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Modulated Fourier expansions for continuous and discrete oscillatory systems

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Abstract

This article reviews some of the phenomena and theoretical results on the long-time energy behaviour of continuous and discretized oscillatory systems that can be explained by modulated Fourier expansions: long-time preservation of total and oscillatory energies in oscillatory Hamiltonian systems and their numerical discretisations, near-conservation of energy and angular momentum of symmetric multistep methods for celestial mechanics, metastable energy strata in nonlinear wave equations. We describe what modulated Fourier expansions are and what they are good for.

1.1 Introduction

As a new analytical tool developed in the past decade, modulated Fourier expansions have been found useful to explain various long-time phenomena in both continuous and discretized oscillatory Hamiltonian systems, ordinary differential equations as well as partial differential equations. In addition, modulated Fourier expansions have turned out useful as a numerical approximation method in oscillatory systems.

In this review paper we first show some long-time phenomena in oscillatory systems, then give theoretical results that explain these phenomena, and finally outline the basics of modulated Fourier expansions with which these results are proved.

1.2 Some phenomena

1.2.1 Time scales in a nonlinear oscillator chain

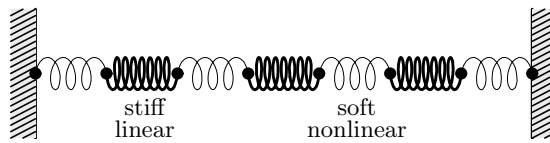
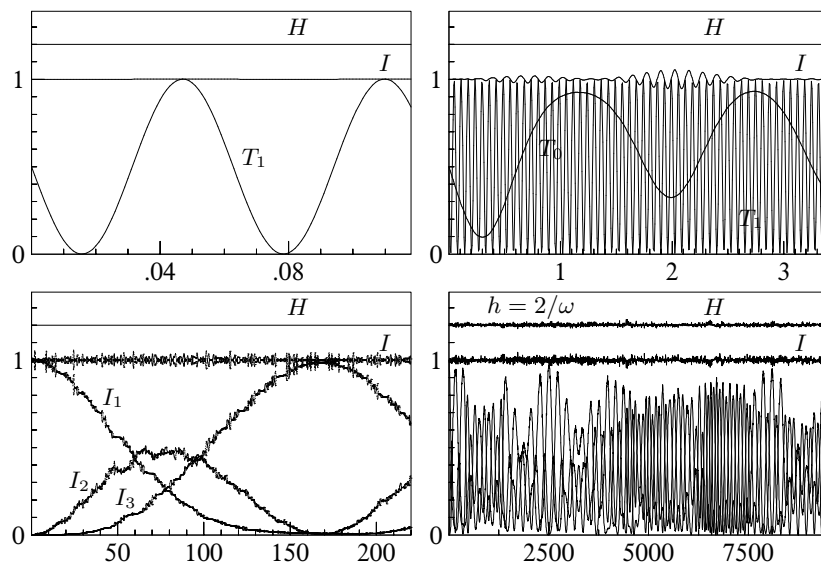


Figure 1.1 Particle chain with alternating soft nonlinear and stiff linear springs.

Following Galgani, Giorgilli, Martinoli & Vanzini [GGMV92], we consider a chain of particles interconnected alternately by stiff linear springs and soft nonlinear springs, as shown in Figure 1.1. We assume that the particles are of unit mass and that the spring constant of the stiff linear springs is ε^{-2} for a small parameter ε . This example was chosen as a model problem for nonlinear oscillatory Hamiltonian problems with a single constant high frequency $\omega = 1/\varepsilon$ in [HLW06, Chap. XIII].

The system shows different behaviour on several time scales. On the fast time scale ε there is the almost-sinusoidal vibration of the stiff springs. The time scale ε^0 is that of the motion of the nonlinear springs. On the slow time scale ε^{-1} , there is an energy transfer between the stiff springs. Over very long times ε^{-N} with $N > 1$ and even over exponentially long times $t \leq e^{c/\varepsilon}$, there is almost-conservation of the sum of the harmonic energies of the stiff springs. The total energy is conserved for all times.

This behaviour is illustrated in Figure 1.2, where various energies in the system are plotted as functions of time. In all four pictures, the upper constant line is the total energy. In the final, long-time picture the total energy does not appear as constant, because the upper line represents the total energy along a numerical solution that was computed with large step size $h > \varepsilon$. It is remarkable that the numerical method, which here is a trigonometric integrator, shows no drift in the total energy

Figure 1.2 Different time scales in the oscillator chain ($\varepsilon = 1/50$).

over such long times, just small oscillations about the correct value. The lower almost-constant line in the pictures represents the oscillatory energy, that is, the sum of the harmonic energies of the stiff springs. It is not exactly conserved, but stays close to its initial value over extremely long times, both in the exact and the numerical solution. This calls for an explanation.

Let us briefly describe the further curves in Figure 1.2: the sinusoidal curve in the first picture represents the kinetic energy of the first stiff spring, the smooth curve in the second picture represents the kinetic energy in the first nonlinear spring. The third and fourth picture show the energy transfer between the stiff springs: the curves show the harmonic energies of the three stiff springs, starting from an initial configuration where only the first spring is excited, while the second and third stiff springs are at rest.

1.2.2 Symmetric multistep methods over long times

We consider the numerical solution of second-order differential equations

$$\ddot{x} = -\nabla U(x)$$

by linear multistep methods. It was reported in the astrophysical literature [QT90] that some *symmetric* multistep methods exhibit excellent long-time behaviour in the computation of planetary orbits, similar to that known for symplectic one-step methods. Since multistep methods cannot be symplectic, as was shown by Tang [Tan93], such behaviour comes unexpected.

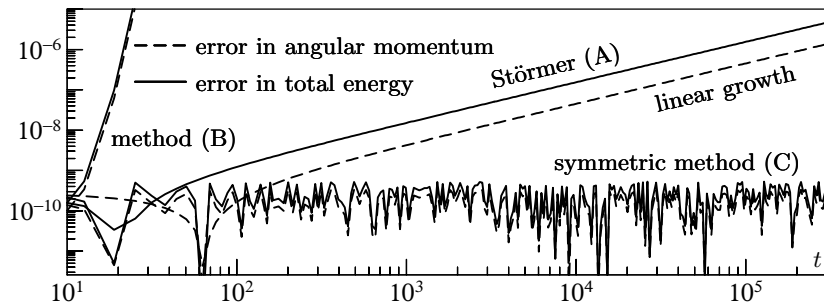


Figure 1.3 Error in energy and angular momentum of three multistep methods applied to the Kepler problem.

Figure 1.3 shows the error in the total energy and the angular momentum of three multistep methods applied to the Kepler problem, all three of the same order 8. The linear error growth in energy and angular momentum corresponds to a non-symmetric method, the eighth-order Störmer method (A). One symmetric method exhibits exponential error growth (B), but another symmetric method shows no drift in energy and angular momentum (C). Such behaviour needs to be explained.

1.2.3 Metastable energy strata in nonlinear wave equations

We consider the nonlinear wave equation $u_{tt} - u_{xx} + \frac{1}{2}u = u^2$ with periodic boundary conditions on a space interval of length 2π and report a numerical experiment from [GHLW11]. The initial data are chosen such that only the first Fourier mode is excited initially, with harmonic energy $E_1(0) = \varepsilon = 10^{-4}$. All higher-mode harmonic energies are initially zero. As is shown in Figure 1.4, due to the presence of the nonlinearity, they become non-zero immediately. Surprisingly, however, the j th mode energy settles quickly at level ε^j (the zero-mode energy at ε^2) and stays there for extremely long times. There is no perceptible energy transfer among the modes.

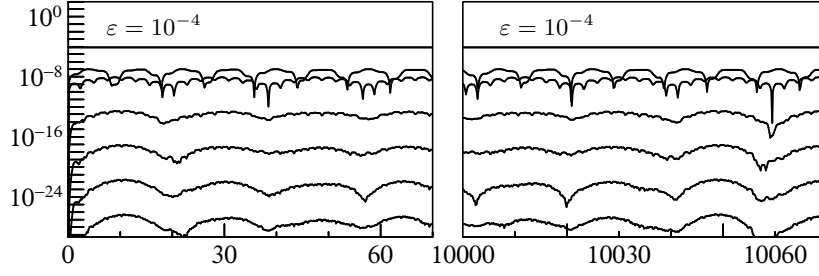


Figure 1.4 Mode energies versus time on different time windows.

1.3 Some theorems

We give theoretical results that explain the long-time phenomena encountered in Section 1.2.

1.3.1 Oscillatory ordinary differential equations

We consider a system of second-order differential equations for $x_0 \in \mathbb{R}^{d_0}$, $x_1 \in \mathbb{R}^{d_1}$,

$$\begin{aligned} \ddot{x}_0 &= -\nabla_{x_0} U(x_0, x_1) \\ \ddot{x}_1 + \frac{1}{\varepsilon^2} x_1 &= -\nabla_{x_1} U(x_0, x_1), \quad 0 < \varepsilon \ll 1. \end{aligned} \tag{1.1}$$

With the momenta $y_0 = \dot{x}_0$, $y_1 = \dot{x}_1$, this is a Hamiltonian system with the Hamilton function

$$H(x_0, x_1, y_0, y_1) = \frac{1}{2} \|y_0\|^2 + \frac{1}{2} \|y_1\|^2 + \frac{1}{2} \varepsilon^{-2} \|x_1\|^2 + U(x_0, x_1).$$

Example. If we describe the position of the $2m$ particles in the non-linear oscillator chain of Figure 1.1 (where $m = 3$) by the coordinates of the centres of the stiff linear springs, $x_0 = (x_{0,1}, \dots, x_{0,m})$, and by their elongations from the rest length, $x_1 = (x_{1,1}, \dots, x_{1,m})$, then the equations of motion take the above form. The potential U is given as $U(x_0, x_1) = V(s_0) + \dots + V(s_m)$, where s_j denotes the elongation of the j th soft nonlinear spring with potential V .

The oscillatory energy

$$E_1 = \frac{1}{2} \|\dot{x}_1\|^2 + \frac{1}{2} \varepsilon^{-2} \|x_1\|^2 = \sum_{j=1}^{d_1} \left(\frac{1}{2} \dot{x}_{1,j}^2 + \frac{1}{2} \varepsilon^{-2} x_{1,j}^2 \right)$$

turns out to be almost invariant. The following result over exponentially long times in $1/\varepsilon$ was proved by Benettin, Galgani & Giorgilli [BGG87] using a sequence of nonlinear coordinate transformations from Hamiltonian perturbation theory, and later by Cohen, Hairer & Lubich [CHL03] using modulated Fourier expansions, working in the original coordinates.

Theorem 1.1 *If U is analytic and the oscillatory energy is bounded by $E_1(0) \leq M$, then*

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

provided that $(x_0(t), 0)$ stays in a compact subset of the domain of analyticity of U . The constants C and c are independent of ε , but depend on M , $\|\dot{x}_0(0)\|$ and bounds of U .

The condition on $x_0(t)$ is satisfied, for example, if $U(x_0, 0) \rightarrow +\infty$ as $\|x_0\| \rightarrow \infty$, since the total energy H is constant along the solution.

Theorem 1.1 explains the almost constant line for E_1 in the lower right picture of Figure 1.2 — at least for the exact solution, whereas the picture was obtained with a numerical method with large step size $h > \varepsilon$, which nevertheless shows remarkably good long-time energy behaviour. The numerical method employed is a *trigonometric integrator*, a method that is exact for $\ddot{x}_1 + \varepsilon^{-2} x_1 = 0$ and reduces to the Störmer-Verlet method for $\ddot{x}_0 = f(x_0)$. The method is of the form

$$x_0^{n+1} = x_0^n + h\dot{x}_0^n + \frac{1}{2}h^2g_0^n$$

$$\dot{x}_0^{n+1} = \dot{x}_0^n + \frac{1}{2}h(g_0^n + g_0^{n+1})$$

$$x_1^{n+1} = \cos\left(\frac{h}{\varepsilon}\right)x_1^n + \varepsilon\sin\left(\frac{h}{\varepsilon}\right)\dot{x}_1^n + \frac{1}{2}h^2\psi\left(\frac{h}{\varepsilon}\right)g_1^n$$

$$\dot{x}_1^{n+1} = -\frac{1}{\varepsilon}\sin\left(\frac{h}{\varepsilon}\right)x_1^n + \cos\left(\frac{h}{\varepsilon}\right)\dot{x}_1^n + \frac{h}{2}(\psi_0\left(\frac{h}{\varepsilon}\right)g_1^n + \psi_1\left(\frac{h}{\varepsilon}\right)g_1^{n+1})$$

with $g_j^n = -\nabla_{x_j} U(x_0^n, \phi(\frac{h}{\varepsilon})x_1^n)$ for $j = 0, 1$ and with filter functions ψ , ψ_0 , ψ_1 , ϕ that take the value 1 at 0. Exchanging $n \leftrightarrow n+1$ and $h \leftrightarrow -h$ in the method, it is seen that the method is symmetric for all values of h and ε if and only if $\psi(\xi) = \text{sinc}(\xi)\psi_1(\xi)$ (where $\text{sinc}(\xi) = \sin(\xi)/\xi$) and $\psi_0(\xi) = \cos(\xi)\psi_1(\xi)$, which we assume in the following. The method is symplectic if and only if $\psi(\xi) = \text{sinc}(\xi)\phi(\xi)$. A popular choice, proposed by Garcia-Archilla, Sanz-Serna & Skeel [GASSS99], is $\phi(\xi) = \text{sinc}(\xi)$, $\psi(\xi) = \text{sinc}(\xi)^2$, but other choices are also favoured in the literature, see Hairer, Lubich & Wanner [HLW06, Chap. XIII] and Grimm & Hochbruck [GH06].

We are interested in the long-time behaviour of the total energy

$$H^n = H(x_0^n, x_1^n, \dot{x}_0^n, \dot{x}_1^n)$$

and oscillatory energy

$$E_1^n = \frac{1}{2} \|\dot{x}_1^n\|^2 + \frac{1}{2} \varepsilon^{-2} \|x_1^n\|^2$$

along the numerical solution. For a numerical analogue of Theorem 1.1 we need the following conditions:

- the energy bound $E_1^0 \leq M$
- a condition on the numerical solution: the values $(x_0^n, 0)$ stay in a compact subset of a domain on which the potential U is smooth;
- conditions on the filter functions: ψ and ϕ have no real zeros other than integral multiples of π ; they satisfy

$$\begin{aligned} |\psi(h/\varepsilon)| &\leq C_1 \operatorname{sinc}^2(\tfrac{1}{2} h/\varepsilon), & |\phi(h/\varepsilon)| &\leq C_2 |\operatorname{sinc}(\tfrac{1}{2} h/\varepsilon)|, \\ |\psi(h/\varepsilon)\phi(h/\varepsilon)| &\leq C_3 |\operatorname{sinc}(h/\varepsilon)|; \end{aligned}$$

- the condition $h/\varepsilon \geq c_0 > 0$;
- a numerical non-resonance condition: for some $N \geq 2$,

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

Theorem 1.2 *Under the above conditions, the total and oscillatory energies along the numerical solution satisfy*

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

The constants symbolized by \mathcal{O} are independent of n, h, ε satisfying the above conditions, but depend on N and the constants in the conditions.

This result from Hairer & Lubich [HL01], see also Hairer, Lubich & Wanner [HLW06, Chap. XIII], was the first long-time result proved with modulated Fourier expansions. That technique could easily be transferred from the continuous to the discrete problem, which does not seem possible for the nonlinear coordinate transforms of Hamiltonian perturbation theory with which Theorem 1.1 was first proved.

The differential equation (1.1) has just a single high frequency $\omega = 1/\varepsilon$. Extensions of Theorem 1.1 to problems with several high frequencies are proved by Benettin, Galgani and Giorgilli [BGG89] (via Hamiltonian perturbation theory) and Cohen, Hairer & Lubich [CHL05] (via modulated Fourier expansions). The latter paper gives a multi-frequency

version of Theorem 1.2 for the numerical solution. An additional difficulty in the multi-frequency case appears because of possible resonances among the frequencies, which need to be studied carefully. In the case of non-resonant frequencies $\omega_j = \lambda_j/\varepsilon$, each of the oscillatory energies $E_j = \frac{1}{2}\|\dot{x}_j\|^2 + \frac{1}{2}\omega_j^2\|x_j\|^2$ is nearly preserved over long times, but in resonant cases only certain linear combinations of the E_j , and in particular their sum, are nearly preserved.

1.3.2 Symmetric multistep methods over long times

We now consider a second-order system of ordinary differential equations with conservative forces (here with just one time scale)

$$\ddot{x} = f(x), \quad f(x) = -\nabla U(x), \quad (1.2)$$

with a smooth potential U . The system is Hamiltonian with

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

For the numerical approximation $x^n \approx x(nh)$ we consider a linear multistep method with step size h ,

$$\sum_{j=0}^k \alpha_j x^{n+j} = h^2 \sum_{j=0}^k \beta_j f(x^{n+j}), \quad (1.3)$$

with the following properties:

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

We recall that the order of the method is characterized by the relation

$$\frac{1}{h^2} \frac{\sum \alpha_j e^{jh}}{\sum \beta_j e^{jh}} = 1 + \mathcal{O}(h^p) \quad \text{for } h \rightarrow 0,$$

which entails a double zero of $\sum \alpha_j \zeta^j$ at 1. The method is completed with a velocity approximation

$$\dot{x}^n \approx \frac{1}{h} \sum_{j=-\ell}^{\ell} \delta_j x^j,$$

which we also assume to be of order p . The velocity approximations are computed *a posteriori* and are not propagated in the scheme. Moreover,

we assume that the error of the starting approximations x^0, \dots, x^{k-1} is $\mathcal{O}(h^{p+1})$.

The following result on the long-time near-conservation of the total energy $H^n = H(x^n, \dot{x}^n)$ is proved in [HL04].

Theorem 1.3 *Under the above assumptions,*

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

The constant symbolized by the \mathcal{O} -notation is independent of n and h with nh in the stated interval. If no root of $\sum \alpha_j \zeta^j$ other than 1 is a product of two other roots, then there is energy conservation up to $\mathcal{O}(h^p)$ even over times $nh \leq h^{-2p-3}$.

Systems with a rotational symmetry preserve angular momentum. This comes about through an invariance

$$U(e^{\tau A}x) = U(x) \quad \text{for all } x \text{ and real } \tau$$

with a skew-symmetric matrix A via Noether's theorem: the system then has the quadratic first integral

$$L(x, \dot{x}) = \dot{x}^T A x.$$

The following result from [HL04] states the long-time near-conservation of angular momentum $L^n = L(x^n, \dot{x}^n)$ along the numerical solution.

Theorem 1.4 *Under the above assumptions,*

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

The constant symbolized by the \mathcal{O} -notation is independent of n and h with nh in the stated interval.

Theorems 1.3 and 1.4 explain the excellent long-time behaviour of the favourable of the three methods of Figure 1.3. The method with the linear error growth in energy and angular momentum is not symmetric, and the method with the exponential error growth is symmetric but its characteristic polynomial has further double roots apart from 1.

At first sight, the problem considered in this subsection bears little resemblance to that of the previous subsection, but in fact both can be viewed as perturbed linear problems. Here, it is the numerical scheme that introduces a fast time scale h on which the solutions of the linear recurrence relation

$$\sum_{j=0}^k \alpha_j x^{n+j} = 0$$

oscillate, with parasitic terms ζ_i^n , where the ζ_i are the zeros of the characteristic polynomial $\sum \alpha_j \zeta^j$ that are different from the principal root 1. The squared norms of parasitic solution components in the nonlinear problem play a similar role to the oscillatory energies E_i of the previous subsection and can be shown to remain almost constant along the numerical solution. The proof uses similar analytical techniques, that is, modulated Fourier expansions.

Bounding parasitic components is the main obstacle to obtaining similarly good long-time results for symmetric multistep methods applied to more general Hamiltonian systems than (1.2), see [HLW06, Chap. XV] and Console & Hairer [CH11].

1.3.3 Metastable energy strata in nonlinear wave equations

We now turn to a surprising long-time result in weakly nonlinear partial differential equations. The *linear* Klein–Gordon equation

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

with initial data $a e^{ik \cdot x} + b e^{-ik \cdot x}$ for some (fixed) wave vector $k \in \mathbb{R}^d$ has a solution that is a linear combination of plane waves $e^{i(\pm k \cdot x \pm \omega t)}$ (with frequency $\omega = \sqrt{|k|^2 + \rho}$). We now consider the nonlinearly perturbed equation

$$u_{tt} - \Delta u + \rho u = g(u) \tag{1.4}$$

with the same initial data and ask the question: *Are plane waves stable under nonlinear perturbations of the equation?*

The solution has a Fourier series

$$u(x, t) = \sum_{j \in \mathbb{Z}} u_j(t) e^{ij k \cdot x},$$

where the coefficient functions satisfy the infinite system of second-order differential equations

$$\ddot{u}_j + \omega_j^2 u_j = -\frac{\partial U}{\partial u_{-j}}(\mathbf{u}), \quad j \in \mathbb{Z},$$

with frequencies $\omega_j = \sqrt{j^2|k|^2 + \rho}$ and the potential

$$U(\mathbf{u}) = - \sum_m \frac{g^{(m-1)}(0)}{m!} \sum_{j_1 + \dots + j_m = 0} u_{j_1} \dots u_{j_m} \quad \text{for } \mathbf{u} = (u_j)_{j \in \mathbb{Z}}.$$

We are interested in the size of the mode energies

$$E_j(t) = \frac{1}{2} |\dot{u}_j(t)|^2 + \frac{1}{2} |\omega_j u_j(t)|^2$$

for large t and in the energy transfer to higher modes.

We note that $E_j(t) = E_{-j}(t)$ for real solutions of (1.4). We assume the following:

- real initial data with $E_1(0) = \varepsilon$, $E_j(0) = 0$ for $|j| \neq 1$
- a real-analytic nonlinearity g with $g(0) = g'(0) = 0$.

The following long-term stability result is proved by Gauckler, Hairer, Lubich & Weiss [GHLW11] using modulated Fourier expansions in time.

Theorem 1.5 *Assume the above conditions and fix an integer $K > 1$. Then the following holds true: For almost all mass parameters $\rho > 0$ and wave vectors k , solutions to the nonlinear Klein–Gordon equation (1.4) satisfy, for sufficiently small ε and over long times*

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

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

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

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

The constants C are independent of ε and t in the stated interval.

This result explains the stable energy strata observed in Figure 1.4. It holds for almost all (with respect to Lebesgue measure) $\rho > 0$ and k , for which it can be shown that the frequencies $\omega_j = \sqrt{j^2|k|^2 + \rho}$ satisfy a non-resonance condition. For $\rho = 0$ the frequencies are fully resonant, and there are no stable energy strata.

1.3.4 Further results

Modulated Fourier expansions have been used to prove a variety of further long-time results for oscillatory ordinary and partial differential equations and their numerical discretisations:

- energy distribution in Fermi–Pasta–Ulam chains of particles [HL10]
- long-time Sobolev regularity of nonlinear wave equations [CHL08b]
- Sobolev stability of plane wave solutions to nonlinear Schrödinger equations [FGL11]
- long-time near-conservation of actions in Hamiltonian partial differential equations [CHL08b, GL10a, Gau10]
- ... and their numerical counterparts [CHL08a, GL10a, GL10b, Gau10, HL08].

A common theme in all these works is the long-time behaviour of nonlinearly perturbed oscillatory systems and their numerical discretisations.

1.4 Modulated Fourier expansions

Modulated Fourier expansions in time have been developed as a technique for analysing weakly nonlinear oscillatory systems, both continuous and discrete, over long times. There are two ingredients:

- a solution approximation over short time (the modulated Fourier expansion properly speaking)
- almost-invariants of the modulation system.

Together they yield long-time results as illustrated in the previous section. The technique can be viewed as embedding the original system in a larger modulation system that turns out to have a Hamiltonian/Lagrangian structure with an invariance property from which the long-time behaviour can be inferred.

The technique was first developed for the long-time analysis of numerical integrators for highly oscillatory ordinary differential equations in [HL01] and was subsequently extended by the authors of the present review together with Cohen, Console, Gauckler and Weiss (see references) to treat analytical and numerical problems in Hamiltonian ODEs, PDEs, and lattice systems over long times. The approach was also taken up by Sanz-Serna [SS09] for analysing the heterogeneous multiscale method for oscillatory ODEs. In addition to the use of modulated Fourier expansions as an analytical technique, they have also been found useful as a numerical approximation method by Hairer, Lubich & Wanner [HLW06, Chap. XIII], Cohen [Coh04], and Condon, Deaño & Iserles [CDI09, CDI10].

We illustrate the procedure on the model problem

$$\ddot{x}_j + \omega_j^2 x_j = \sum_{j_1+j_2=j \bmod N} x_{j_1} x_{j_2} \quad \text{for } j = 1, \dots, N \quad (1.5)$$

for large frequencies $\omega_j = \lambda_j/\varepsilon$, with $\lambda_j \geq 1$. We assume that the oscillatory energies $E_j = \frac{1}{2}\dot{x}_j^2 + \frac{1}{2}\omega_j^2 x_j^2$ are initially bounded independently of ε .

We make the approximation ansatz

$$x_j(t) \approx \sum_{\mathbf{k}} z_j^{\mathbf{k}}(t) e^{i(\mathbf{k} \cdot \boldsymbol{\omega})t} \quad (1.6)$$

with slowly varying modulation functions $z_j^{\mathbf{k}}$, all derivatives of which should be bounded independently of ε . The sum is taken over a finite set of multi-indices $\mathbf{k} = (k_1, \dots, k_N) \in \mathbb{Z}^N$, and $\mathbf{k} \cdot \boldsymbol{\omega} = \sum k_j \omega_j$. The slowly changing modulation functions appear multiplied with the highly oscillatory exponentials $e^{i(\mathbf{k} \cdot \boldsymbol{\omega})t} = \prod_{j=1}^N (e^{i\omega_j t})^{k_j}$, which are products of solutions to the linear equations $\ddot{x}_j + \omega_j^2 x_j = 0$.

Modulation system and non-resonance condition. When we insert this ansatz into the differential equation (1.5) and collect the coefficients corresponding to the same exponential $e^{i(\mathbf{k} \cdot \boldsymbol{\omega})t}$, we obtain the infinite system of modulation equations

$$(\omega_j^2 - (\mathbf{k} \cdot \boldsymbol{\omega})^2) z_j^{\mathbf{k}} + 2i(\mathbf{k} \cdot \boldsymbol{\omega}) \dot{z}_j^{\mathbf{k}} + \ddot{z}_j^{\mathbf{k}} = -\frac{\partial \mathcal{U}}{\partial z_{-j}^{\mathbf{k}}}(\mathbf{z}). \quad (1.7)$$

The left-hand side results from the linear part in (1.5) and the right-hand side from the nonlinearity. It turns out to have a gradient structure with the modulation potential

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

The infinite system is truncated and can be solved approximately (up to a defect ε^K) for polynomial modulation functions $z_j^{\mathbf{k}}$ under a non-resonance condition: we require that small denominators $\omega_j^2 - (\mathbf{k} \cdot \boldsymbol{\omega})^2$ are not too small. For example, we might suppose, as in [CHL05],

$$|\mathbf{k} \cdot \boldsymbol{\lambda}| \geq c\sqrt{\varepsilon} \quad \text{for } \mathbf{k} \in \mathbb{Z}^N \quad \text{with } 0 < |\mathbf{k}| \leq 2K,$$

where $|\mathbf{k}| = |k_1| + \dots + |k_N|$. Under such a non-resonance condition one can construct and suitably bound the modulation functions $z_j^{\mathbf{k}}$, and the modulated Fourier expansion (1.6) is an $\mathcal{O}(\varepsilon^K)$ approximation to the solution over a short time interval $t = \mathcal{O}(1)$.

The case of resonant frequencies can also be treated by requiring a non-resonance condition outside a resonance module; cf. [BGG89, CHL05]. The situation is at present less clear for almost-resonances.

Almost-invariants of the modulation system. With the functions $y_j^{\mathbf{k}}(t) = z_j^{\mathbf{k}}(t)e^{i(\mathbf{k}\cdot\boldsymbol{\omega})t}$, the modulation equations (1.7) take the Newtonian form

$$\ddot{y}_j^{\mathbf{k}} + \omega_j^2 y_j^{\mathbf{k}} = -\frac{\partial \mathcal{U}}{\partial y_{-j}^{-\mathbf{k}}}(\mathbf{y}).$$

The modulation potential has the obvious, but important invariance property

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

Formally applying Noether's theorem, this leads to formal invariants

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

which are almost-invariants of the truncated modulation system (1.7). They turn out to be close to the oscillatory energies E_ℓ . By patching together many short time intervals, the drift in the almost-invariants \mathcal{E}_ℓ can be controlled to remain small over long times, and in this way also the drift in the oscillatory energies E_ℓ is under control.

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

1.5 Conclusion

We close this review with a citation from the very influential paper by Fermi, Pasta & Ulam [FPU55] (see [Gal08] for a reprint and review):

“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.”

This is just what modulated Fourier expansions are good for, both for continuous problems and their numerical discretisations.

References

- [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.
- [BGG89] 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 II. *Comm. Math. Phys.*, 121:557–601, 1989.
- [CDI09] M. Condon, A. Deaño, and A. Iserles. On highly oscillatory problems arising in electronic engineering. *M2AN*, 43:785–804, 2009.
- [CDI10] M. Condon, A. Deaño, and A. Iserles. On second order differential equations with highly oscillatory forcing terms. *Proc. Royal Soc. A*, 466:1809–1828, 2010.
- [CH11] P. Console and E. Hairer. Long-term stability of symmetric partitioned linear multistep methods. *Preprint*, 2011.
- [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.
- [CHL08a] D. Cohen, E. Hairer, and C. Lubich. Conservation of energy, momentum and actions in numerical discretizations of nonlinear wave equations. *Numer. Math.*, 110:113–143, 2008.
- [CHL08b] D. Cohen, E. Hairer, and C. Lubich. Long-time analysis of nonlinearly perturbed wave equations via modulated Fourier expansions. *Arch. Ration. Mech. Anal.*, 187:341–368, 2008.
- [Coh04] D. Cohen. *Analysis and numerical treatment of highly oscillatory differential equations*. PhD thesis, Univ. Genève, 2004.
- [FGL11] E. Faou, L. Gauckler, and C. Lubich. Sobolev stability of plane wave solutions to the cubic nonlinear Schrödinger equation on a torus. *Preprint*, 2011.
- [FPU55] E. Fermi, J. Pasta, and S. Ulam. Studies of non linear problems. Technical Report LA-1940, Los Alamos, 1955.
- [Gal08] G. Gallavotti, editor. *The Fermi-Pasta-Ulam problem. A status report*, volume 728 of *Lecture Notes in Physics*. Springer, Berlin, 2008.
- [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.
- [Gau10] L. Gauckler. *Long-time analysis of Hamiltonian partial differential equations and their discretizations*. PhD thesis, Univ. Tübingen, 2010.
- [GGMV92] L. Galgani, A. Giorgilli, A. Martinoli, and S. Vanzini. On the

- problem of energy equipartition for large systems of the Fermi-Pasta-Ulam type: analytical and numerical estimates. *Physica D*, 59:334–348, 1992.
- [GH06] V. Grimm and M. Hochbruck. Error analysis of exponential integrators for oscillatory second-order differential equations. *J. Phys. A*, 39(19):5495–5507, 2006.
- [GHLW11] L. Gauckler, E. Hairer, C. Lubich, and D. Weiss. Metastable energy strata in weakly nonlinear wave equations. *Preprint*, 2011.
- [GL10a] L. Gauckler and C. Lubich. Nonlinear Schrödinger equations and their spectral semi-discretizations over long times. *Found. Comput. Math.*, 10:141–169, 2010.
- [GL10b] L. Gauckler and C. Lubich. Splitting integrators for nonlinear Schrödinger equations over long times. *Found. Comput. Math.*, 10:275–302, 2010.
- [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 weakly nonlinear wave equations over long times. *Found. Comput. Math.*, 8:319–334, 2008.
- [HL10] E. Hairer and C. Lubich. On the energy distribution in Fermi-Pasta-Ulam lattices. *Preprint*, 2010.
- [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.
- [QT90] G. D. Quinlan and S. Tremaine. Symmetric multistep methods for the numerical integration of planetary orbits. *Astron. J.*, 100:1694–1700, 1990.
- [SS09] J. M. Sanz-Serna. Modulated Fourier expansions and heterogeneous multiscale methods. *IMA J. Numer. Anal.*, 29:595–605, 2009.
- [Tan93] Y.-F. Tang. The symplecticity of multi-step methods. *Computers Math. Applic.*, 25:83–90, 1993.