Modulated Fourier expansions for oscillatory differential equations

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Topic related to four workshops of this conference:

- Geometric integration and computational mechanics
- Asymptotic analysis and high oscillation
- Computational dynamics
- Foundations of numerical PDEs

Outline

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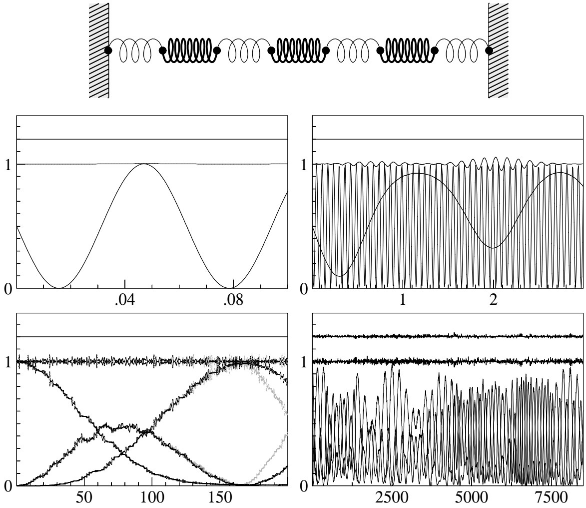
Some phenomena

Some theorems

Modulated Fourier expansions

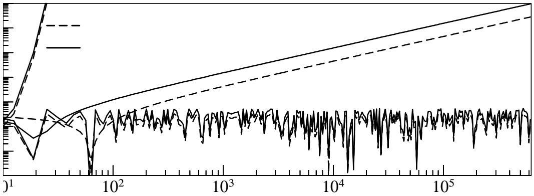
Time scales in a nonlinear oscillator chain



Galgani, Giorgilli, Martinoli & Vanzini, Physica D 1992

Hairer & L., SINUM 2000, % & Wanner, GNI book 2002/2006

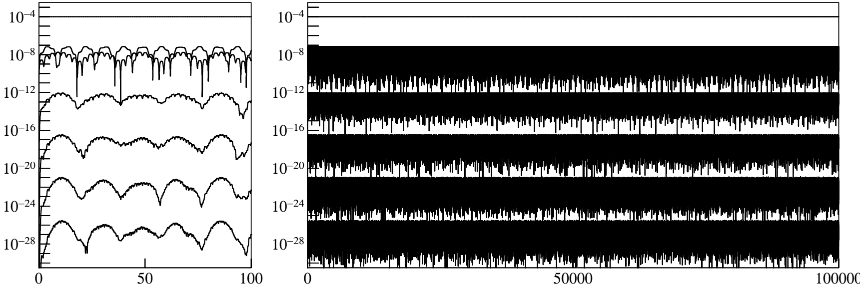
Symmetric linear multistep methods over long times



error in total energy and angular momentum (Kepler problem)

Hairer & L., Numer. Math. 2004

Metastable energy cascades in nonlinear wave eqs.



mode energies in a nonlinear wave equation $u_{tt} - u_{xx} + \frac{1}{2}u = u^2$ with periodic b.c., only first Fourier mode excited initially

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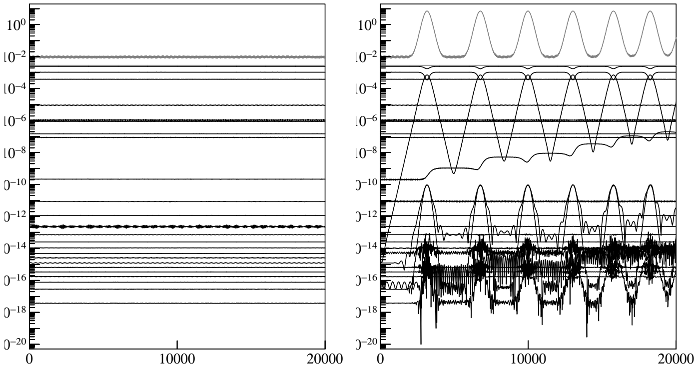
Gauckler, Hairer, L. & Weiss, Preprint 2011

Splitting integrator for a nonlinear Schrödinger eq.



actions $|u_j|^2$ in a full discretisation:
non-resonant step size $\Delta t = 2\pi/\omega_6 + 0.005$
vs. resonant step size $\Delta t = 2\pi/\omega_6$

Gauckler & L., JFoCM 2010

Outline

Oscillatory ODEs

$$\begin{aligned} \ddot{x}_0 &= -\nabla_{x_0} U(x_0, x_1) \\ \ddot{x}_1 + \frac{1}{\varepsilon^2} x_1 &= -\nabla_{x_1} U(x_0, x_1), \qquad 0 < \varepsilon \ll 1 \end{aligned}$$

Oscillatory energy $E_1 = \frac{1}{2}|\dot{x}_1|^2 + \frac{1}{2\varepsilon^2}|x_1|^2$ is an almost-invariant:

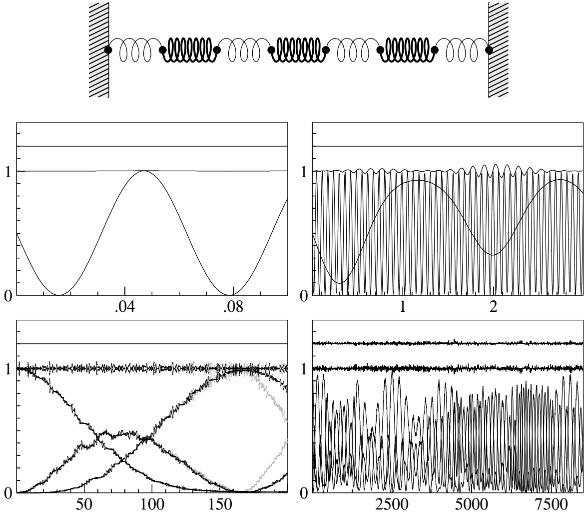
If U is analytic and $E_1(0) \leq M$, then

$$|E_1(t) - E_1(0)| \leq C\varepsilon \quad \text{for} \quad t \leq e^{c/\varepsilon},$$

provided that x_0 stays in a compact set.

Benettin, Galgani & Giorgilli, CMP 1989
Cohen, Hairer & L., JFoCM 2003

Time scales in a nonlinear oscillator chain



Trigonometric integrator for oscillatory ODEs

same ODE

$$\begin{aligned} \ddot{x}_0 &= -\nabla_{x_0} U(x_0, x_1) \\ \ddot{x}_1 + \frac{1}{\varepsilon^2} x_1 &= -\nabla_{x_1} U(x_0, x_1), \qquad 0 < \varepsilon \ll 1 \end{aligned}$$

trigonometric integrator with step size $h \geq c\varepsilon$:
exact for $\ddot{x}_1 + \frac{1}{\varepsilon^2} x_1 = 0$, Störmer-Verlet for $\ddot{x}_0 = f(x_0)$

Under the non-resonance condition

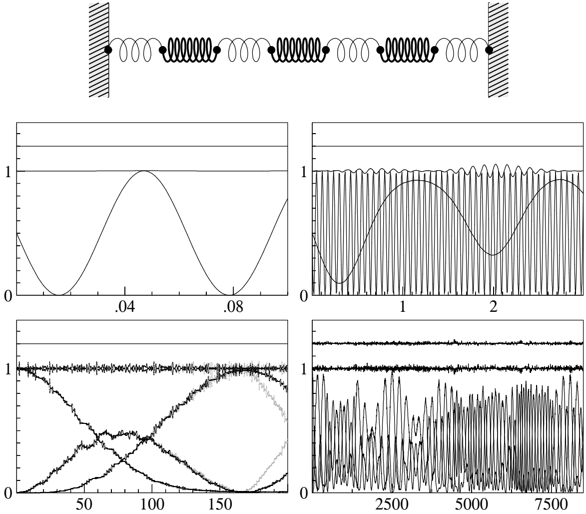
$$\left| \sin\left(\frac{kh}{2\varepsilon}\right) \right| \geq c\sqrt{h} \quad \text{for} \quad k = 1, \dots, N,$$

long-time near-conservation of total and oscillatory energies:

$$\begin{aligned} H^n - H^0 &= O(h) \\ E_1^n - E_1^0 &= O(h) \end{aligned} \qquad \text{for} \quad nh \leq h^{-N+1}.$$

Hairer & L., SINUM 2000

Time scales in a nonlinear oscillator chain



Symmetric linear multistep methods over long times

$$\ddot{y} = f(y), \qquad f(y) = -\nabla U(y)$$

linear multistep method $\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f_{n+j}$

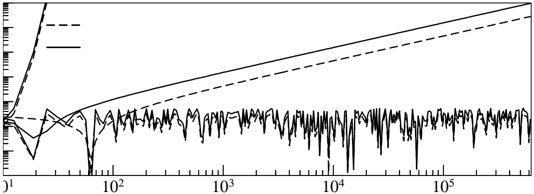
- symmetric: $\alpha_j = \alpha_{k-j}$, $\beta_j = \beta_{k-j}$
- all zeros of $\sum \alpha_j \zeta^j$ are simple, except double root at 1
- order $p \geq 2$

long-time near-conservation of energy:

$$H^n - H^0 = O(h^p) \quad \text{for} \quad nh \leq h^{-p-2}$$

Hairer & L., Numer. Math. 2004

Symmetric linear multistep methods over long times



error in total energy and angular momentum (Kepler problem)

Weakly nonlinear wave equations

1. Linear Klein–Gordon equation:

$$u_{tt} - \Delta u + \rho u = 0 \quad (x \in \mathbb{R}^d, t \in \mathbb{R}); \qquad \text{with} \quad \rho \geq 0$$

initial data $a\, e^{ik\cdot x} + b\, e^{-ik\cdot x}$ for some wave vector $k \in \mathbb{R}^d$

The solution is a linear combination of plane waves $e^{i(\pm k\cdot x \pm \omega t)}$.

(with frequency $\omega = \sqrt{|k|^2 + \rho}$)

2. Nonlinear perturbation: $u_{tt} - \Delta u + \rho u = g(u)$, same initial data

The solution has a Fourier series $u(x,t) = \sum_{j\in\mathbb{Z}} u_j(t)\, e^{ijk\cdot x}$.

Size of mode energies $E_j(t) = \frac{1}{2}|\omega_j u_j(t)|^2 + \frac{1}{2}|\dot{u}_j(t)|^2$ for large t?

(with frequencies $\omega_j = \sqrt{j^2|k|^2 + \rho}$)

Energy transfer to higher modes?

Are plane waves stable under nonlinear perturbations?

Weakly nonlinear wave equations (cont.)

- real initial data with $E_1(0) = \varepsilon, \;\; E_j(0) = 0$ for $j \neq 1$
- real-analytic nonlinearity $g(u)$ at least quadratic at 0

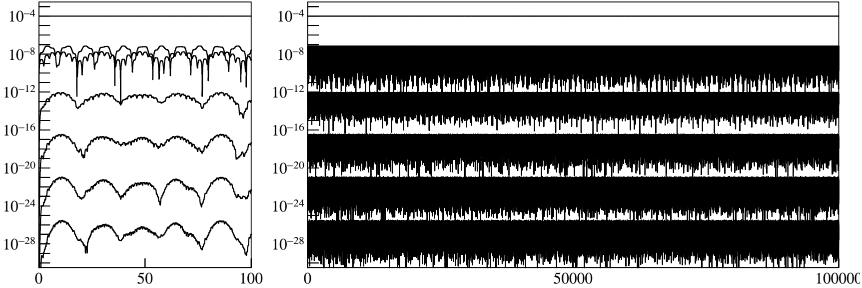
Fix an integer $K > 1$. Then:
For almost all mass parameters $\rho > 0$ and wave vectors k, solutions to the nonlinear Klein–Gordon equation satisfy, over long times

$$t \leq c\,\varepsilon^{-K/4},$$

the bounds $\quad |E_1(t) - E_1(0)| \leq C\varepsilon^2, \quad E_0(t) \leq C\varepsilon^2,$

$$\begin{aligned} E_j(t) &\leq C\varepsilon^j, \quad 0 < j < K, \\ \sum_{j=K}^{\infty} \varepsilon^{-(j-K)/2} E_j(t) &\leq C\varepsilon^K. \end{aligned}$$

Metastable energy cascades in nonlinear wave eqs.



mode energies in a nonlinear wave equation $u_{tt} - u_{xx} + \frac{1}{2}u = u^2$, only first mode excited initially

Further results on ...

- energy distribution in FPU chains, particle lattices
- long-time Sobolev regularity of nonlinear wave equations
- Sobolev stability of plane wave solutions to NLS
- long-time near-conservation of actions in NLW and NLS
- ... and their numerical counterparts

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general theme: long-time behaviour of weakly nonlinear systems and their numerical discretizations

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Some phenomena

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Modulated Fourier expansions

Modulated Fourier expansions

technique for analysing weakly nonlinear systems over long times

two ingredients:

- solution approximation over short time (MFE)
- almost-invariants of the modulation system

$\rightarrow$ long-time results on the energy behaviour

Hairer & L. 2000 for long-time analysis of numerical integrators for highly oscillatory ODEs

Hairer & L. and Cohen, Gauckler 2003-2011, Sanz-Serna 2009

for analytical and numerical problems in Hamiltonian ODEs, PDEs, lattice systems over long times

Hairer, L. & Wanner 2002, Cohen 2003, Condon, Deaño & Iserles 2010

MFE as a numerical approximation method

Modulated Fourier expansion in time

Model problem:

$$\ddot{x}_j + \omega_j^2 x_j = \sum_{j_1+j_2=j \ mod \ N} x_{j_1} x_{j_2} \quad \text{for} \quad j = 1, \dots, N$$

for frequencies $\omega_j = \lambda_j/\varepsilon$, with $\lambda_j \geq 1$.

Assume: Harmonic energies $E_j = \frac{1}{2}\omega_j^2 x_j^2 + \frac{1}{2}\dot{x}_j^2$ are initially bounded independently of ε.

Approximation ansatz:

$$x_j(t) \approx \sum_{\mathbf{k}} z_j^{\mathbf{k}}(t)\, e^{i(\mathbf{k}\cdot\boldsymbol{\omega})t}$$

with slowly varying modulation functions $z_j^{\mathbf{k}}$
finite sum over $\mathbf{k} = (k_1, \dots, k_N) \in \mathbb{Z}^N$, and $\mathbf{k} \cdot \boldsymbol{\omega} = \sum k_j \omega_j$

Modulation system

$$\left(\omega_j^2 - (\mathbf{k}\cdot\boldsymbol{\omega})^2\right) z_j^{\mathbf{k}} + 2i(\mathbf{k}\cdot\boldsymbol{\omega})\dot{z}_j^{\mathbf{k}} + \ddot{z}_j^{\mathbf{k}} = -\frac{\partial \mathcal{U}}{\partial z_{-j}^{-\mathbf{k}}}(\mathbf{z})$$

with the modulation potential

$$\mathcal{U}(\mathbf{z}) = -\tfrac{1}{3} \sum_{j_1+j_2+j_3=0 \ mod \ N} \ \sum_{\mathbf{k}^1+\mathbf{k}^2+\mathbf{k}^3=0} z_{j_1}^{\mathbf{k}^1} z_{j_2}^{\mathbf{k}^2} z_{j_3}^{\mathbf{k}^3}.$$

The infinite system is truncated and solved approximately (up to a defect ε^K) for polynomial modulation functions $z_j^{\mathbf{k}}$ under a

non-resonance condition:
Small denominators $\omega_j^2 - (\mathbf{k}\cdot\boldsymbol{\omega})^2$ are not too small.

Formal invariants of the modulation system

The invariance property

$$\mathcal{U}(S_\ell(\theta)\mathbf{z}) = \mathcal{U}(\mathbf{z}) \quad \text{for} \quad S_\ell(\theta)\mathbf{z} = (e^{ik_\ell\theta} z_j^{\mathbf{k}})_{j,\mathbf{k}}$$

leads to formal invariants (Noether's theorem)

$$\mathcal{E}_\ell\Big(\mathbf{z}, \frac{d\mathbf{z}}{d\tau}\Big) = \tfrac{1}{2} \sum_j \sum_{\mathbf{k}} k_\ell \omega_\ell \Big((\mathbf{k}\cdot\boldsymbol{\omega}) |z_j^{\mathbf{k}}|^2 - i z_{-j}^{-\mathbf{k}} \frac{d\mathbf{z}_j^{\mathbf{k}}}{d\tau} \Big),$$

which are almost-invariants of the truncated modulation system and turn out to be close to the harmonic energies E_ℓ.

With these ingredients and many problem-specific technical details and estimates we obtain results on the long-time behaviour of the harmonic energies E_ℓ.

"This report is intended to be the first one in a series dealing with the behavior of certain nonlinear physical systems where the non-linearity is introduced as a perturbation to a primarily linear problem. The behavior of the systems is to be studied for times which are long compared to the characteristic periods of the corresponding linear problem."

Fermi, Pasta & Ulam 1955

... which is just what modulated Fourier expansions are good for.