Summary: Chapter 6

- In this chapter, we consider *highly oscillatory differential equations* of the form

$$\begin{aligned} \ddot{x} &+ \Omega^2 x = g(x) := -\nabla U(x) \\ x(0) &= \tilde{x}_0,\ \dot{x}(0) = \dot{\tilde{x}}_0, \end{aligned} \tag{1}$$

where $\Omega = \begin{pmatrix} 0 & 0 \\ 0 & \omega I \end{pmatrix}$ with $\omega \gg 1$. We partition the vector $x = (x_0, x_1)$ according to the blocks of the matrix Ω. Moreover, we assume that the initial values are bounded

$$\frac{1}{2}\left\|\dot{\tilde{x}}_0\right\|^2 + \frac{1}{2}\left\|\Omega\tilde{x}_0\right\|^2 \leq E,$$

where the constant E does not depend on ω. We also assume that the potential is *smooth*, i.e. with derivatives bounded independently of ω.

This problem is Hamiltonian with Hamiltonian function given by

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

and has another quantity of interest, the *oscillatory energy*

$$I(x, \dot{x}) = \frac{1}{2}\dot{x}_1^T\dot{x}_1 + \frac{\omega^2}{2}x_1^T x_1.$$

Below, we will show that this quantity is almost preserved for very long time intervals along the exact solution of (1).

Example: Modified Fermi-Pasta-Ulam problem.

- A proper numerical treatment of the above problem is done by the *trigonometric methods*

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

where $g_n := g(\Phi x_n)$ and $\Phi = \Phi(h\Omega), \Psi = \Psi(h\Omega), \Psi_0 = \Psi_0(h\Omega), \Psi_1 = \Psi_1(h\Omega)$ are called *filter functions*, see the yellow book for precise assumptions and examples. One thus obtain a numerical approximation $x_n \approx x(nh)$ of the exact solution of (1).

These numerical methods reduce to the Störmer-Verlet method if $\Omega = 0$; are exact if $g(x) = 0$; are explicit; work well for large step sizes $h\omega \geq c_1 > 0$; and almost preserve the energy $H(x, \dot{x})$ and the oscillatory energy $I(x, \dot{x})$ for very long times, see below.

- The main ingredient to prove the near-preservation of the oscillatory energy along the exact solution of (1) is the *modulated Fourier expansion*. This consists in writing the exact solution as

$$x(t) = y(t) + \sum_{|k|<N} \mathrm{e}^{\mathrm{i}k\omega t} z^k(t) + R_N(t), \quad 0 \le t \le T,$$

  with smooth functions $y(t)$, $z^k(t)$ and with a very small defect $R_N(t) = \mathcal{O}(\omega^{-N})$. Analysing the system that determines the *modulated coefficients* $y(t)$ and $z^k(t)$, one finds two formal invariants that are close to the original energy $H(x,\dot{x})$ and oscillatory energy $I(x,\dot{x})$. This is then used to prove the near-conservation of the oscillatory energy for the exact solution:

$$I(x(t),\dot{x}(t)) = I(\tilde{x}_0,\dot{\tilde{x}}_0) + \mathcal{O}(\omega^{-1}) + \mathcal{O}(t\omega^{-N}), \quad 0 \le t \le \omega^N.$$

- To explain the good long-time behaviour of the numerical solution by the trigonometric methods, we proceed as for the exact solution and write the numerical solution as a modulated Fourier expansion. Following the same program as above and using additional assumptions, one can show that

$$\begin{aligned} H(x_n,\dot{x}_n) &= H(\tilde{x}_0,\dot{\tilde{x}}_0) + \mathcal{O}(h) \\ I(x_n,\dot{x}_n) &= I(\tilde{x}_0,\dot{\tilde{x}}_0) + \mathcal{O}(h) \end{aligned}$$

  along the numerical solution given by the trigonometric methods for $0 \le nh \le h^{-N+1}$.