Summerschool in Aveiro (Sept. 2018), Ernst Hairer

- **Part I. Geometric numerical integration**
  - Hamiltonian systems, symplectic mappings, geometric integrators, Störmer–Verlet, composition and splitting, variational integrator
  - Backward error analysis, modified Hamiltonian, long-time energy conservation, application to charged particle dynamics

- **Part II. Differential equations with multiple time-scales**
  - Highly oscillatory problems, Fermi–Pasta–Ulam-type problems, trigonometric integrators, adiabatic invariants
  - Modulated Fourier expansion, near-preservation of energy and of adiabatic invariants, application to wave equations

Lecture 3. Highly oscillatory systems

1. **Numerical energy conservation**
   - Molecular dynamics model
   - Oscillatory energy – FPU-type problem
   - Conservation of oscillatory energy (exact solution)

2. **Numerical integrators**
   - Step size restriction for Störmer–Verlet
   - Exponential integrators
   - IMEX (implicit–explicit) integrators
   - Conservation of energies (numerical solution)

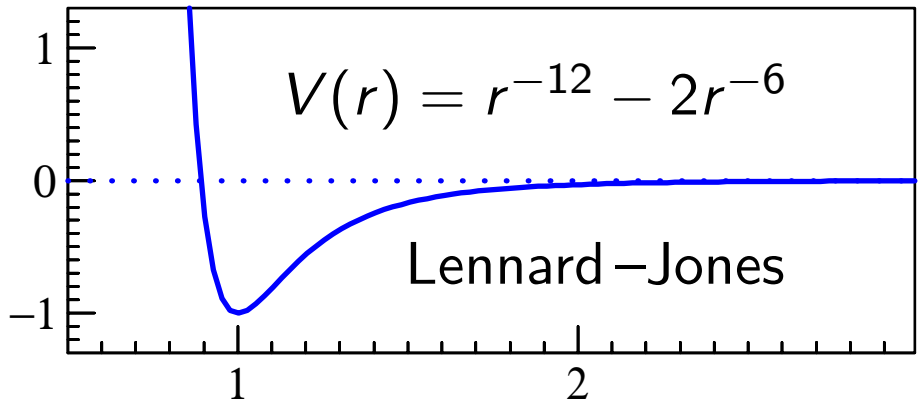
3. **Several high frequencies – resonances**
   - FPU type problem
   - Example with resonant frequencies
   - Numerical energy conservation

Example 1. Molecular dynamics model

Consider the N-body problem

$$\ddot{q} = -\nabla U(q), \qquad U(q) = \sum_{i=2}^{N} \sum_{j=1}^{i-1} V_{ij}\Big(\|q_i - q_j\|\Big),$$

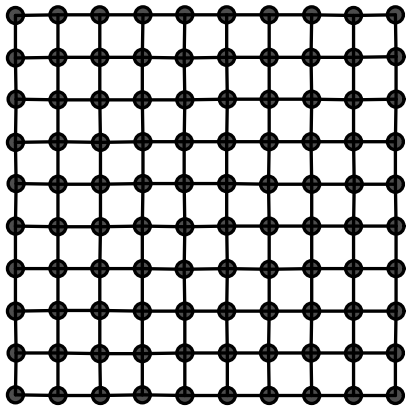
where $V_{ij}(r) = V(r)$



Initial values:

positions q : randomly perturbed values on a grid (see the figure)

momenta $p = \dot{q}$: zero



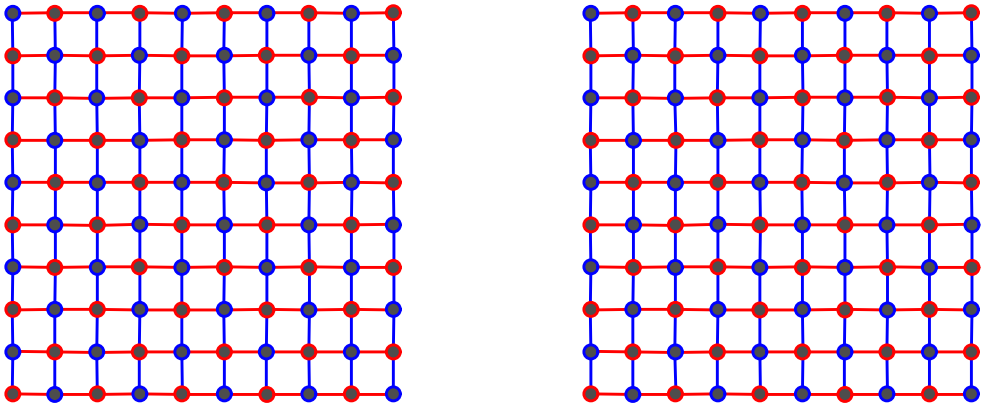
Numerical simulation

Störmer–Verlet method

$$\begin{aligned} p_{n+1/2} &= p_n - \tfrac{h}{2} \nabla U(q_n) \\ q_{n+1} &= q_n + h\, p_{n+1/2} \\ p_{n+1} &= p_{n+1/2} - \tfrac{h}{2} \nabla U(q_{n+1}) \end{aligned}$$

with two different step sizes

$h = 0.08$ $\qquad$ $t = 0.00$ $\qquad$ $h = 0.04$



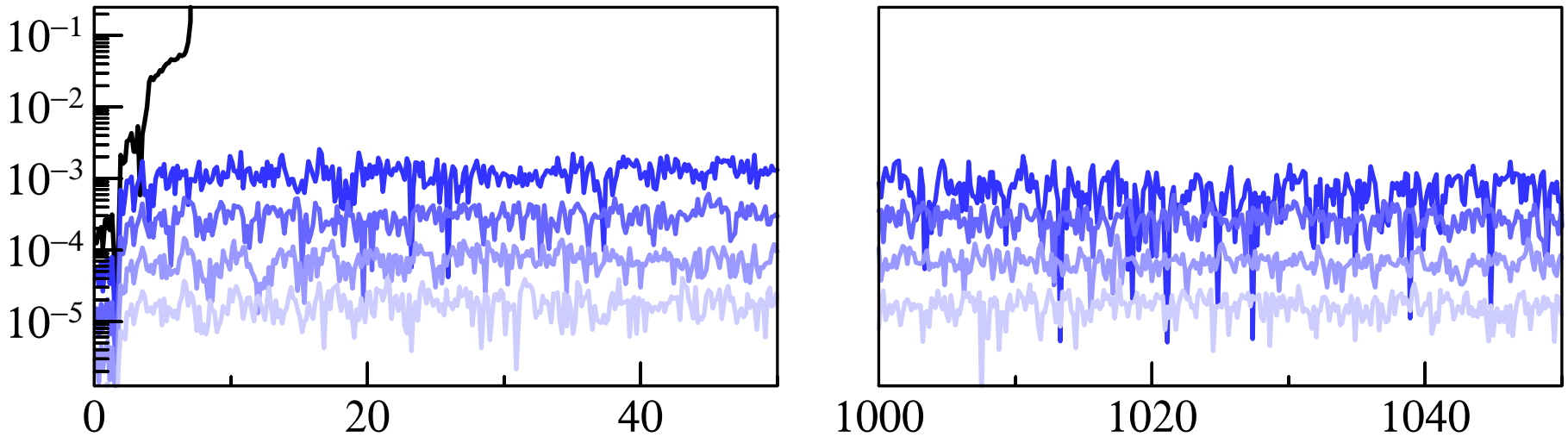
Let us look at the Hamiltonian

We plot the total energy

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

as a function of time for step sizes:

$$h = 0.08 \text{ (black)}, \quad h = 0.04,\ 0.02,\ 0.01,\ 0.005 \text{ (blue)}$$



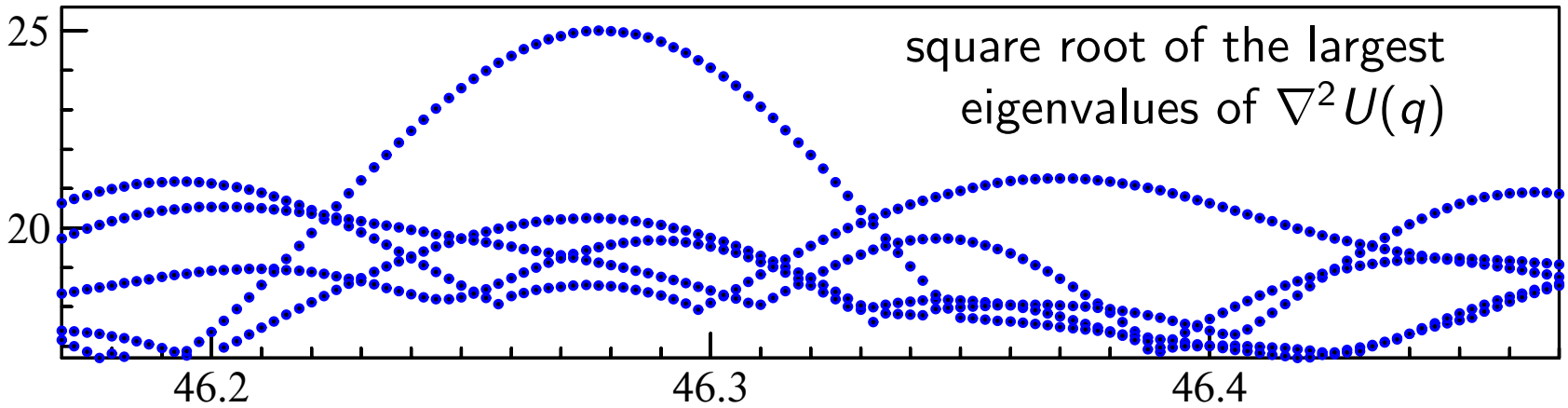
Is the step size small (compared to the frequency)?

For the harmonic oscillator $\ddot{q} = -\omega^2 q$ the Störmer–Verlet scheme leads to the recursion

$$q_{n+1} - 2\Big(1 - \frac{1}{2}(h\omega)^2\Big) q_n + q_{n-1} = 0,$$

which is stable for $0 < h\omega < 2$.

For the N-body problem $\ddot{q} = -\nabla U(q)$ we linearise the vector field, we approximate ω^2 by the largest eigenvalue of the Hessian $\nabla^2 U(q)$, and we approximate ω by the square root of the largest eigenvalues.



The largest ω is between 20 and 25.

In the situation of our experiment we have $\omega_{\max} \approx 25$. Therefore

step sizes $h = 0.08,\ 0.04,\ 0.02,\ 0.01,\ 0.005$

correspond to $h\,\omega_{\max} \approx 2,\ 1,\ 0.5,\ 0.25,\ 0.125$

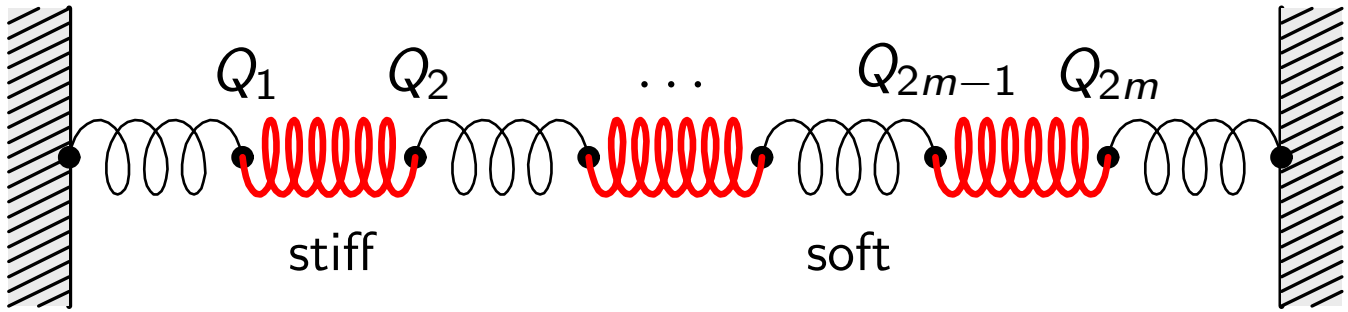
Comments

- **divergence** for $h = 0.08$, because $h\omega \approx 2$ is too close to the linear stability limit
- **backward error analysis** cannot be applied for the considered step sizes, because $h\omega$ is not small

Conclusion

- it is an **open problem** to explain the long-time behaviour of the previous experiment
- Let us turn to **simpler problems** which still have high oscillations.

Example 2. Chain of alternating soft and stiff springs



$$H(Q,\dot{Q}) = \frac{1}{2}\sum_{k=1}^{2m}\dot{Q}_k^2 + \frac{1}{4}\sum_{j=1}^{m}\omega_j^2\,(Q_{2j}-Q_{2j-1})^2 + \sum_{j=0}^{m}(Q_{2j+1}-Q_{2j})^4$$

$q_j = (Q_{2j}-Q_{2j-1})/\sqrt{2}$ compression/extension of a stiff spring

$q_{j+m} = (Q_{2j}+Q_{2j-1})/\sqrt{2}$ its mean position

$$\begin{aligned}\ddot{q}_j + \omega_j^2\, q_j &= -\nabla_j\, U(q)\\ \ddot{q}_{j+m} &= -\nabla_{j+m}\, U(q)\end{aligned} \qquad j = 1,\dots,m$$

Oscillatory energies

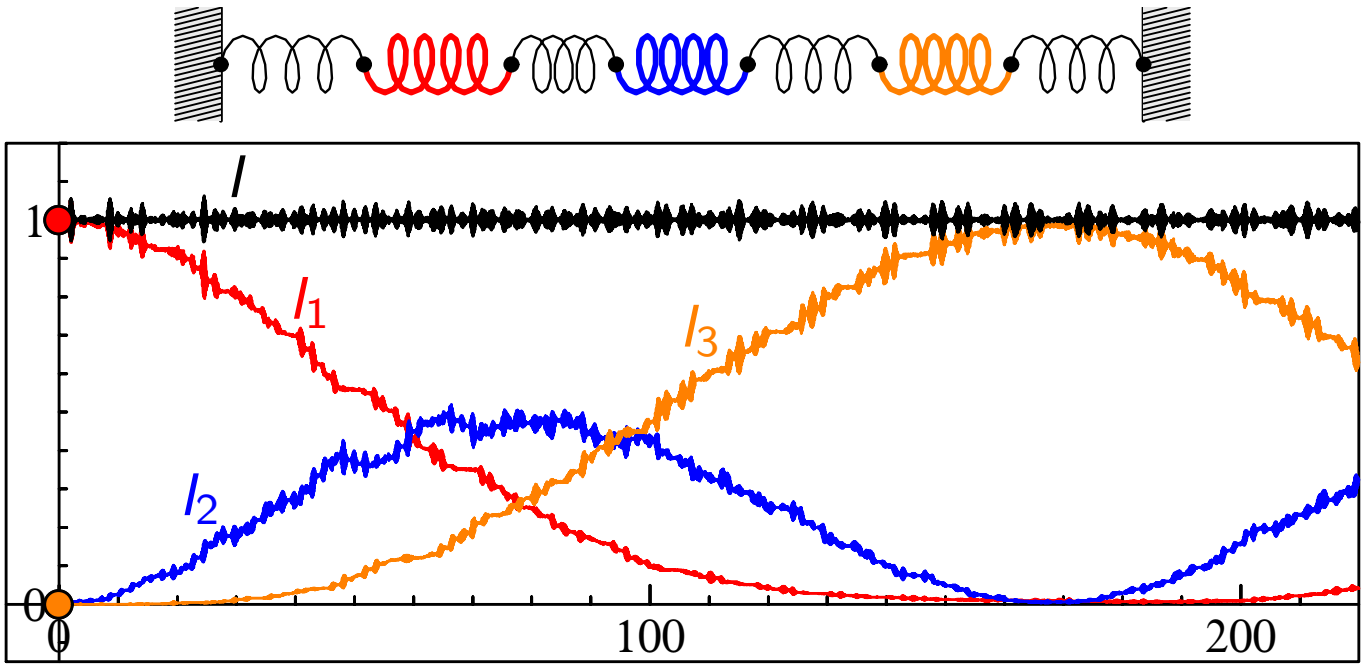
Oscillatory energies of the stiff springs

$$I_j(q_j, \dot{q}_j) = \frac{1}{2}\left(\dot{q}_j^2 + \omega_j^2 q_j^2\right)$$

$$\begin{aligned} \ddot{q}_j + \omega_j^2 q_j &= -\nabla_j U(q) \\ \ddot{q}_{j+m} &= -\nabla_{j+m} U(q) \end{aligned}$$

Total oscillatory energy

$$I(q, \dot{q}) = I_1(q_1, \dot{q}_1) + \ldots + I_m(q_m, \dot{q}_m)$$



Highly oscillatory differential equations

Oscillatory Hamiltonian system $\ddot{q}_j + \omega_j^2\, q_j \;=\; -\,\nabla_j U(q) \qquad j = 0, 1$

Total energy $H(q,\dot{q}) = \frac{1}{2}\Big(|\dot{q}_0|^2 + |\dot{q}_1|^2\Big) + \frac{1}{2}\,\omega^2\,|q_1|^2 + U(q)$

Oscillatory energy $I(q_1,\dot{q}_1) = \frac{1}{2}\Big(|\dot{q}_1|^2 + \omega^2\,|q_1|^2\Big)$

- $\omega_0 = 0$ and $\omega_1 = \omega \geq 1$ arbitrarily large
- there exist $\delta > 0$ and a set K such that the potential U has bounded derivatives of all orders in a δ-neighborhood of $K \times \{0\}$.
- the initial values satisfy

$$q_0(0) = \mathcal{O}(1), \quad \dot{q}_0(0) = \mathcal{O}(1), \quad q_1(0) = \mathcal{O}(\omega^{-1}), \quad \dot{q}_1(0) = \mathcal{O}(1),$$

such that $I\big(q_1(0),\dot{q}_1(0)\big) \leq E$, where the bound E is independent of ω.

Preservation of the oscillatory energy

We know that $H\big(q(t),\dot q(t)\big) - H\big(q(0),\dot q(0)\big) = 0 \qquad \text{for all } t.$

Theorem (Benettin, Galgani & Giorgilli, 1987)

For an arbitrarily fixed integer $N \geq 1$ there exist $C > 0$ and $\omega^* > 0$ such that the following holds for $\omega \geq \omega^*$: along the exact solution the total oscillatory energy deviates from its starting value by no more than

$$\big|I\big(q_1(t),\dot q_1(t)\big) - I\big(q_1(0),\dot q_1(0)\big)\big| \leq C\,\omega^{-1} \quad \text{for} \quad 0 \leq t \leq \omega^N,$$

provided that $q_0(t)$ stays in the set K for such long times. The threshold ω^* and the constant C depend on N, on the energy bound E and on bounds of derivatives of the potential U.

This result explains the excellent long-time preservation of the total oscillatory energy in Example 2 (for the exact solution).

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Step size restriction for Störmer–Verlet

Harmonic oscillator

$$\ddot{q} + \omega^2 q = 0$$

Störmer–Verlet

$$q_{n+1} - 2q_n + q_{n-1} + (h\omega)^2 q_n = 0$$

The characteristic equation of this difference relation is

$$\zeta^2 - 2\Big(1 - \frac{(h\omega)^2}{2}\Big)\zeta + 1 = 0$$

and we have stability (bounded solutions) if and only if

$$\Big|1 - \frac{(h\omega)^2}{2}\Big| < 1 \qquad \text{i.e.} \qquad 0 < h\omega < 2$$

Aim. Consider numerical integrators without such a severe step size restriction.

Exponential integrators

For a system $\ddot{q} + \Omega^2 q = -\nabla U(q)$ we consider

$$q_{n+1} - 2\cos(h\Omega)\, q_n + q_{n-1} = -h^2 \Psi \nabla U(\Phi q_n)$$

$$2h\,\mathrm{sinc}\,(h\Omega)\, p_n = q_{n+1} - q_{n-1}$$

where $\Psi = \psi(h\Omega)$, $\Phi = \phi(h\Omega)$ and $\psi(x)$, $\phi(x)$ are even functions satisfying $\psi(0) = 1$, $\phi(0) = 1$.

Exponential integrators

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where $\Psi = \psi(h\Omega)$, $\Phi = \phi(h\Omega)$ and $\psi(x)$, $\phi(x)$ are even functions satisfying $\psi(0) = 1$, $\phi(0) = 1$.

One-step formulation

$$\begin{aligned} q_{n+1} &= \cos(h\Omega)\, q_n + h\,\mathrm{sinc}\,(h\Omega)\, p_n + \tfrac{1}{2} h^2 \Psi g_n \\ p_{n+1} &= -\Omega \sin(h\Omega)\, q_n + \cos(h\Omega)\, p_n + \tfrac{1}{2} h \left(\Psi_0 g_n + \Psi_1 g_{n+1}\right) \end{aligned}$$

where $g_n = -\nabla U(\phi q_n)$, $\Psi_0 = \psi_0(h\Omega)$, $\Psi_1 = \psi_1(h\Omega)$, and the functions $\psi_0(x)$ and $\psi_1(x)$ are given by

$$\psi(x) = \mathrm{sinc}\,(x)\,\psi_1(x), \qquad \psi_0(x) = \cos(x)\,\psi_1(x).$$

Interpretation as splitting method

The previous one-step formulation can be split into

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} \mapsto \begin{pmatrix} p_n^+ \\ q_n \end{pmatrix} \mapsto \begin{pmatrix} p_{n+1}^- \\ q_{n+1} \end{pmatrix} \mapsto \begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix}$$

where

$$\begin{aligned} p_n^+ &= p_n - \frac{h}{2}\Psi_1 \nabla U(\Phi q_n) \\ p_{n+1} &= p_{n+1}^- - \frac{h}{2}\Psi_1 \nabla U(\Phi q_{n+1}) \end{aligned}$$

and the central mapping is the exact flow of the differential equation $\ddot{q} + \Omega^2 q = 0$.

Exponential integrators

Properties.

- For $\Omega = 0$ we get the Störmer–Verlet method.
- This method is symmetric, and of order 2
- It is symplectic, if and only if $\psi(x) = \operatorname{sinc}(x)\,\phi(x)$
- It is (linearly) unconditionally stable
- it gives the exact solution, when $\nabla U(x) \equiv 0$.

Examples.

(A)	$\psi(x) = \operatorname{sinc}^2(x/2)$	$\phi(x) = 1$	Gautschi (1961)
(B)	$\psi(x) = \operatorname{sinc}(x)$	$\phi(x) = 1$	Deuflhard (1979)
(C)	$\psi(x) = \operatorname{sinc}(x)\,\phi(x)$	$\phi(x) = \operatorname{sinc}(x)$	García-Archilla (1999)
(D)	$\psi(x) = \operatorname{sinc}^2(x)$	$\phi(x) = 1$	H. & Lubich (2000)

IMEX (implicit–explicit) integrators

For a system $\ddot{q} + \Omega^2 q = -\nabla U(q)$ we consider

$$q_{n+1} - 2q_n + q_{n-1} + h^2\Omega^2 q_n + \alpha h^2\Omega^2\big(q_{n+1} - 2q_n + q_{n-1}\big) = -h^2\nabla U(q_n)$$

$$2hp_n = (I + \alpha h^2\Omega^2)(q_{n+1} - q_{n-1})$$

- This method is symmetric, symplectic and of order 2.
- It is linearly stable for $h\omega < 2/\sqrt{1-4\alpha}$ and
- unconditionally stable for $\alpha \geq 1/4$.

Special cases:

$\alpha = 0$: Störmer–Verlet

$\alpha = 1/4$: IMEX scheme (Zhang & Skeel 1997, Stern & Grinspun 2009)

IMEX scheme as modified exponential integrator

modified exponential integrator

$$q_{n+1} - 2\cos(h\widetilde{\Omega})\, q_n + q_{n-1} = -h^2 \widetilde{\Psi} \nabla U(\widetilde{\Phi} q_n)$$
$$2h\, \widetilde{\chi}\, p_n = q_{n+1} - q_{n-1}$$

where $\widetilde{\Psi} = \psi(h\widetilde{\Omega})$, $\widetilde{\Phi} = \phi(h\widetilde{\Omega})$, $\widetilde{\chi} = \chi(h\widetilde{\Omega})$. The modified exponential integrator is symplectic if $\psi(h\omega) = \chi(h\omega)\phi(h\omega)$.

$$q_{n+1} - 2q_n + q_{n-1} + h^2\Omega^2 q_n + \alpha h^2 \Omega^2 \big(q_{n+1} - 2q_n + q_{n-1}\big) = -h^2 \nabla U(q_n)$$
$$2hp_n = (I + \alpha h^2 \Omega^2)(q_{n+1} - q_{n-1})$$

is a modified exponential integrator with $h\widetilde{\omega} \in [0, \pi]$ defined by

$$\cos(h\widetilde{\omega}) = \frac{1 + (\alpha - \frac{1}{2})h^2\omega^2}{1 + \alpha h^2 \omega^2} \quad \text{or equiv.} \quad \sin\Big(\frac{1}{2} h\widetilde{\omega}\Big) = \frac{\frac{1}{2} h\omega}{\sqrt{1 + \alpha h^2 \omega^2}}$$

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

Numerical energy conservation

In addition to the assumption for the analytic solution

we require that

- finite energy $\frac{1}{2}\|\dot{x}(0)\|^2 + \frac{\omega^2}{2}\|x_1(0)\|^2 \leq E$
- non-resonance $|\sin(\frac{h}{2}k\omega)| \geq c\sqrt{h}$ for $k = 1, \ldots N$
- filter functions $|\psi(h\omega)| \leq C_1 \operatorname{sinc}^2(\frac{h\omega}{2}), \ldots$
- the numerical solution Φx_n stays in a compact set
- the condition $h\omega \geq c_0 > 0$

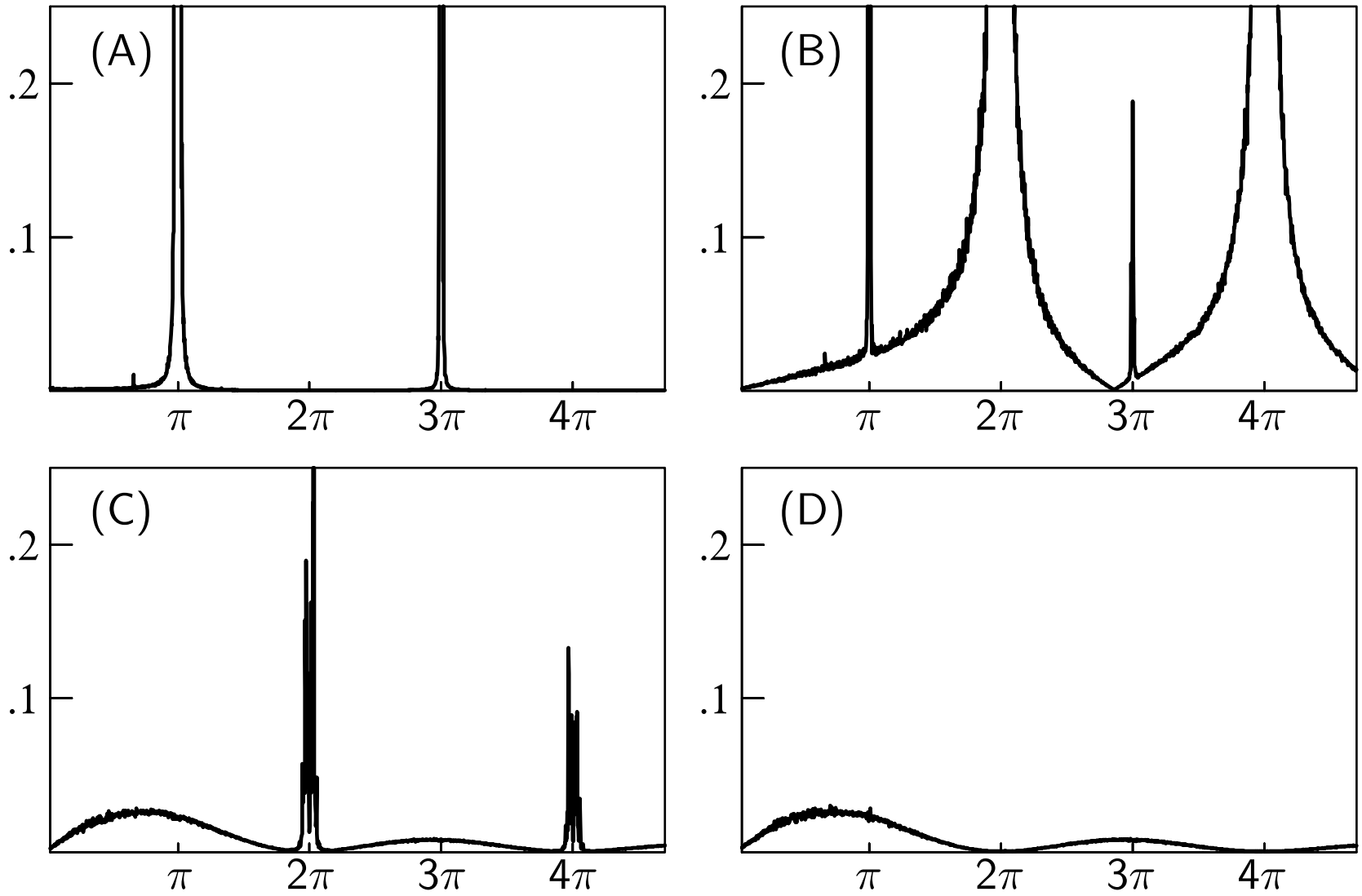
Theorem (H. & Lubich, 2001)

Under these assumptions, we have

$$\begin{aligned} H(q_n, p_n) &= H(q_0, p_0) + \mathcal{O}(h) \\ I(q_n, p_n) &= I(q_0, p_0) + \mathcal{O}(h) \end{aligned} \qquad \text{for} \quad 0 \leq nh \leq h^{-N+1}$$

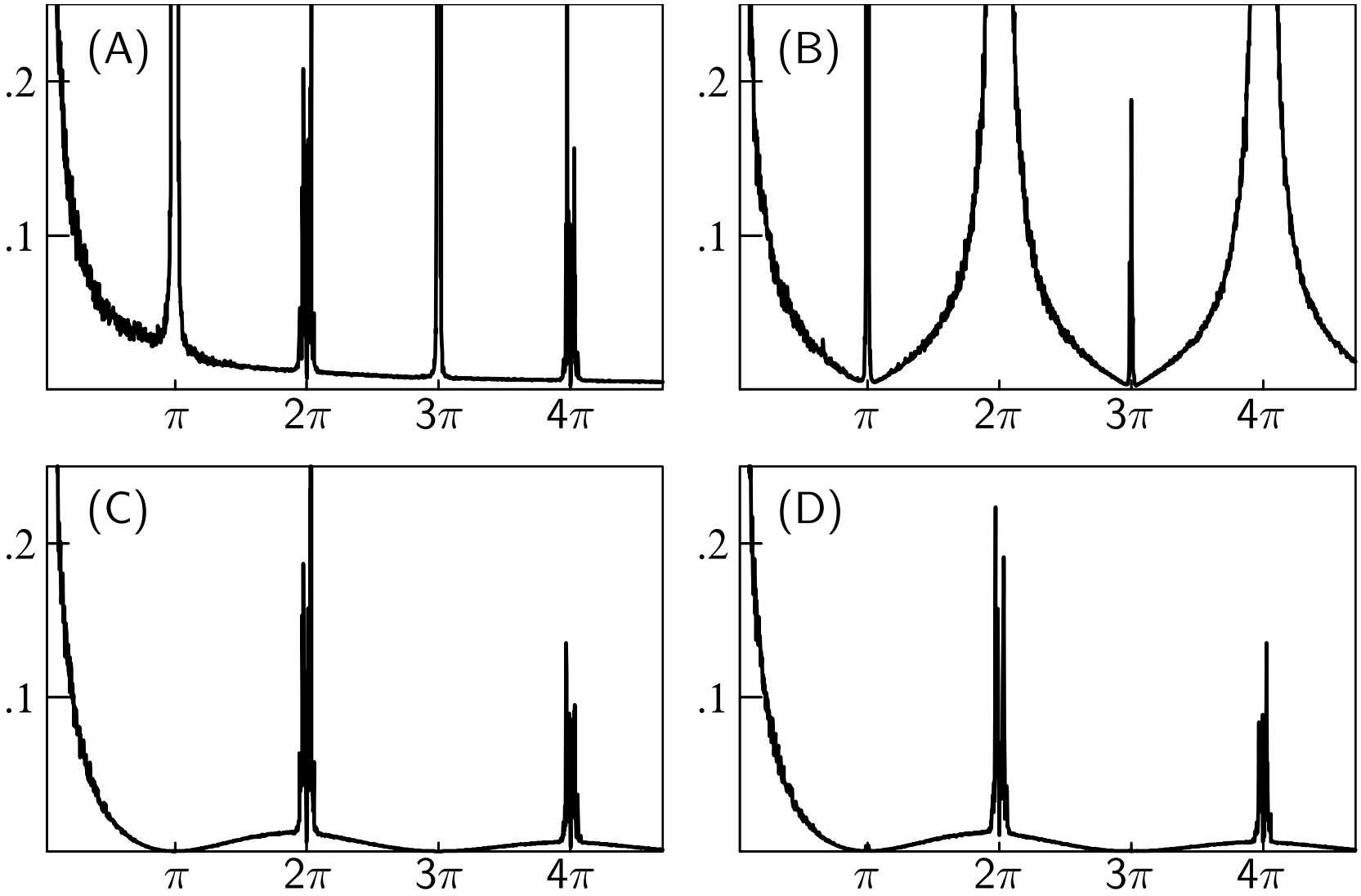
Numerical illustration: Hamiltonian

Error in Hamiltonian as function of $h\omega$ (step size $h = 0.02$)



Numerical illustration: oscillatory energy

Error in oscillatory energy as function of $h\omega$ (step size $h = 0.02$)



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3. **Several high frequencies – resonances**
   - FPU type problem
   - Example with resonant frequencies
   - Numerical energy conservation

FPU type problem

We consider the problem $\ddot{q} + \Omega^2 q = -\nabla U(q)$ where

$$q = \begin{pmatrix} q_0 \\ q_1 \\ \vdots \\ q_\ell \end{pmatrix} \qquad \Omega = \begin{pmatrix} 0 & & & \\ & \omega_1 & & \\ & & \ddots & \\ & & & \omega_\ell \end{pmatrix}$$

It is Hamiltonian with ($\omega_0 = 0$)

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

We assume that the ω_j are well separated, i.e.,

$$\omega_j = \frac{\lambda_j}{\varepsilon}, \qquad 0 < \lambda_1 < \lambda_2 < \ldots < \lambda_\ell, \quad 0 < \varepsilon \ll 1$$

Example with resonant frequencies

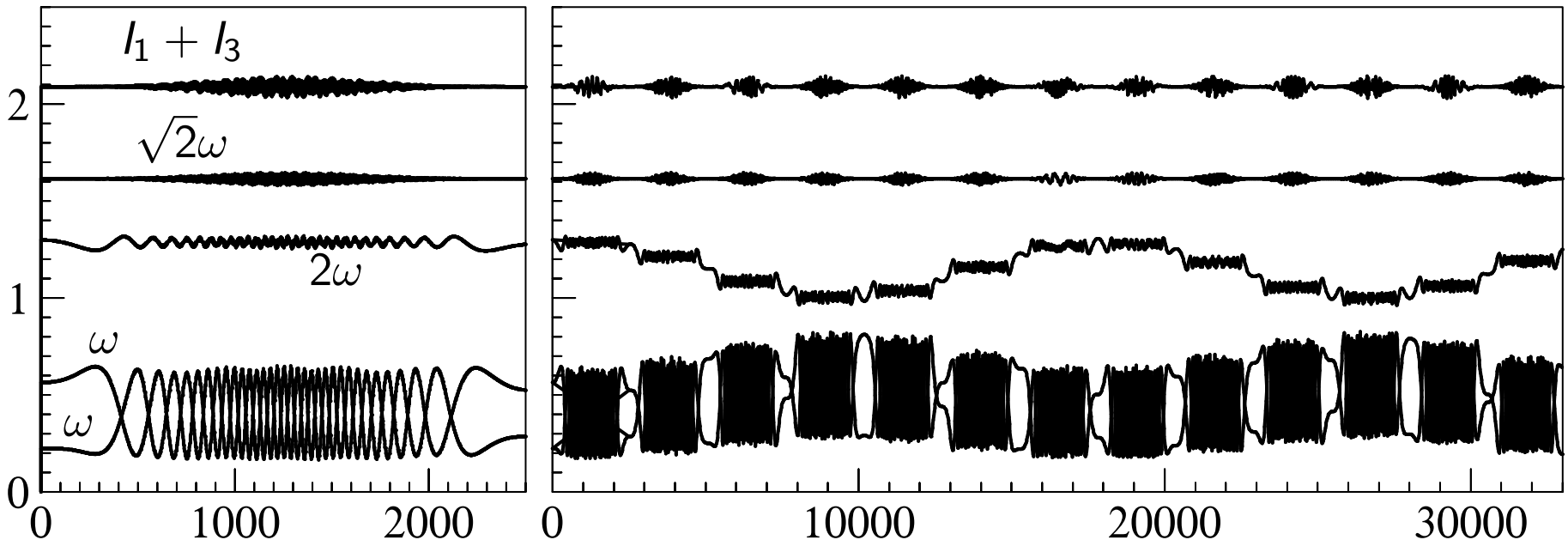
Three frequencies, two of them in resonance:

$$\lambda_1 = 1 \text{ (double)}, \ \lambda_2 = \sqrt{2}, \ \lambda_3 = 2, \qquad \omega = \varepsilon^{-1} = 70.$$

The first one is a double eigenvalue of Ω.

$$U(q) = (0.001q_0 + q_{11} + q_{12} + q_2 + q_3)^4$$

Figure shows the oscillatory energies of all 4 components.



Resonance module

We consider the resonance module

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

For our **example**, where

$$\lambda_1 = 1 \text{ (double)}, \ \lambda_2 = \sqrt{2}, \ \lambda_3 = 2,$$

we have

$$\mathcal{M} = \{(-2k_3, 0, k_3) \ ; \ k_3 \in \mathbb{Z}\}$$

Numerical energy conservation

Theorem (Cohen, H. & Lubich, 2005)

Under suitable assumptions (similar to those for one high frequency), the numerical solution of the exponential integrator satisfies

$$\begin{aligned} H(q_n, \dot{q}_n) &= H(q_0, \dot{q}_0) + \mathcal{O}(h) \\ I_\mu(q_n, \dot{q}_n) &= I_\mu(q_0, \dot{q}_0) + \mathcal{O}(h) \end{aligned} \qquad \text{for} \quad 0 \le nh \le h^{-N+1}$$

for $\mu \in \mathbb{R}^\ell$ *with* $\mu \perp \mathcal{M}_N = \{k \in \mathcal{M}\,;\, |k| \le N\}$, *where*

$$I_\mu(q, \dot{q}) = \sum_{j=1}^{\ell} \frac{\mu_j}{\lambda_j}\, I_j(q_j, \dot{q}_j), \quad I_j(q_j, \dot{q}_j) = \frac{1}{2}\left(\|\dot{q}_j\|^2 + \frac{\lambda_j^2}{\varepsilon^2} \|q_j\|^2 \right)$$

Reference for the analogous result for the analytic solution:

Benettin, Galgani & Giorgilli (1989)

Example (cont.)

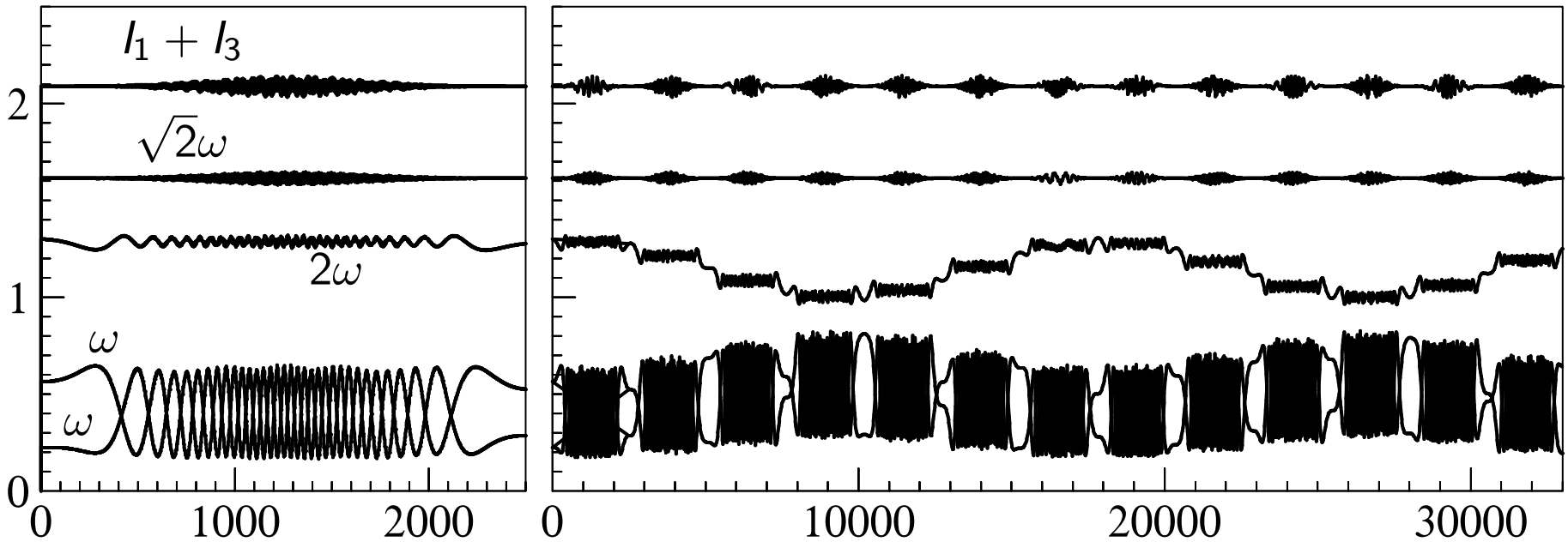
For the previous example, where $\lambda_1 = 1,\ \lambda_2 = \sqrt{2},\ \lambda_3 = 2$, we have

$$\mathcal{M} = \{(-2k_3, 0, k_3)\ ;\ k_3 \in \mathbb{Z}\}$$

and

$$\mathcal{M}^{\perp} = \langle (1, 0, 2), (0, \sqrt{2}, 0) \rangle$$

In this example: $I_1 + I_3$ and I_2 are well conserved.
There is an energy exchange between I_1 and I_3.

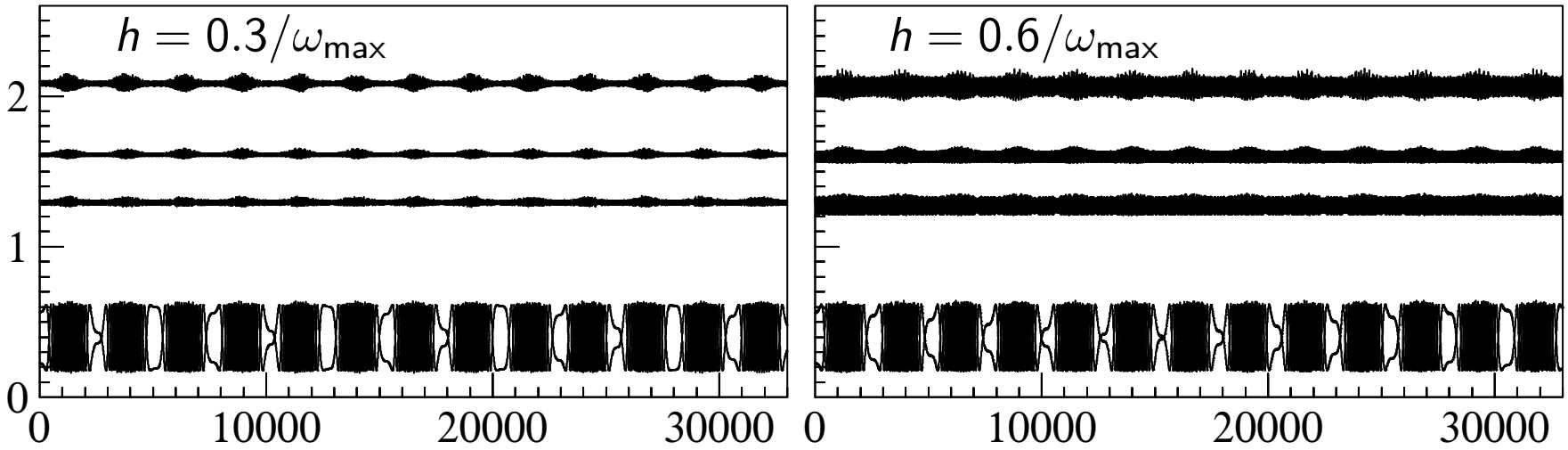


Numerical experiment

Three frequencies, two of them in resonance:

$$\lambda_1 = 1 \ \text{(double)}, \ \lambda_2 = \sqrt{2}, \ \lambda_3 = 2.$$

Oscillatory energies of all 4 components with Störmer–Verlet:



Observation. The numerical solution completely misses the energy exchange between I_1 and I_3. **Why ?**

Numerical experiment – explanation

The Störmer–Verlet method, applied to

$$\ddot{q} + \Omega^2 q = -\nabla U(q) \qquad \text{with} \qquad \Omega = \text{diag}\,(0, \omega_1, \ldots, \omega_\ell)$$

can be interpreted as an exponential integrator with modified frequencies given by

$$\cos(h\widetilde{\omega}_j) = \frac{1 - \frac{1}{2}h^2\omega_j^2}{1 + \frac{1}{2}h^2\omega_j^2} \quad \text{or equiv.} \quad \sin\left(\frac{1}{2}h\widetilde{\omega}_j\right) = \frac{1}{2}h\omega_j.$$

The frequencies $\omega_1 = 1$ and $\omega_3 = 2$ are in resonance, but the modified frequencies $\widetilde{\omega}_1$ and $\widetilde{\omega}_3$ are not.