Modulated Fourier expansions for oscillatory differential equations

Christian Lubich
Univ. Tübingen

joint work with Ernst Hairer
and David Cohen, Ludwig Gauckler, Daniel Weiss

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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

Some phenomena

Some theorems

Modulated Fourier expansions
Some phenomena

Some theorems

Modulated Fourier expansions
Time scales in a nonlinear oscillator chain

Galgani, Giorgilli, Martinoli & Vanzini, Physica D 1992
Symmetric linear multistep methods over long times

error in total energy and angular momentum (Kepler problem)

Hairer & L., Numer. Math. 2004
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

*Gauckler, Hairer, L. & Weiss, Preprint 2011*
actions $|u_j|^2$ in a full discretisation:

non-resonant step size $\Delta t = 2\pi/\omega_6 + 0.005$

vs. resonant step size $\Delta t = 2\pi/\omega_6$
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Modulated Fourier expansions
Oscillatory ODEs

\[ \ddot{x}_0 = -\nabla_{x_0} U(x_0, x_1) \]
\[ \ddot{x}_1 + \frac{1}{\varepsilon^2} x_1 = -\nabla_{x_1} U(x_0, x_1), \quad 0 < \varepsilon \ll 1 \]

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

\[
\begin{align*}
\ddot{x}_0 & = -\nabla_{x_0} U(x_0, x_1) \\
\ddot{x}_1 + \frac{1}{\varepsilon^2} x_1 & = -\nabla_{x_1} U(x_0, x_1), \quad 0 < \varepsilon \ll 1
\end{align*}
\]

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

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

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

\[
\begin{align*}
H^n - H^0 & = O(h) \quad \text{for} \quad nh \leq h^{-N+1}.
\end{align*}
\]

Hairer & L., SINUM 2000
Time scales in a nonlinear oscillator chain
Symmetric linear multistep methods over long times

\[
\ddot{y} = f(y), \quad f(y) = -\nabla U(y)
\]

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:

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

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

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

$$E_j(t) \leq C\varepsilon^j, \quad 0 < j < K,$$

$$\sum_{j=K}^{\infty} \varepsilon^{-(j-K)/2} E_j(t) \leq C\varepsilon^K.$$

metastable energy cascade     Gauckler, Hairer, L. & Weiss 2011
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

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

→ 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


MFE as a numerical approximation method
Modulated Fourier expansion in time

Model problem:

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

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 \( \varepsilon \).

Approximation ansatz:

\[ x_j(t) \approx \sum_k z_j^k(t) e^{i(k \cdot \omega)t} \]

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

\[(\omega_j^2 - (k \cdot \omega)^2) z_j^k + 2i(k \cdot \omega) \dot{z}_j^k + \ddot{z}_j^k = -\frac{\partial U}{\partial z_{-j}^k}(z)\]

with the modulation potential

\[U(z) = -\frac{1}{3} \sum_{j_1+j_2+j_3=0 \mod N} \sum_{k^1+k^2+k^3=0} z_{j_1}^{k_1} z_{j_2}^{k_2} z_{j_3}^{k_3}.\]

The infinite system is truncated and solved approximately (up to a defect \(\varepsilon^K\)) for polynomial modulation functions \(z_j^k\) under a non-resonance condition:

Small denominators \(\omega_j^2 - (k \cdot \omega)^2\) are not too small.
Formal invariants of the modulation system

The invariance property

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

leads to formal invariants (Noether’s theorem)

$$E_\ell(z, \frac{d\bar{z}}{d\tau}) = \frac{1}{2} \sum_j \sum_k k_\ell \omega_\ell \left( (k \cdot \omega)|z_j^k|^2 - iz_{-j}^{-k} \frac{dz_j^k}{d\tau} \right),$$

which are almost-invariants of the truncated modulation system and turn out to be close to the harmonic energies $E_\ell$.

With these ingredients and many problem-specific technical details and estimates we obtain results on the long-time behaviour of the harmonic energies $E_\ell$. 
“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.