Trondheim, October 18, 2006

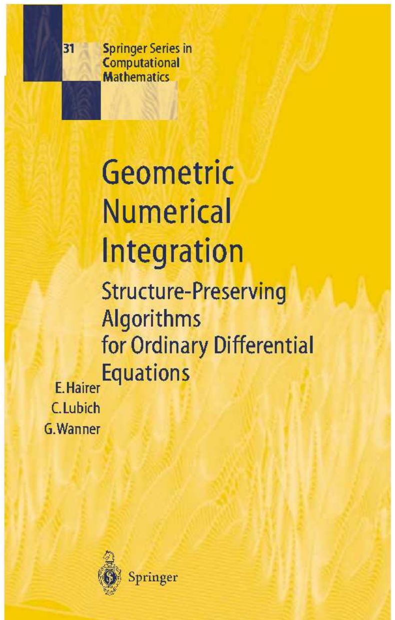
# A lot of oscillations . . .

David Cohen, Trondheim

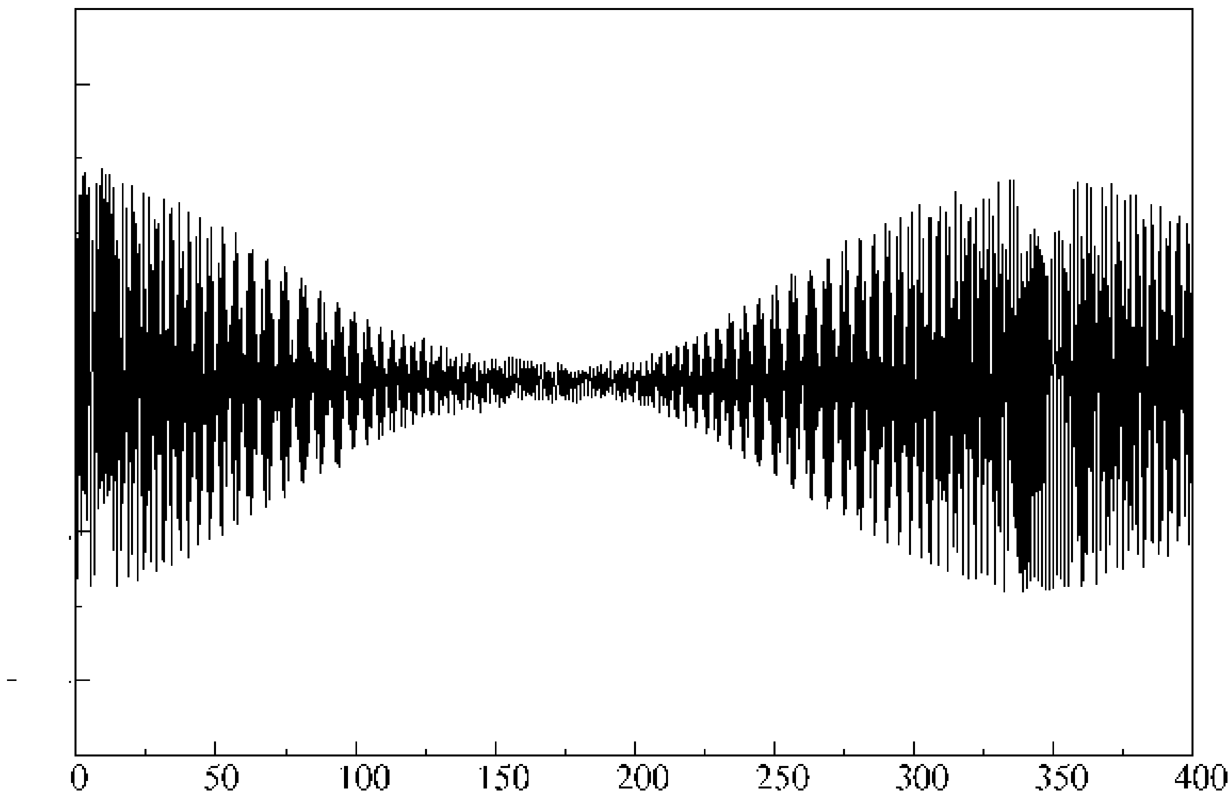
Joint work with E. Hairer & C. Lubich

# Outline

- Highly oscillatory systems with one frequency
- The numerical schemes
- Several high frequencies
- Systems with non-constant mass matrix
- Infinitely many frequencies



# I. Highly oscillatory systems with one frequency



# The problem

We consider Hamiltonian problems with

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

where $\Omega = \begin{pmatrix} 0 & 0 \\ 0 & \omega I \end{pmatrix}$, $x = (x_1, x_2)$ and $\omega \gg 1$.

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The equations of motion are

$$\begin{aligned} \tfrac{d}{dt}\dot{x} &= -\nabla_x H(x,\dot{x}) = -\Omega^2 x - \nabla_x U(x) \\ \tfrac{d}{dt}x &= \nabla_{\dot{x}} H(x,\dot{x}) = \dot{x}, \end{aligned}$$

or

$$\ddot{x} + \Omega^2 x = -\nabla_x U(x).$$

# An example

Recall

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**Example**: Modified Fermi-Pasta-Ulam problem (FPU).

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**Example**: Modified Fermi-Pasta-Ulam problem (FPU).

We are interested in the almost conservation of the oscillatory energy

$$I(x, \dot{x}) = \frac{1}{2}\dot{x}_2^T \dot{x}_2 + \frac{\omega^2}{2} x_2^T x_2.$$

# The result

Assumptions:

- Bounded initial energy $H(x(0), \dot{x}(0)) \leq E$ (indep. of $\omega \gg 1$).
- The potential $U$ is analytic and bounded.

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- Bounded initial energy $H(x(0), \dot{x}(0)) \leq E$ (indep. of $\omega \gg 1$).
- The potential $U$ is analytic and bounded.

Result:

$$|I(x(t), \dot{x}(t)) - I(x(0), \dot{x}(0))| \leq \mathit{Const} \cdot \omega^{-1}$$

for exponentially long times $t \leq \mathrm{e}^{c \cdot \omega}$.

Benettin, Galgani, Giorgilli 1987 (Hamiltonian perturbation theory).

C, Hairer, Lubich 2003 (modulated Fourier expansion).

# The modulated Fourier expansion (I)

Motivation:

For a linear ODE $\ddot{x}(t) + \omega^2 x(t) = g(t)$.

Particular sol.: $x_P(t) = c_0(t) + \omega^{-1} c_1(t) + \omega^{-2} c_2(t) + \ldots$.

Homogeneous sol.: $x_H(t) = d_1 \mathrm{e}^{\mathrm{i}\omega t} + d_2 \mathrm{e}^{-\mathrm{i}\omega t}$.

The solution of the linear ODE is given by

$$x(t) = x_P(t) + x_H(t) = y(t) + \mathrm{e}^{\mathrm{i}\omega t} z(t) + \mathrm{e}^{-\mathrm{i}\omega t} \bar{z}(t),$$

with $y(t), z(t)$ smooth functions, i.e. with derivatives bounded independently of $\omega \gg 1$.

# The modulated Fourier expansion (II)

For more complicated problems, the solution admits, on a short time interval, the following expansion, for (an arbitrary large) $N \geq 1$,

$$x(t) = y(t) + \sum_{0<|k|<N} \mathrm{e}^{\mathrm{i}k\omega t} z^k(t) + \mathcal{O}(\omega^{-N}).$$

with $z^0(t) = y(t), z^k(t)$ smooth functions satisfying $\overline{z^k}(t) = z^{-k}(t)$.

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with $z^0(t) = y(t), z^k(t)$ smooth functions satisfying $\overline{z^k}(t) = z^{-k}(t)$.

We find the modulation functions $z^k$ by inserting the MFE into our ODE

$$\ddot{x} + \Omega^2 x = g(x) := -\nabla U(x).$$

# The modulated Fourier expansion (III)

$$\begin{pmatrix} \ddot{y}_1 \\ \omega^2 y_2 \end{pmatrix} + \begin{pmatrix} 0 \\ \ddot{y}_2 \end{pmatrix} = g(y) + \sum_{s(\alpha)=0} \frac{1}{m!} g^{(m)}(y) z^\alpha$$

$$\begin{pmatrix} -\omega^2 z_1^1 \\ 2\mathrm{i}\omega \dot{z}_2^1 \end{pmatrix} + \begin{pmatrix} 2\mathrm{i}\omega \dot{z}_1^1 \\ \ddot{z}_2^1 \end{pmatrix} = \sum_{s(\alpha)=1} \frac{1}{m!} g^{(m)}(y) z^\alpha$$

$$\begin{pmatrix} -k^2\omega^2 z_1^k \\ (1-k^2)\omega^2 z_2^k \end{pmatrix} + \begin{pmatrix} 2\mathrm{i}k\omega \dot{z}_1^k + \ddot{z}_1^k \\ 2\mathrm{i}k\omega \dot{z}_2^k + \ddot{z}_2^k \end{pmatrix} = \sum_{s(\alpha)=k} \frac{1}{m!} g^{(m)}(y) z^\alpha$$

where for the multi-indices $\alpha = (\alpha_1, \ldots, \alpha_m)$, with integers $\alpha_j$, we denote $s(\alpha) = \sum_j \alpha_j$ and $g^{(m)}(y) z^\alpha = g^{(m)}(y)(z^{\alpha_1}, \ldots, z^{\alpha_m})$.

# The modulated Fourier expansion (IV)

We thus obtain

$$
\begin{aligned}
\ddot{y}_1 &= F_{10}(y_1, \dot{y}_1, z_2^1) \\
&+ \omega^{-1} F_{11}(y_1, \dot{y}_1, z_2^1) + \ldots && \text{second order ODE} \\
\omega \dot{z}_2^1 &= \ldots && \text{first order ODE} \\
\omega^2 z_j^k &= \ldots && \text{algebraic equations.}
\end{aligned}
$$

In general, these formal series (in power of $\omega^{-1}$) diverge.

# MFE:Hamiltonian structure of the modulation system

Let us note the MFE $x_*(t) = \sum_k z^k(t)\mathrm{e}^{\mathrm{i}k\omega t} = \sum_k y^k(t)$, and $\mathbf{y} = (y^k)$.

By construction, the coefficients $y^k$ verify

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

for an extended potential $\mathcal{U}(\mathbf{y})$.

This system is Hamiltonian for

$$\mathcal{H}(\mathbf{y}, \dot{\mathbf{y}}) = \sum_k \frac{1}{2}(\dot{y}^k)^T \dot{y}^k + \frac{1}{2}(y^k)^T \Omega^2 y^k + \mathcal{U}(\mathbf{y}).$$

# Conservation of the oscillatory energy

The system that define the modulation functions has a formal invariant

$$\mathcal{I}(\mathbf{y}, \dot{\mathbf{y}}) = -\mathrm{i}\omega \sum_k k(y^{-k})^T \dot{y}^k.$$

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- $\mathcal{I}$ is close to the oscillatory energy $I$:
  $\mathcal{I}(\mathbf{y}(t), \dot{\mathbf{y}}(t)) = I(x(t), \dot{x}(t)) + \mathcal{O}(\omega^{-1})$ for $0 \le t \le 1$.

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- $I(x(t), \dot{x}(t)) = I(x(0), \dot{x}(0)) + \mathcal{O}(\omega^{-1})$ for $0 \leq t \leq \omega^N$.

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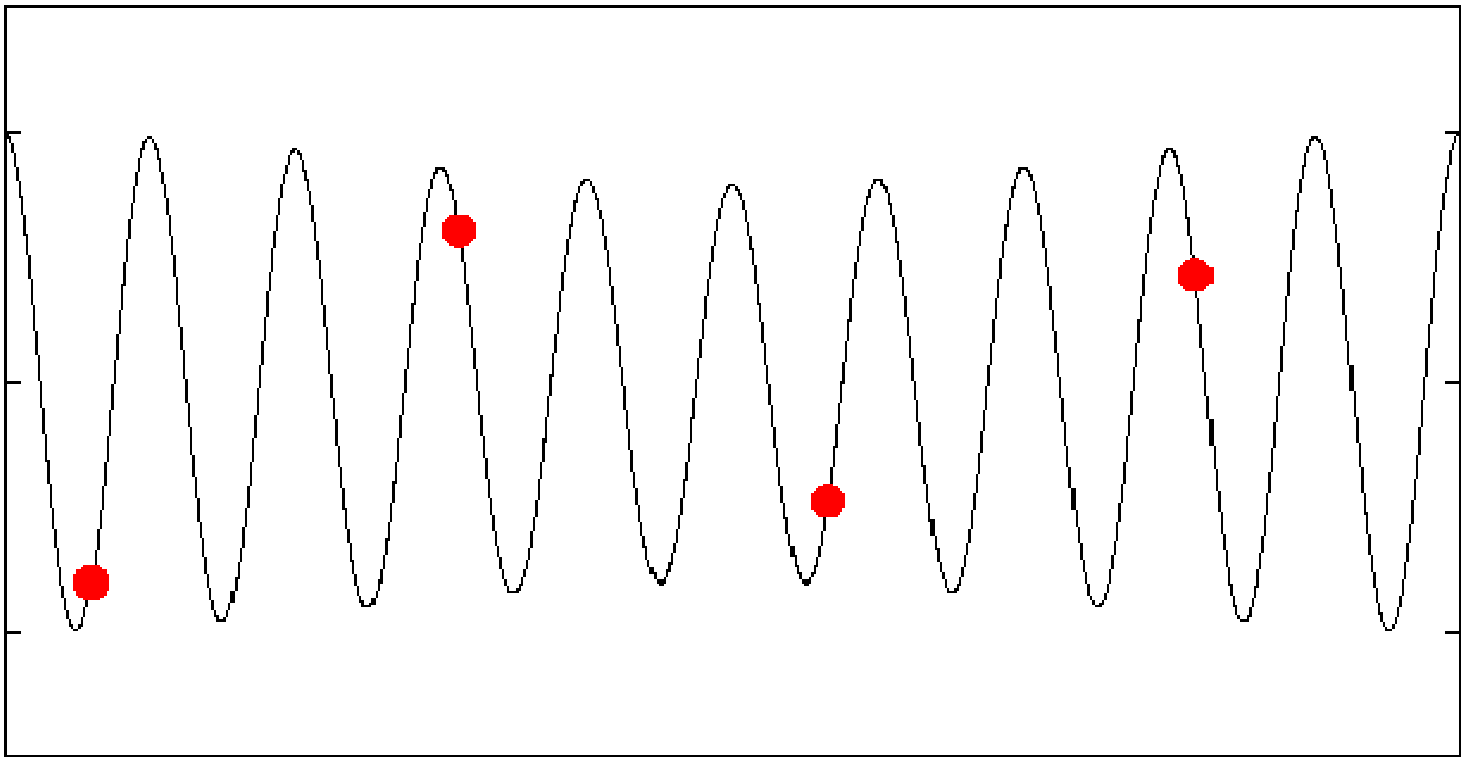
- $I(x(t),\dot{x}(t)) = I(x(0),\dot{x}(0)) + \mathcal{O}(\omega^{-1})$ for $0 \le t \le \mathrm{e}^{c\cdot\omega}$.

# II. The numerical schemes



# The Störmer-Verlet scheme

Recall

$$\ddot{x} = -\Omega^2 x - \nabla_x U(x).$$

Störmer-Verlet scheme (1907-1967) :

$$x_{n+1} - 2x_n + x_{n-1} = -h^2(\Omega^2 x_n + \nabla_x U(x_n))$$

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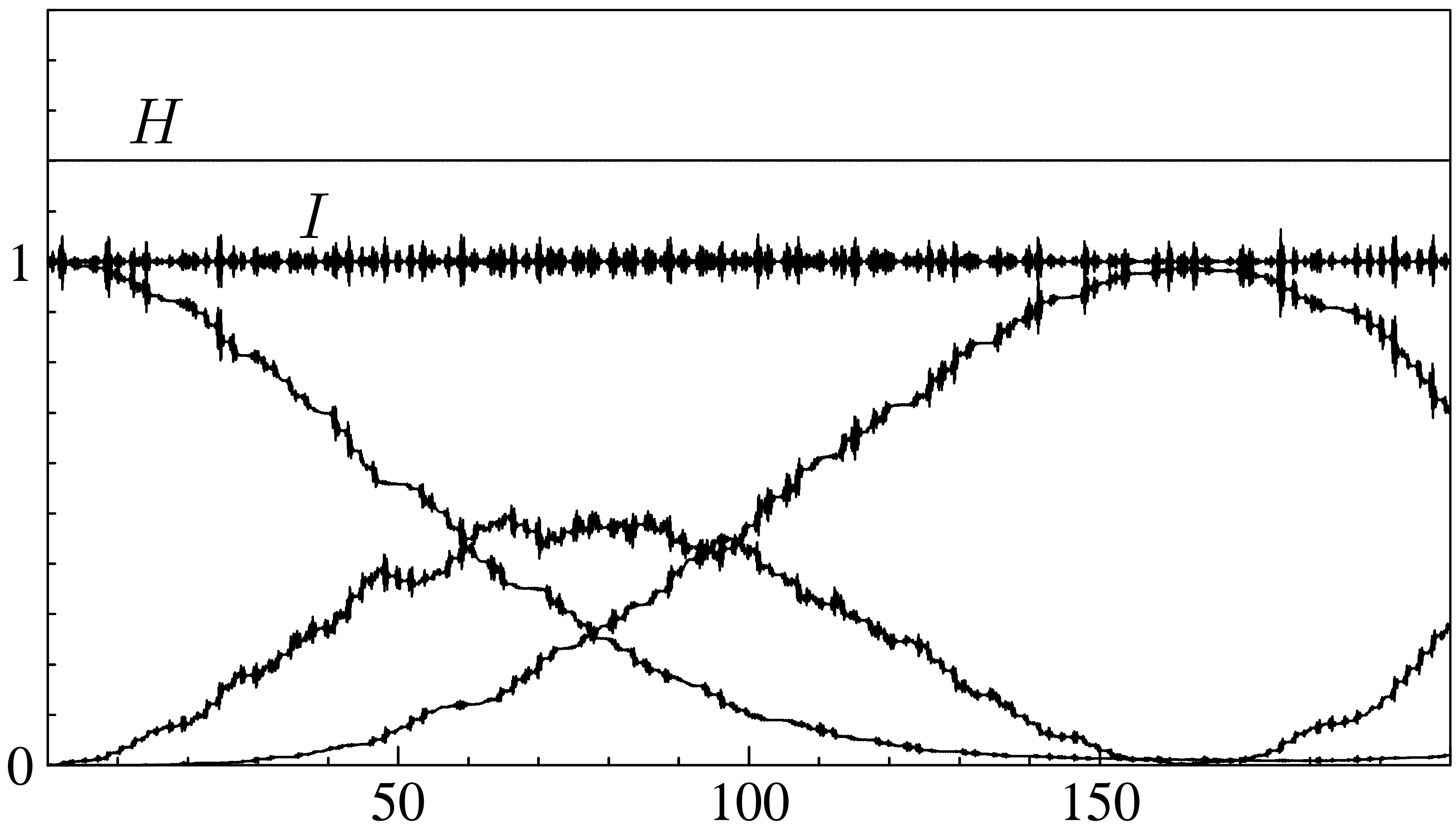
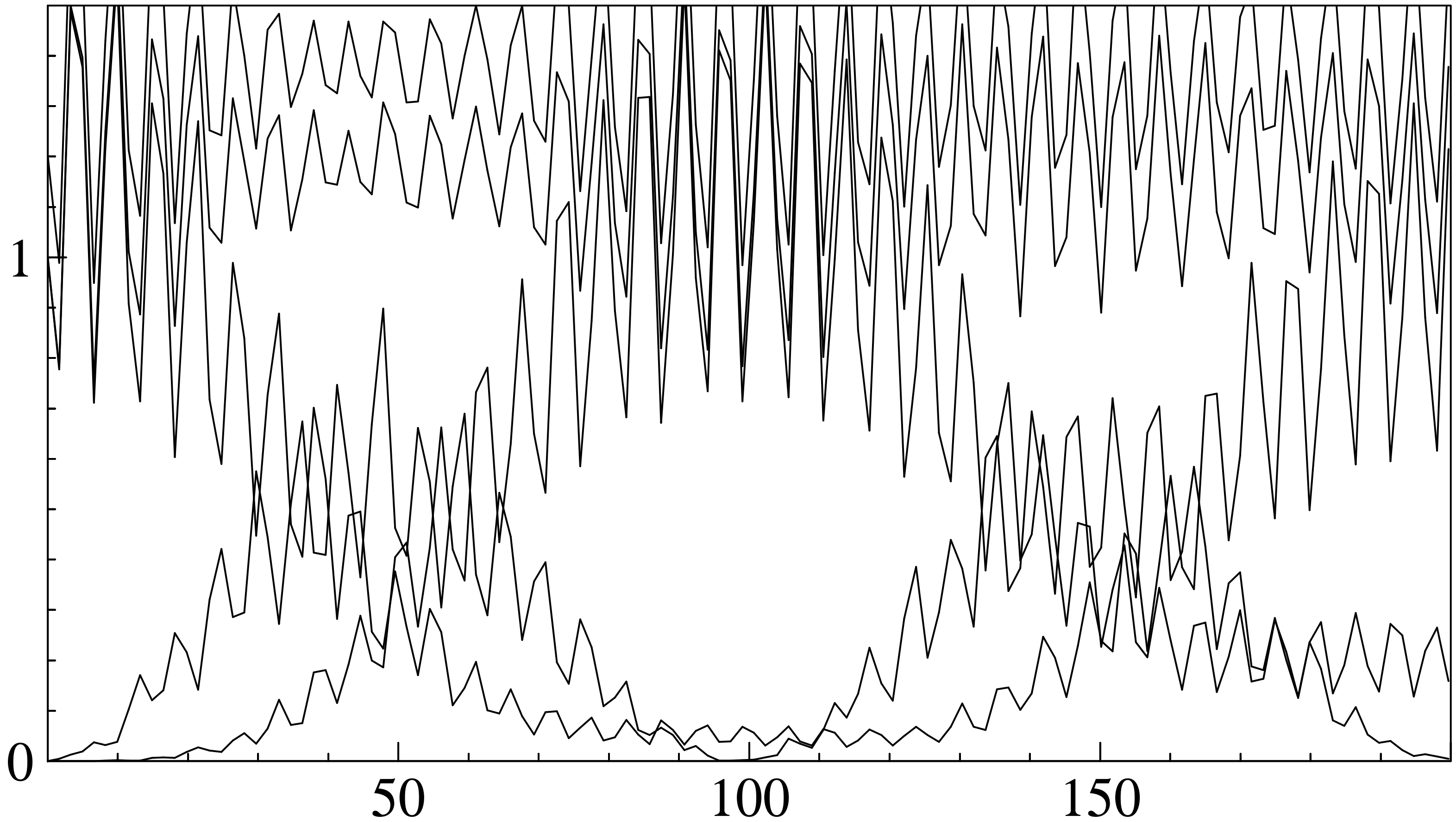



Störmer-Verlet, $h = 0.001$, $\omega = 50$

# The Störmer-Verlet scheme

Step size restriction for Störmer-Verlet: $h\omega < 2$




Störmer-Verlet, $h = 0.03$, $\omega = 50$

# The trigonometric methods

$$\ddot{x} = -\Omega^2 x - \nabla U(x), \qquad \frac{\mathrm{d}}{\mathrm{dt}}\begin{pmatrix} x \\ \dot{x} \end{pmatrix} = \begin{pmatrix} 0 & I \\ -\Omega^2 & 0 \end{pmatrix}\begin{pmatrix} x \\ \dot{x} \end{pmatrix} + \begin{pmatrix} 0 \\ g(x) \end{pmatrix}.$$

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By the variation of constants formula, the solution satisfies

$$\begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix} = \begin{pmatrix} \cos(t\Omega) & \Omega^{-1}\sin(t\Omega) \\ -\Omega\sin(t\Omega) & \cos(t\Omega) \end{pmatrix}\begin{pmatrix} x_0 \\ \dot{x}_0 \end{pmatrix} + \int_0^t \mathrm{R}(t-s)\begin{pmatrix} 0 \\ g(x(s)) \end{pmatrix}\mathrm{d}s,$$

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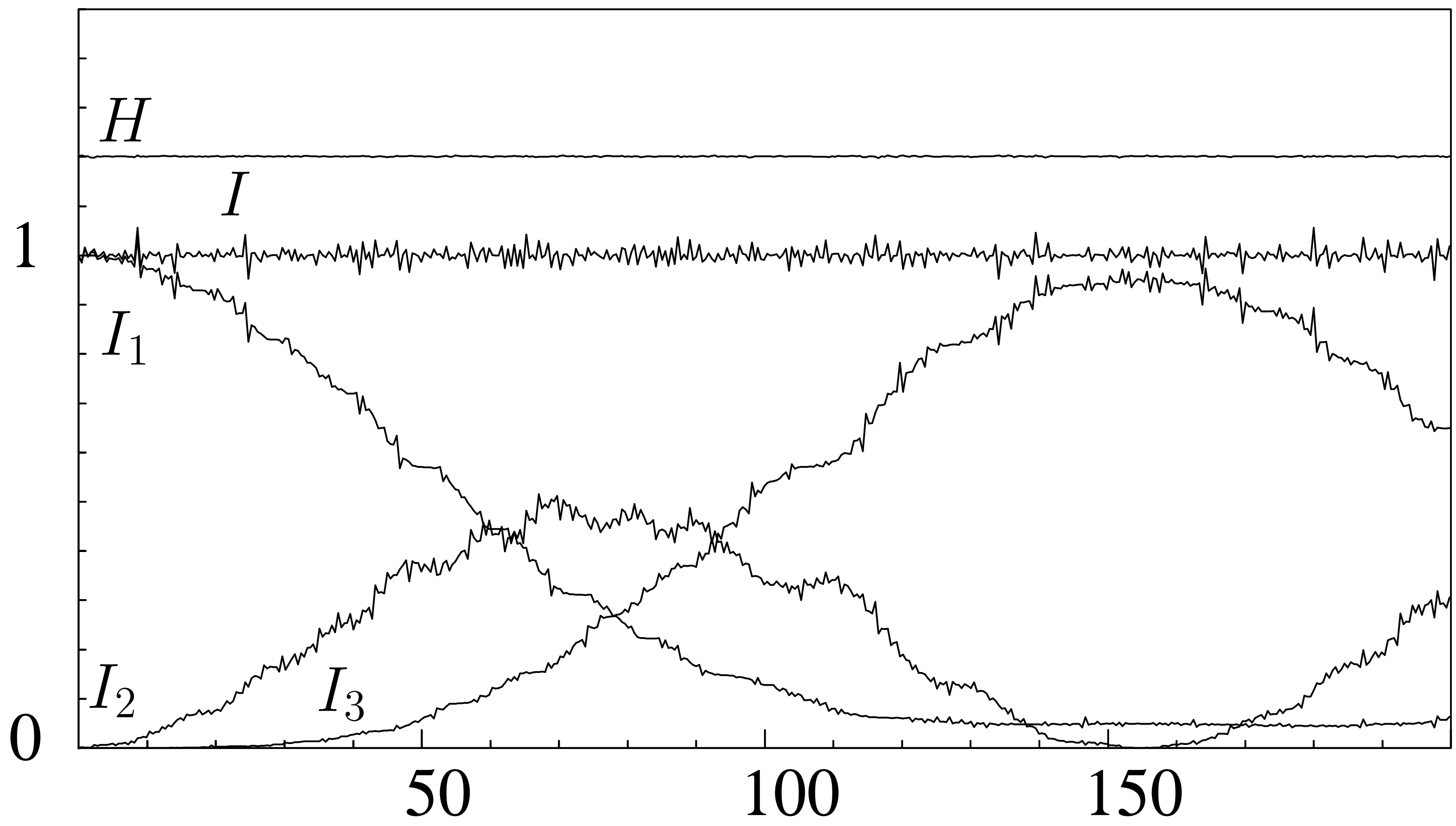
Trigonometric methods (Gautschi, Hairer, Hochbruck, Lubich, Sanz-Serna, . . . ):

$$\begin{aligned} x_{n+1} &= \cos(h\Omega)x_n + \Omega^{-1}\sin(h\Omega)\dot{x}_n + \frac{h^2}{2}\Psi g_n \\ \dot{x}_{n+1} &= -\Omega\sin(h\Omega)x_n + \cos(h\Omega)\dot{x}_n + \frac{h}{2}(\Psi_0 g_n + \Psi_1 g_{n+1}) \end{aligned}$$

where $g_n = g(\phi(h\Omega)x_n)$ and $\phi, \psi, \ldots$ are some filter functions.

# The trigonometric methods




Hochbruck, Lubich, $h = 0.03$

# The results

Assumptions:

- Bounded initial energy $H(x_0, \dot{x}_0) \leq E$ (indep. of $\omega \gg 1$).
- Conditions on the filter functions (not symplectic).
- $h\omega \geq c_0 > 0$.
- Non-resonance condition: $|\sin(\frac{1}{2}hk\omega)| \geq c\sqrt{h}$ for $k = 1, \ldots, N$.

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Results:

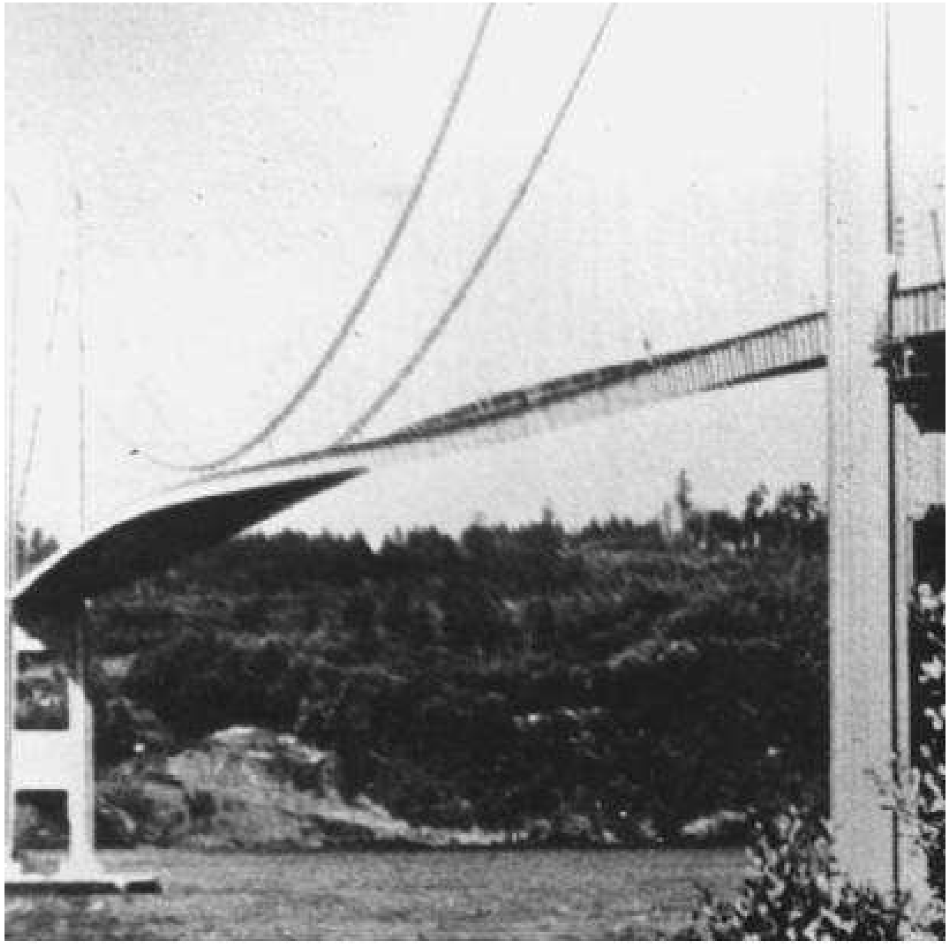
Near-conservation of the total energy $H$ and of the oscillatory energy $I$ for long time intervals $0 \leq t \leq h^{-N+1}$.

Hairer & Lubich 2000.

Proof:

We adapt the techniques of the first part !

# III. Several high frequencies



# Several frequencies

We consider

$$\ddot{x} + \Omega^2 x = -\nabla U(x)$$

where $\Omega = \text{diag}(\omega_j I)$, with $\omega_j = \lambda_j/\varepsilon$, $\lambda_0 = 0$, $\lambda_j \geq 1$ for $j = 1, \dots, \ell$, and $\varepsilon \ll 1$.

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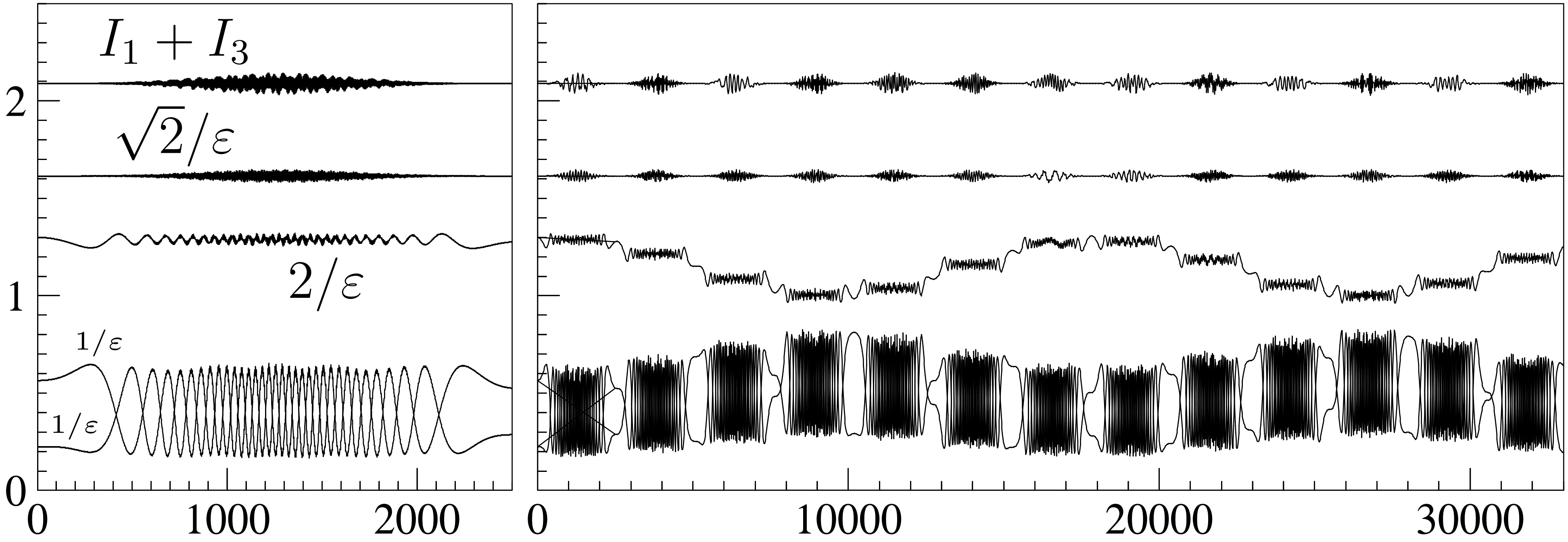
We are interested in the near-conservation of the oscillatory energy of the $j^{th}$ frequency

$$I_j(x, \dot{x}) = \frac{1}{2}||\dot{x}_j||^2 + \frac{1}{2}\frac{\lambda_j^2}{\varepsilon^2}||x_j||^2.$$

And, for $\mu = (\mu_1, \ldots, \mu_\ell)$ in $I_\mu(x, \dot{x}) = \sum_{j=1}^{\ell} \frac{\mu_j}{\lambda_j} I_j(x, \dot{x})$. In particular, $\mu = \lambda$ —–> total oscillatory energy.

# Several frequencies




$$\lambda = (1, 1, \sqrt{2}, 2), \varepsilon = 70^{-1}$$

# Several frequencies: results

Assumptions:

- Bounded initial energy $H(x(0), \dot{x}(0)) \leq E$ (indep. of $\varepsilon \ll 1$).
- Weak non-resonance condition: $|k \cdot \lambda| \geq c\sqrt{\varepsilon}$ for $k \in \mathbb{Z}^\ell \backslash \mathcal{M}$, $|k| \leq N$ where $\mathcal{M} = \{k \in \mathbb{Z}^\ell : k_1\lambda_1 + \ldots + k_\ell\lambda_\ell = 0\}$.

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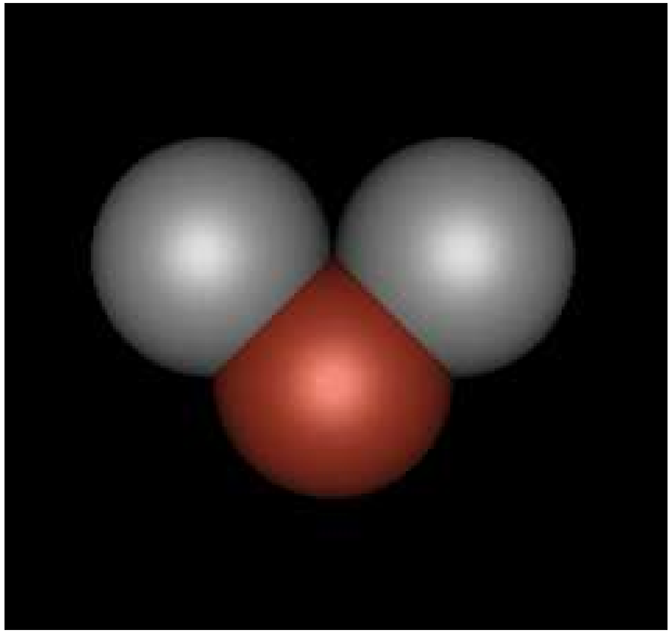
Results:

- $I_j(x(t),\dot{x}(t)) = I_j(x(0),\dot{x}(0)) + \mathcal{O}(\varepsilon)$ for $t \le \varepsilon^{-K+1}$ with $K = \min(N, M+1)$ where $M = \min\{|k| : 0 \ne k \in \mathcal{M}\}$.
- $I_\mu(x(t),\dot{x}(t)) = I_\mu(x(0),\dot{x}(0)) + \mathcal{O}(\varepsilon)$ for $t \le \varepsilon^{-N+1}$ and $\mu \perp \mathcal{M}_N = \{k \in \mathcal{M} : |k| \le N\}$.
- Also for the numerical solution (cond. on the filters and some num. non-resonance condition).
  C., Hairer, Lubich 2005. Benettin, Galgani, Giorgilli 1989.

# IV. Systems with non-constant mass matrix



# The problem

$$H(p,q) = T(p,q) + \frac{\omega^2}{2} q^T A q + U(q), \text{ with } \omega \gg 1.$$

Where $A = \begin{pmatrix} 0 & 0 \\ 0 & A_+ \end{pmatrix}$, with $A_+$ symmetric positive definite

$$T(p,q) = \frac{1}{2} p_1^T M_1(q)^{-1} p_1 + \frac{1}{2} p_2^T p_2 + \frac{1}{2} p^T R(q) p,$$

$M_1(q)$ symmetric positive definite matrix,

$R(q)$ symmetric with $R(q_1, 0) = 0$.

**Examples** : Triatomic molecule, Elastic dumbbell spacecraft

# The results

$$H(p,q) = \frac{1}{2} p_1^T M_1(q)^{-1} p_1 + \frac{1}{2} p^T R(q) p + \frac{1}{2} p_2^T p_2 + \frac{\omega^2}{2} q_2^T q_2 + U(q)$$

$$I(p,q) = \frac{1}{2} p_2^T p_2 + \frac{\omega^2}{2} q_2^T q_2$$

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- num. sol.: near cons. of $H$ and $I$ over long time intervals.

  C. $2004 - 2005$.

# Some ideas

**Problem:**

$$H(p,q) = \frac{1}{2}p_1^T M_1(q)^{-1} p_1 + \frac{1}{2}p^T R(q) p + \frac{1}{2}p_2^T p_2 + \frac{\omega^2}{2} q_2^T q_2 + U(q).$$

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- Adapt the trigonometric methods (splitting+mix, explicit).
- Find a modulated Fourier expansion (short time interval).
- Find two formal invariants $\widehat{\mathcal{H}}_h$ and $\widehat{\mathcal{I}}_h$ for the modulated functions.
- Near conservation of $H$ and $I$ for the numerical methods over long time intervals.

# V. Infinitely many frequencies

# The nonlinear wave equation

A pseudo-spectral discretisation in space of the nonlinear equation

$$u_{tt}(t,x) - u_{xx}(t,x) + \rho u(t,x) - g(u(t,x)) = 0$$

leads to

$$\ddot{q}(t) + \Omega^2 q(t) = \mathcal{F} g(\mathcal{F}^{-1} q(t)),$$

where $q$ is the vector of Fourier coefficients, $\mathcal{F}$ is the Fourier series and

$$\Omega = diag(\omega_j I) \text{ with } \omega_j = \sqrt{\rho + j^2}.$$

# Conservation properties

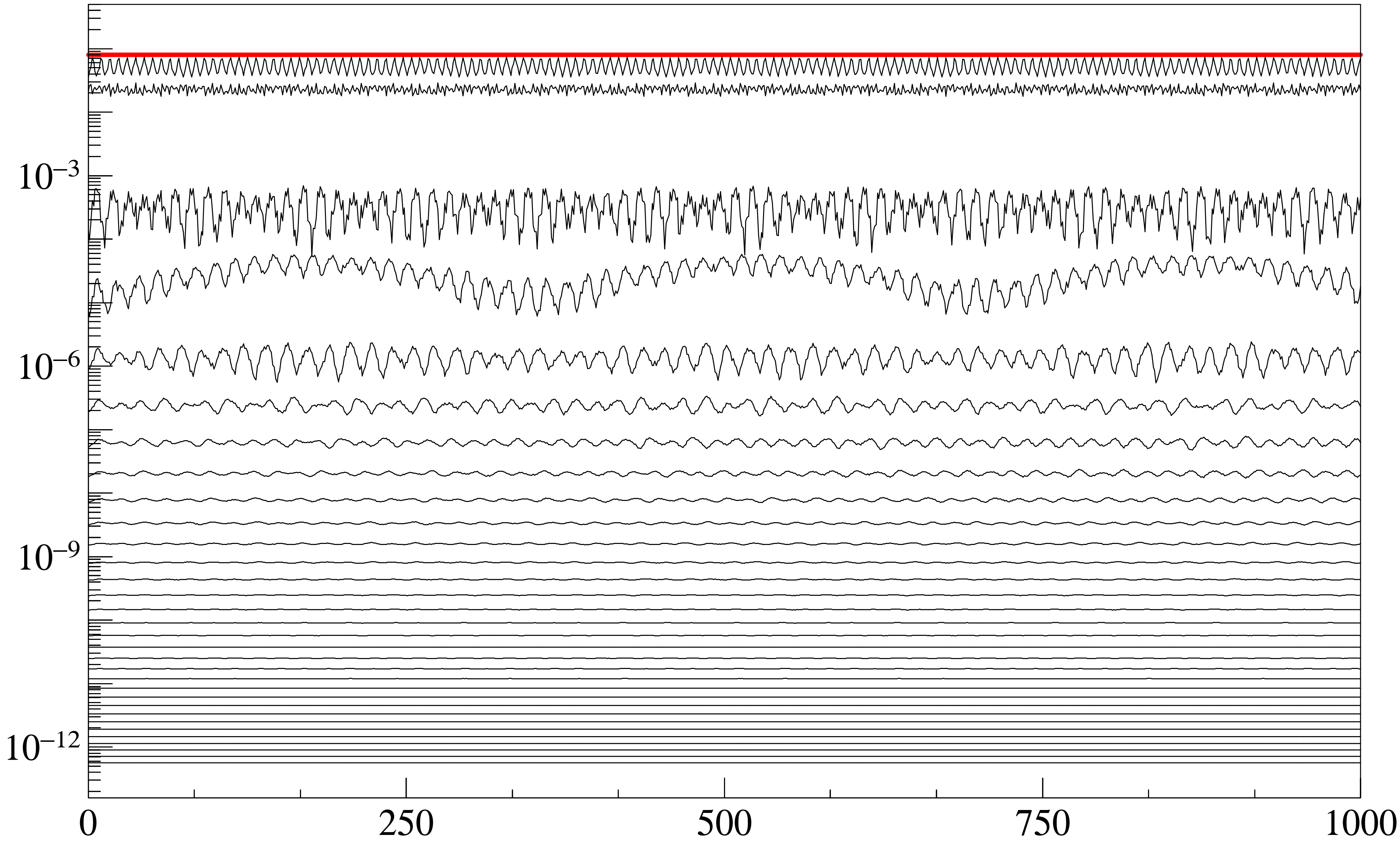
We are interested in the near-conservation, over long time intervals, of the actions

$$J_\ell(t) = I_\ell(t) + I_{-\ell}(t)\,, \quad \ell \geq 1,$$

where

$$I_j(t) = \frac{1}{2\omega_j}|\dot{q}_j(t)|^2 + \frac{\omega_j}{2}|q_j(t)|^2.$$

# Conservation properties




$$\partial_t^2 u(t,x) - \partial_x^2 u(t,x) + u(t,x) - u(t,x)^2 = 0$$

# The results

Assumptions:

- Small initial values $u(\cdot, 0)$ and $\partial_t u(\cdot, 0)$ in an appropriate Sobolev space.
- Non-resonance condition (of the type of the one used by Bambusi) on the frequencies $\omega_\ell = \sqrt{\rho + \ell^2}$.

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Results:

- The actions $J_\ell$ are nearly-preserved over long time intervals along the exact solution of the problem.
- In the same norm that specifies the smallness condition on the initial data, the solution remains nearly constant for long time intervals.

C., Hairer, Lubich 2006. Bambusi 2003. Bourgain 1996.