) + \mathcal{O}(h)
\end{aligned}$$

on intervals of length $\mathcal{O}(h^{-N+1})$, where the constant symbolising the $\mathcal{O}(h)$ reminder may depend on N.

1.3.4 Several high frequencies and resonance

The results of the previous sections can be extended to more than one high frequencies. We consider the Hamiltonian system (1.11), where the entries of the diagonal matrix Ω are $\omega_j = \lambda_j\omega$ (for $j = 0, \dots, \ell$) with $\lambda_0 = 0$ and $\lambda_j \geq 1$ for $j \geq 1$. As before, ω is a large parameter. The Hamiltonian of this system is

$$H(q, \dot q) = \frac{1}{2}\sum_{j=0}^{\ell}\Big(\|\dot q_j\|^2 + \omega_j^2\|q_j\|^2\Big) + U(q), \tag{1.30}$$

where the components q_j of q can themselves be vectors in different dimensions. With the aim of extending the analysis of Sect. 1.3.1 we are led to consider oscillators $\mathrm{e}^{\pm\mathrm{i}\omega_j t}$ and products thereof, i.e., $\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\omega)t}$, where $\mathbf{k}\cdot\omega$ is the scalar product of $\mathbf{k} = (k_1, \dots, k_\ell) \in \mathbb{Z}^\ell$ and $\omega = (\omega_1, \dots, \omega_\ell)$.

To avoid redundancy in a linear combination of such expressions, we introduce the resonance module

$$\mathcal{M} = \{\mathbf{k} \in \mathbb{Z}^\ell \,;\, k_1\lambda_1 + \ldots + k_\ell\lambda_\ell = 0\}, \tag{1.31}$$

and we consider the equivalence relation $\mathbf{k} \sim \mathbf{j}$ defined by $\mathbf{k}-\mathbf{j} \in \mathcal{M}$. We choose a set $\mathcal{K}$ of representatives which is such that $|\mathbf{k}| = |k_1| + \ldots + |k_\ell|$ is minimal within the equivalence class $\mathbf{k}+\mathcal{M}$, and such that with $\mathbf{k} \in \mathcal{K}$ also $-\mathbf{k} \in \mathcal{K}$. Extending (1.12) we make the ansatz

$$q(t) = \sum_{\mathbf{k}\in\mathcal{K}} z^{\mathbf{k}}(t)\, \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\omega)t} \tag{1.32}$$

for the solution of (1.11). Here, the smooth function $z^{\mathbf{k}}$ is partitioned into $z_j^{\mathbf{k}}$ in the same as q into q_j.

The whole programme of Sects. 1.3.1 and 1.3.3 can now be repeated to get information on the long-time behaviour of the analytic and the numerical solution in the case of several high frequencies. Let us just mention a few crucial steps.

Inserting (1.32) into the differential equation (1.11), a Taylor series expansion and a comparison of the coefficients of $\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\omega)t}$ yields

$$\ddot{z}_j^{\mathbf{k}} + 2\mathrm{i}(\mathbf{k}\cdot\omega)\dot{z}_j^{\mathbf{k}} + \big(\omega_j^2 - (\mathbf{k}\cdot\omega)^2\big) z_j^{\mathbf{k}} = \sum_{m\ge 0} \frac{1}{m!} \sum_{s(\boldsymbol{\alpha})\sim\mathbf{k}} g^{(m)}(z^{\mathbf{0}})\, z^{\boldsymbol{\alpha}}, \tag{1.33}$$

where $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_m)$ is a multi-index of elements in $\mathcal{K}$, $\boldsymbol{\alpha}_j \neq \mathbf{0}$, and $s(\boldsymbol{\alpha}) = \sum_{j=1}^m \boldsymbol{\alpha}_j$. Since there is only a fixed finite number of frequencies and since we restrict all considerations to indices $\mathbf{k} \in \mathcal{K}$ with $|\mathbf{k}| \le N$, the situation is very similar to that for one high frequency. We obtain a second order differential equation for $z_0^{\mathbf{0}}$, first order differential equations for $z_j^{\pm\langle j\rangle}$ where $\langle j\rangle \in \mathcal{K}$ is the vector with value 1 at position j and 0 else, and algebraic relations for the remaining coefficient functions. As in Sect. 1.3.1, the equations (1.33) can be interpreted as a complex Hamiltonian system with potential

$$\mathcal{U}(\mathbf{z}) = U(z^{\mathbf{0}}) + \sum_{m\ge 1} \frac{1}{m!} \sum_{s(\boldsymbol{\alpha})\sim\mathbf{0}} U^{(m)}(z^{\mathbf{0}}) z^{\boldsymbol{\alpha}}, \tag{1.34}$$

where $\mathbf{z} = (z^{\mathbf{k}})_{\mathbf{k}\in\mathcal{K}}$. This is again a time average of the potential $U(q)$.

This time, the potential (1.34) is invariant under the one-parameter group of transformations $z^{\mathbf{k}} \to \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\mu})\tau} z^{\mathbf{k}}$ for all $\boldsymbol{\mu} \perp \mathcal{M}$. We always have $(\lambda_1, \ldots, \lambda_\ell) \perp \mathcal{M}$, but there may be many more vectors perpendicular to $\mathcal{M}$. For example, if the λ_j are rationally independent, then $\mathcal{M} = \{\mathbf{0}\}$ and all vectors $\boldsymbol{\mu}$ are perpendicular to $\mathcal{M}$. Therefore,

Noether's theorem yields for every $\boldsymbol{\mu} \perp \mathcal{M}$ a conserved quantity which, with $y^{\mathbf{k}}(t) = z^{\mathbf{k}}(t)\,\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\omega)t}$ is given by

$$\mathcal{I}_{\boldsymbol{\mu}}(\mathbf{y},\dot{\mathbf{y}}) = -\mathrm{i}\sum_{\mathbf{k}\in\mathcal{K}} (\mathbf{k}\cdot\boldsymbol{\mu})(y^{-\mathbf{k}})^T \dot{y}^{\mathbf{k}}. \tag{1.35}$$

This invariant turns out to be $\mathcal{O}(\omega^{-1})$ close to

$$I_{\boldsymbol{\mu}}\big(q(t),\dot{q}(t)\big) = \sum_{j=1}^{\ell} \frac{\mu_j}{\lambda_j}\, I_j\big(q(t),\dot{q}(t)\big)$$

where

$$I_j\big(q(t),\dot{q}(t)\big) = \tfrac{1}{2}\big(\|\dot{q}_j(t)\|^2 + \omega_j^2\,\|q_j(t)\|^2\big)$$

is the harmonic energy corresponding to the frequency ω_j.

It is possible to continue the analysis as for the case with one high frequency. This yields the long-time near conservation of the quantities $I_{\boldsymbol{\mu}}\big(q(t),\dot{q}(t)\big)$. These ideas can be extended to the numerical solution of exponential integrators, and they lead to statements on the near conservation of total and harmonic energies over long time intervals (see [CHL05] for an elaboration of the details).

1.3.5 Störmer–Verlet as exponential integrator

Applying the Störmer–Verlet discretisation (1.4) to the highly oscillatory differential equation (1.11) yields

$$\begin{aligned} q^{n+1} - 2q^n + q^{n-1} &= -(h\Omega)^2 q^n + h^2 g(q^n) \\ q^{n+1} - q^{n-1} &= 2h\,p^n. \end{aligned} \tag{1.36}$$

This can be written as an exponential integrator

$$\begin{aligned} \tilde{q}^{n+1} - 2\cos(h\tilde{\Omega})\,\tilde{q}^n + \tilde{q}^{n-1} &= h^2\,\Psi g(\Phi\tilde{q}^n) \\ \tilde{q}^{n+1} - \tilde{q}^{n-1} &= 2h\ \mathrm{sinc}\,(h\tilde{\Omega})\,\tilde{p}^n, \end{aligned}$$

where $\Psi = \psi(h\tilde{\Omega})$, $\Phi = \phi(h\tilde{\Omega})$ with $\psi(\xi) = \phi(\xi) = 1$, the diagonal matrix $\tilde{\Omega}$ is related to Ω via

$$I - \tfrac{1}{2}\,(h\Omega)^2 = \cos(h\tilde{\Omega}) \qquad \text{or} \qquad \sin\Big(\frac{h\tilde{\Omega}}{2}\Big) = \frac{h\Omega}{2},$$

and the numerical approximations are related by

$$\tilde{q}^n = q^n \qquad \text{and} \qquad \mathrm{sinc}\,(h\tilde{\Omega})\,\tilde{p}^n = p^n.$$

This interpretation permits us to apply all the results that we know

for the long-time behavior of exponential integrators (1.21) to get information for the numerical solution of the Störmer–Verlet discretisation.

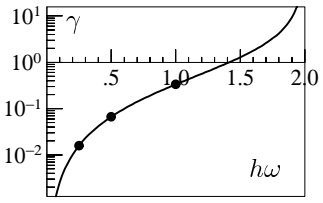
A linear stability analysis (i.e., vanishing non-linearity in (1.36)) shows that a necessary condition for stability is $h\omega_j \leq 2$ which corresponds to $h\tilde{\omega}_j \leq \pi$. Assumption (1.27) is therefore automatically satisfied for $h\tilde{\omega}_j$.

The results of Sect. 1.3.3 imply that $\tilde{H}(\tilde{q}^n, \tilde{p}^n)$ and $\tilde{I}(\tilde{q}^n, \tilde{p}^n)$ are conserved up to an error of size $\mathcal{O}(h)$ on intervals of length $\mathcal{O}(h^{-N+1})$. Here, $\tilde{H}$ and $\tilde{I}$ are defined in the same way as H and I, but with $\tilde{\omega}_j$ in place of ω_j. Rewritten in the original variables, this implies that on intervals of size $\mathcal{O}(h^{-N+1})$

$$\begin{aligned} H(q^n, p^n) + \frac{\gamma(h\omega)}{2} \|p^n\|^2 &= const + \mathcal{O}(h) \\ I(q^n, p^n) + \frac{\gamma(h\omega)}{2} \|p^n\|^2 &= const + \mathcal{O}(h), \end{aligned}$$

where

$$\gamma(h\omega) = \frac{(h\omega/2)^2}{1 - (h\omega/2)^2}.$$



If $h\omega$ is not too close to 2, say $h\omega \leq 1/2$, the perturbation in the above formula is small and, what is even more important, bounded without any drift.

The extension to several high frequencies is more delicate, and one has to pay attention. We still have that $\tilde{I}_{\boldsymbol{\mu}}(\tilde{q}^n, \tilde{p}^n)$ is well conserved over long times when $\boldsymbol{\mu}$ is perpendicular to the resonance module $\tilde{\mathcal{M}}$ corresponding to the frequencies $\tilde{\omega}_j$. However, $\boldsymbol{\mu}$ need not be perpendicular to $\mathcal{M}$. This means that a quantity is nearly conserved over long times by the numerical solution, but not by the analytic solution of the problem. Also the converse situation is possible.

1.4 Nonlinear wave equation

We consider the one-dimensional wave equation (non-linear Klein–Gordon)

$$\partial_t^2 u - \partial_x^2 u + \rho\, u + g(u) = 0 \tag{1.37}$$

for $t \geq 0$ and $-\pi \leq x \leq \pi$ subject to periodic boundary conditions. We assume $\rho > 0$, a smooth non-linearity $g(u)$ satisfying $g(0) = g'(0) = 0$, and initial data that are small in a Sobolev norm of sufficiently high

differentiation order s:

$$\Big(\big\|u(\cdot,0)\big\|_{s+1}^2 + \big\|\partial_t u(\cdot,0)\big\|_s^2\Big)^{1/2} \le \varepsilon\,, \qquad 0<\varepsilon\ll 1. \tag{1.38}$$

We expand the solution into a Fourier series

$$u(x,t) = \sum_{j=-\infty}^{\infty} u_j(t)\mathrm{e}^{\mathrm{i}jx}, \qquad \partial_t u(x,t) = \sum_{j=-\infty}^{\infty} v_j(t)\mathrm{e}^{\mathrm{i}jx},$$

so that, in terms of the Fourier coefficients, the wave equation (1.37) becomes

$$\partial_t^2 u_j + \omega_j^2 u_j + \mathcal{F}_j g(u) = 0 \qquad \text{for} \qquad j\in\mathbb{Z}, \tag{1.39}$$

where $\omega_j = \sqrt{j^2+\rho}$ and $\mathcal{F}_j v$ denotes the jth Fourier coefficient of a function $v(x)$. We consider only real solutions, so that $u_{-j} = \overline{u_j}$. The system (1.39) can be viewed as an infinite-dimensional version of (1.11) with an infinite number of frequencies.

1.4.1 Modulated Fourier expansion of the analytic solution

For the analytic solution we an make an ansatz analogous to (1.12) and (1.32),

$$u_j(t) \;\approx \sum_{\|\mathbf{k}\|\le 2N} z_j^{\mathbf{k}}(\varepsilon t)\,\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\omega})t},$$

where we use the multi-index notation $\mathbf{k}=(k_1,k_2,k_3,\ldots)$ with $k_j\in\mathbb{Z}$, $\|\mathbf{k}\| = |k_1|+|k_2|+|k_3|+\ldots$, and $\mathbf{k}\cdot\boldsymbol{\omega} = k_1\omega_1 + k_2\omega_2 + k_3\omega_3 + \ldots$. We insert this ansatz by a modulated Fourier expansion into the wave equation and compare the coefficients of $\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\omega})t}$. This yields relations of the form

$$(\omega_j^2 - |\mathbf{k}\cdot\boldsymbol{\omega}|^2) z_j^{\mathbf{k}} + 2\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\omega})\varepsilon \dot z_j^{\mathbf{k}} + \varepsilon^2 \ddot z_j^{\mathbf{k}} + \ldots = 0, \tag{1.40}$$

where $\dot z_j^{\mathbf{k}}$ and $\ddot z_j^{\mathbf{k}}$ are derivatives with respect to the slow time $\tau=\varepsilon t$ and the three dots indicate the contribution due to the non-linearity. We separate the dominant term, i.e.,

for $(\mathbf{k},j)$ with $\mathbf{k}\cdot\omega = \pm\omega_j$ the second term in (1.40);
for $(\mathbf{k},j)$ with $\big|\omega_j - |\mathbf{k}\cdot\omega|\big| \ge \varepsilon^{1/2}$ the first term in (1.40);
for $(\mathbf{k},j)$ with $\big|\omega_j - |\mathbf{k}\cdot\omega|\big| < \varepsilon^{1/2}$ it is undecidable.

We put $z_j^{\mathbf{k}} = 0$ in the third case, and estimate the defect with the help of a non-resonance condition, which imposes a restriction on the choice of ρ, but holds for almost all ρ. We refer the reader to [CHL07b] for more details.

The theory then follows the following steps:

- Proving existence of smooth functions $z_j^{\mathbf{k}}$ with derivatives bounded independently of ε (on intervals of length ε^{-1}).
- Establishing a Hamiltonian structure and the existence of formal invariants in the differential and algebraic equations for the $z_j^{\mathbf{k}}$.
- Proving closeness (on intervals of length ε^{-1}) of the formal invariants to actions

$$I_j(t) = \frac{\omega_j}{2}|u_j(t)|^2 + \frac{1}{2\omega_j}|v_j(t)|^2$$

and to the total energy

$$H(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{1}{2}\Big((\partial_t u)^2 + (\partial_x u)^2 + \rho\, u^2\Big) + U\big(u\big)\right)dx,$$

and the momentum

$$K(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \partial_x u\ \partial_t u\, dx.$$

(Unlike the actions I_j, energy and momentum are exactly conserved along solutions of the wave equation (1.37).)
- Stretching from short to long intervals of length ε^{-N+1} by patching together previous results along an invariant.

Carrying out this programme yields, in particular, an estimate on the long-time near-conservation of the harmonic actions:

$$\sum_{\ell=0}^{\infty} \omega_\ell^{2s+1}\, \frac{|I_\ell(t) - I_\ell(0)|}{\varepsilon^2} \le C\,\varepsilon \qquad \text{for} \qquad 0 \le t \le \varepsilon^{-N+1}. \tag{1.41}$$

The proof of this result is given in full detail in [CHL07b]. Related results on the long-time near-conservation of actions were previously obtained in [Bou96, Bam03] by different techniques.

We note that N can be chosen arbitrarily (but with s and C depending on N via the non-resonance condition). The near-conservation of harmonic actions is thus valid on time intervals that are much longer than the natural time scale of the problem. Moreover, the result implies spatial regularity over long times

$$\big\|u(\cdot,t)\big\|_{s+1}^2 + \big\|\partial_t u(\cdot,t)\big\|_s^2 \le \varepsilon^2(1 + C\varepsilon) \qquad \text{for} \qquad 0 \le t \le \varepsilon^{-N+1}.$$

1.4.2 Pseudo-spectral semi-discretisation

We approximate the solution of (1.37) by a trigonometric polynomial

$$u^M(x,t) = \sum_{|j|\le M}{}' q_j(t) \mathrm{e}^{\mathrm{i}jx},$$

where the prime on the sum indicates a factor $\frac{1}{2}$ in the first and last terms. The $2M$-periodic sequence $q = (q_j)$ is solution of the system

$$\frac{d^2 q_j}{dt^2} + \omega_j^2 q_j = f_j(q) \qquad \text{with} \qquad f(q) = -\mathcal{F}_{2M}\, g(\mathcal{F}_{2M}^{-1} q), \tag{1.42}$$

where $\mathcal{F}_{2M}$ stands for the discrete Fourier transform. This is in fact a finite-dimensional Hamiltonian system with Hamiltonian

$$H_M(q,p) = \frac{1}{2} \sum_{|j|\le M}{}' \Big(|p_j|^2 + \omega_j^2 |q_j|^2 \Big) + V(q),$$

$$V(q) = \frac{1}{2M} \sum_{k=-M}^{M-1} U\big((\mathcal{F}_{2M}^{-1} q)_k \big).$$

The above programme can again be carried out in the semi-discrete case. It yields the near-conservation over long times, uniformly in the discretization parameter M, of the harmonic actions as in (1.41) and of the continuous total energy H (which stays close to H_M) and the momentum K along semi-discrete solutions [HL08].

1.4.3 Full discretisation

The system (1.42), which we also write as $\frac{d^2 q}{dt^2} + \Omega^2 q = f(q)$, is an ordinary differential equation, and we can apply the exponential integrators of Section 1.3.2 and the Störmer–Verlet method.

Combining the techniques addressed in Sections 1.3.3 and 1.4, we obtain under a numerical non-resonance condition that along the numerical solution of a symplectic exponential integrator (1.23), for $0 \le t_n \le \varepsilon^{-N+1}$,

$$\begin{aligned} \frac{|H(t_n) - H(0)|}{\varepsilon^2} &\le C\,\varepsilon \\ \frac{|K(t_n) - K(0)|}{\varepsilon^2} &\le C(\varepsilon + M^{-s} + t_n\,\varepsilon\, M^{-s+1}) \\ \sum_{\ell=0}^{\infty} \omega_\ell^{2s+1} \frac{|I_\ell(t_n) - I_\ell(0)|}{\varepsilon^2} &\le C\,\varepsilon. \end{aligned}$$

Here, the functions $u(x,t_n)$ and $\partial_t u(x,t_n)$ in $H(t)$, $K(t)$, and $I_\ell(t)$ have to be replaced by the trigonometric interpolation polynomial with Fourier coefficients q^n and p^n, respectively.

For the Störmer–Verlet discretisation (1.5) this holds with an additional $\mathcal{O}(h^2)$ term on the right-hand side of these estimates, if in addition the step size is restricted by the CFL condition $h\omega_M \le c < 2$.

These results, which are proved in [CHL07a], are apparently the first rigorous results on the long-time near-conservation of energy (and momentum and actions) for symplectic discretisations of a non-linear partial differential equation.

1.5 Linear multistep methods

There is an interesting connection between the numerical solution of special linear multistep methods for non-stiff Hamiltonian equations $\ddot q = -\nabla U(q)$ and the analytic solution of the highly oscillatory problem (1.11). An analogue of the technique of modulated Fourier expansion (Sect. 1.3) will provide new insight into the long-time behaviour of such methods. In particular, the long-time conservation of harmonic actions corresponds to the bounded-ness of parasitic solutions in the multistep discretisation.

1.5.1 Multistep methods for second order problems

For the second order differential equation

$$\ddot q = f(q) \qquad \text{with} \qquad f(q) = -\nabla U(q) \tag{1.43}$$

we consider linear multistep methods of the form

$$\sum_{j=0}^{k} \alpha_j \, q^{n+j} \;=\; h^2 \sum_{j=0}^{k} \beta_j \, f\big(q^{n+j}\big) \tag{1.44}$$

together with an approximation to the derivative $p(t) = \dot q(t)$ which is obtained by a finite difference formula and does not affect the propagation of errors:

$$p^n = \frac{1}{h} \sum_{j=-k}^{k} \gamma_j q^{n+j}. \tag{1.45}$$

A special case is the Störmer–Verlet discretisation (1.4). The general method (1.44) is characterised by its generating polynomials

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \, \zeta^j, \qquad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \, \zeta^j. \tag{1.46}$$

The classical theory of Dahlquist tells us that zero-stability (all roots of $\rho(\zeta) = 0$ satisfy $|\zeta| \leq 1$ and those on the unit circle have at most multiplicity two) and consistency ($\rho(1) = \rho'(1) = 0$, $\rho''(1) = 2\sigma(1) \neq 0$) imply convergence to the analytic solution on intervals of length $\mathcal{O}(1)$.

For the case of a Hamiltonian system (1.43) we are often interested in the long-time behaviour of numerical solutions and, in particular, in the near conservation of the total energy

$$H(t) = \frac{1}{2} \, \dot{q}^T \dot{q} + U(q) \tag{1.47}$$

along numerical solutions. For methods that are

- *symmetric,* i.e., $\alpha_{k-j} = \alpha_j$ and $\beta_{k-j} = \beta_j$ for all j,
- *s-stable,* i.e., all roots of $\rho(\zeta) = 0$ are on the unit circle and they are simple roots with the exception of $\zeta = 1$ which is a double root,
- *order r,* i.e., $\rho(\mathrm{e}^h) - h^2 \sigma(\mathrm{e}^h) = \mathcal{O}(h^{p+2})$ asymptotically for $h \to 0$,

we shall prove that with sufficiently accurate starting approximations the total energy is nearly conserved over long times

$$H(q_n, p_n) = H(q_0, p_0) + \mathcal{O}(h^r) \qquad \text{for} \qquad nh \leq \mathcal{O}(h^{-r-2}). \tag{1.48}$$

For methods, where no zero of $\rho(\zeta)$ other than 1 can be written as the product of two other zeros, the estimate holds even on intervals of length $\mathcal{O}(h^{-2r-3})$.

A similar statement holds for quadratic first integrals of the form $p^T C q$ such as the angular momentum in N-body problems, and for all action variables in nearly integrable Hamiltonian systems.

1.5.2 Parasitic solutions

We consider a linear multistep method (1.44) where $\zeta_0 = 1$ is a double root of $\rho(\zeta) = 0$, and $\zeta_j, \zeta_{-j} = \overline{\zeta}_j$ are pairs of complex conjugate roots for $j = 1, \ldots, \ell$. In the limit $h \to 0$, (1.44) becomes a linear difference relation with characteristic polynomial $\rho(\zeta)$. Its solution is a linear combination of 1, n, and ζ_j^n, ζ_{-j}^n for $j = 1, \ldots, \ell$. Similar to the analytic solution of (1.11), we are also here confronted with two time scales:

- fast time t/h in oscillations of the form $\zeta_j^n = \zeta_j^{t/h}$;
- slow time t due to the zero root and the dynamics of (1.43).

In the general situation, ζ_j will be slightly perturbed leading to a modulation of the coefficients, and the non-linearity in the differential equation provokes the presence of products of ζ_j^n in the numerical solution. This motivates the following ansatz with smooth functions $z^j(t)$

$$q^n = \widetilde{q}(nh), \qquad \widetilde{q}(t) = \sum_{j \in \mathcal{I}} z^j(t)\, \zeta_j^{t/h} \tag{1.49}$$

which is in complete analogy to (1.12). Here, the sum is not only over $|j| \le \ell$, but the index-set $\mathcal{I}$ includes also finite products of roots of $\rho(\zeta) = 0$ which are denoted by $\zeta_{\ell+1}, \zeta_{\ell+2}, \ldots$ and $\zeta_{-j} = \overline{\zeta}_j$. The set $\mathcal{I}$ can be finite (e.g., if the roots of $\rho(\zeta) = 0$ are all roots of unity) or infinite. In the latter case the sum will be truncated suitably for a rigorous analysis. In the representation (1.49) only the function $z^0(t)$ contributes to an approximation of the solution of (1.43), the other coefficient functions are called parasitic solutions.

For determining the smooth functions $z^j(t)$, we insert q^n from (1.49) into the multistep formula (1.44), we expand the non-linearity around z^0, and we compare the coefficients of ζ_j^n. This yields

$$\rho(\zeta_j\, \mathrm{e}^{hD})\, z^j = h^2 \sigma(\zeta_j\, \mathrm{e}^{hD}) \sum_{m \ge 0} \frac{1}{m!} \sum_{p(\alpha)=j} f^{(m)}(z^0)\, z^\alpha,$$

where D represents differentiation with respect to time, so that the Taylor series expansion of a function $z(t+h)$ is given by $\mathrm{e}^{hD} z(t)$, and the second sum is over multi-indices $\alpha = (\alpha_1, \ldots, \alpha_m)$ such that the product $\zeta_{\alpha_1} \cdot \ldots \cdot \zeta_{\alpha_m}$ equals ζ_j. This is symbolised by $p(\alpha) = j$. We divide this relation formally by $\sigma(\zeta_j\, \mathrm{e}^{hD})$ and we introduce the notation

$$\frac{\rho(\zeta_j \mathrm{e}^{\mathrm{i}x})}{\sigma(\zeta_j \mathrm{e}^{\mathrm{i}x})} = \nu_{j,0} + \nu_{j,1}\, x + \nu_{j,2}\, x^2 + \nu_{j,3}\, x^3 + \ldots . \tag{1.50}$$

Due to the symmetry of the method (i.e., $\rho(\zeta) = \zeta^k \rho(\zeta^{-1})$ and $\sigma(\zeta) = \zeta^k \sigma(\zeta^{-1})$) the coefficients $\nu_{j,0}, \nu_{j,1}, \ldots$ are all real. The functions $z^j(t)$ of (1.49) are thus determined by

$$\begin{aligned} \nu_{j,0}\, z^j + \nu_{j,1}(-\mathrm{i}h)\, \dot{z}^j + \nu_{j,2}(-\mathrm{i}h)^2\, \ddot{z}^j + \ldots \\ = h^2 \sum_{m \ge 0} \frac{1}{m!} \sum_{p(\alpha)=j} f^{(m)}(z^0)\, z^\alpha. \end{aligned} \tag{1.51}$$

For $j = 0$, we have from $\rho(1) = \rho'(1) = 0$ and $\rho''(1) = 2\sigma(1) \neq 0$ that

$\nu_{0,0} = \nu_{0,1} = 0$ and $\nu_{0,2} = -1$ so that we get a second order differential equation for $z^0(t)$ which is a perturbation of (1.43). For $0 < |j| \le \ell$, where ζ_j is a simple root of $\rho(\zeta) = 0$, we get a first order differential equation for $z^j(t)$. Finally, for $|j| > \ell$, where $\rho(\zeta_j) \neq 0$ we get an algebraic relation for $z^j(t)$ (to avoid technical difficulties, we assume $\sigma(\zeta_j) \neq 0$ also in this case).

1.5.3 Long-term stability

From now on we assume that the differential equation (1.43) is Hamiltonian, i.e., $f(q) = -\nabla U(q)$. We introduce the extended potential

$$\mathcal{U}(\mathbf{z}) = U(z^0) + \sum_{m \ge 1} \frac{1}{m!} \sum_{p(\alpha)=0} U^{(m)}(z^0) z^\alpha \tag{1.52}$$

in complete analogy to (1.15), so that the relation (1.51) becomes

$$\nu_{j,0}\, z^j + \nu_{j,1}(-\mathrm{i}h)\, \dot z^j + \nu_{j,2}(-\mathrm{i}h)^2\, \ddot z^j + \ldots \;=\; -\,h^2 \nabla_{-k}\, \mathcal{U}(\mathbf{z}). \tag{1.53}$$

Here, the situation is very similar to formula (1.29). In the left-hand side the derivatives of z^j are multiplied with the corresponding power of h, and the coefficients are real for even derivatives and purely imaginary for odd derivatives. To get a conserved quantity close to the Hamiltonian of the system, we take the scalar product of (1.53) with $\dot z^{-j}$ and sum over all $j \in \mathcal{I}$. The same miracle which helped us in Sect.1.3.3 to obtain a conserved quantity, applies also here. We thus get a formally conserved quantity $\mathcal{H}(\mathbf{z}, \dot{\mathbf{z}})$ that is close to the Hamiltonian of the system.

Concerning further conserved quantities of the system (1.53) we encounter a serious difficulty. The extended potential (1.52) is invariant with respect to the transformation $z^j \to \zeta_j^n z^j$ only for integral values of n, so that Noether's theorem cannot be applied. Nevertheless, we take the scalar product of (1.53) with $\mathrm{i}j z^{-j}$, but this time we sum up only the relation for j and that for $-j$ (for $1 \le j \le \ell$). Since $\nu_{j,0} = \nu_{-j,0} = 0$ and $\nu_{j,1} = -\nu_{-j,1} \neq 0$, we obtain as in Sect. 1.3 that the left-hand side is the total derivative of an expression which is close to $ch\|z^j\|^2$ with a constant $c \neq 0$. The dominant term of the right-hand side which, up to the factor $-h^2/2$, equals $U''(z^0)(\mathrm{i}j z^{-j}, z^j) + U''(z^0)(-\mathrm{i}j z^j, z^{-j})$, vanishes due to the symmetry of the Hessian $U''(z^0)$ of the potential. Consequently, all terms of the right-hand side contain at least three times a factor z^j with $j \neq 0$. As long as $\|z^j\| \le \delta$ for $j \neq 0$, we thus get an expression $\mathcal{I}_j(\mathbf{z}, \dot{\mathbf{z}})$ close to $\|z_j\|^2$ whose time derivative is bounded by $\mathcal{O}(h\delta^3)$.

If the starting approximations $q^0, q^1, \ldots, q^{k-1}$ for the multistep formula (1.44) are such that $\|z^j(0)\| \leq \delta$, then the parasitic solutions $z^j(t)$ for $j \neq 0$ remain bounded by 2δ on a time interval of length $\mathcal{O}(h^{-1}\delta^{-1})$. In a typical situation, when the multistep method is of order r and the starting approximations are obtained by a one-step method of order r, we have $\delta = \mathcal{O}(h^{r+1})$. The parasitic solutions are then bounded by $\mathcal{O}(h^{r+1})$ on intervals of length $\mathcal{O}(h^{-r-2})$. This implies that also the Hamiltonian is nearly conserved on a time interval of this length.

A rigorous elaboration of these ideas can be found in the publication [HL04] and in [HLW06, Chap. XV].

Bibliography

[Bam03] D. Bambusi. Birkhoff normal form for some nonlinear PDEs. *Comm. Math. Phys.*, 234:253–285, 2003.

[BG94] G. Benettin and A. Giorgilli. On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms. *J. Statist. Phys.*, 74:1117–1143, 1994.

[BGG87] G. Benettin, L. Galgani, and A. Giorgilli. Realization of holonomic constraints and freezing of high frequency degrees of freedom in the light of classical perturbation theory. Part I. *Comm. Math. Phys.*, 113:87–103, 1987.

[Bou96] J. Bourgain. Construction of approximative and almost periodic solutions of perturbed linear Schrödinger and wave equations. *Geom. Funct. Anal.*, 6:201–230, 1996.

[CHL03] D. Cohen, E. Hairer, and C. Lubich. Modulated Fourier expansions of highly oscillatory differential equations. *Foundations of Comput. Math.*, 3:327–345, 2003.

[CHL05] D. Cohen, E. Hairer, and C. Lubich. Numerical energy conservation for multi-frequency oscillatory differential equations. *BIT*, 45:287–305, 2005.

[CHL07a] D. Cohen, E. Hairer, and C. Lubich. Conservation of energy, momentum and actions in numerical discretizations of nonlinear wave equations. Technical report, Isaac Newton Institute, 2007.

[CHL07b] D. Cohen, E. Hairer, and C. Lubich. Long-time analysis of nonlinearly perturbed wave equations via modulated Fourier expansions. *Arch. Ration. Mech. Anal.*, 2007.

[Deu79] P. Deuflhard. A study of extrapolation methods based on multistep schemes without parasitic solutions. *Z. Angew. Math. Phys.*, 30:177–189, 1979.

[GASSS99] B. García-Archilla, J. M. Sanz-Serna, and R. D. Skeel. Long-time-step methods for oscillatory differential equations. *SIAM J. Sci. Comput.*, 20:930–963, 1999.

[Gau61] W. Gautschi. Numerical integration of ordinary differential equations based on trigonometric polynomials. *Numer. Math.*, 3:381–397, 1961.

[HL97] E. Hairer and C. Lubich. The life-span of backward error analysis for numerical integrators. *Numer. Math.*, 76:441–462, 1997. Erratum: http://www.unige.ch/math/folks/hairer/.

[HL01] E. Hairer and C. Lubich. Long-time energy conservation of numerical methods for oscillatory differential equations. *SIAM J. Numer. Anal.*, 38:414–441, 2001.

[HL04] E. Hairer and C. Lubich. Symmetric multistep methods over long times. *Numer. Math.*, 97:699–723, 2004.

[HL08] E. Hairer and C. Lubich. Spectral semi-discretisations of nonlinear wave equations over long times. *Foundations of Comput. Math.*, 2008.

[HLW03] E. Hairer, C. Lubich, and G. Wanner. Geometric numerical integration illustrated by the Störmer–Verlet method. *Acta Numerica*, 12:399–450, 2003.

[HLW06] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics 31. Springer-Verlag, Berlin, 2nd edition, 2006.

[HNW93] E. Hairer, S. P. Nørsett, and G. Wanner. *Solving Ordinary Differential Equations I. Nonstiff Problems*. Springer Series in Computational Mathematics 8. Springer, Berlin, 2nd edition, 1993.

[HW96] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*. Springer Series in Computational Mathematics 14. Springer-Verlag, Berlin, 2nd edition, 1996.

[Rei99] S. Reich. Backward error analysis for numerical integrators. *SIAM J. Numer. Anal.*, 36:1549–1570, 1999.