TRAVELING WAVES AND MONODROMY IN ANHARMONIC LATTICES

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The study of anharmonic lattices can be considerably simplified by imposing a spatial periodicity condition on solutions. This reduces the infinite dimensional lattice equations to a finite dimensional system of ordinary differential equations for which we have at our disposal Birkhoff normal forms, invariant theory, singular reduction and the Kolmogorov Arnol'd Moser theorem. As an example we study the famous Fermi Pasta Ulam lattice for which we find traveling wave solutions. These traveling waves can become unstable and reverse their directions. Moreover, although the lattice is nearly integrable, the integrable approximation has monodromy and hence does not admit global action angle coordinates.

1. Anharmonic lattices

One-dimensional mono-atomic structures such as crystals and nonlinear strings are often modelled as an anharmonic lattice. This lattice consists of an infinite row of point masses that each move in their own on-site potential field and interact with neighbouring masses. Let $q_j \in \mathbb{R}$ ($j \in \mathbb{Z}$) measure the displacement of the j-th particle with respect to a certain reference position and let p_j be its conjugate momentum. Then, under the assumption that all particles are equal and interact only with their nearest neighbours, the Hamiltonian function governing the equations of motion of the anharmonic lattice is

$$H = \sum_{j\in\mathbb{Z}} \frac{1}{2}p_j^2 + V(q_j) + W(q_j - q_{j-1}) \ . \tag{1}$$

Well-known choices for V and W are for instance

- Klein-Gordon lattice: $V(x) = \frac{1}{2}x^2 + \frac{\alpha}{3}x^3 + \ldots$, $W(x) = \frac{1}{2}x^2$
- Fermi Pasta Ulam lattice: $V(x) = 0$, $W(x) = \frac{1}{2}x^2 + \frac{\alpha}{3}x^3 + \ldots$

One can be interested in special solutions of this infinite dimensional system of differential equations. Traveling waves are found from the Ansatz $q_j(t) = \phi(j-ct)$ and solving the functional equation that results for ϕ, see [1]. Breathers on the other hand are spatially localized time-periodic solutions. They can for instance be found by variational methods in spaces of time-periodic functions. But in this paper we shall avoid functional analytic methods by imposing a spatial periodicity condition on solutions. More precisely, after fixing an $n \in \mathbb{N}$, we look for solutions that lie in the fixed point space of the symplectic symmetry

$$R^n : q_j \mapsto q_{j+n} \ , \ p_j \mapsto p_{j+n} \ . \tag{2}$$

The fixed point space Fix $R^n = \{(q,p)|R^n(q,p)=(q,p)\}$ is a $2n$-dimensional invariant manifold for the infinite dimensional flow of the lattice equations and it consists of solutions with spatial period n. Thus we have a finite dimensional subsystem for the variables $(q_1,\ldots,q_n,p_1,\ldots,p_n) \in T^*\mathbb{R}^n$. The Hamiltonian is (1) in which the summation over $\mathbb{Z}$ is replaced by a summation over $\mathbb{Z}/_{n\mathbb{Z}}$. The subsystem is simply described by a finite set of ordinary differential equations.

2. Normal modes

It is natural to make a symplectic Fourier transformation $(q,p) \mapsto (\bar{q},\bar{p})$ on $T^*\mathbb{R}^n$ which is induced from a transformation of the positions:

$$q_j = \sqrt{\frac{2}{n}} \sum_{1 \le k < \frac{n}{2}} \left(\cos(\frac{2\pi jk}{n})\bar{q}_k + \sin(\frac{2\pi jk}{n})\bar{q}_{n-k} \right) + \frac{(-1)^j}{\sqrt{n}}\bar{q}_{\frac{n}{2}} + \frac{1}{\sqrt{n}}\bar{q}_n \tag{3}$$

In the new canonical coordinates, the Hamiltonian reads

$$H = \sum_{k=1}^{n} \frac{1}{2}(\bar{p}_k^2 + \omega_k^2 \bar{q}_j^2) + H_3(\bar{q}) + \ldots = H_2(\bar{q},\bar{p}) + H_3(\bar{q}) + \ldots \tag{4}$$

and it is a perturbation of n harmonic oscillators with frequencies ω_k. From (3) we infer that the normal mode coordinates $\bar{q}_k$ and $\bar{q}_{n-k}$ $(1 \le k < n/2)$ are the Fourier components of respectively a cosine-wave and a sine-wave with wavelength n/k. Moreover, as waves of equal wavelength have of course the same linear vibrational frequency, we note that $\omega_k = \omega_{n-k}$. This means that the Hamiltonian (4) contains many $1:1$-resonances. For example in the Fermi Pasta Ulam lattice the frequencies are given by the well-known formula

$$\omega_k = 2\sin(\frac{k\pi}{n}) \ . \tag{5}$$

3. The Birkhoff normal form

Well-known in the study of Hamiltonian perturbations of harmonic oscillators is the Birkhoff normal form:

Theorem 3.1. *For every $m \geq 3$, there is an open neighbourhood $0 \in U \subset T^*\mathbb{R}^n$ and a symplectic near-identity transformation $\Phi : U \to T^*\mathbb{R}^n$ with the property that*

$$\Phi^* H = H \circ \Phi = \overline{H} + \mathcal{O}(||(\bar{q}, \bar{p})||^m) = \overline{H}_2 + \ldots + \overline{H}_{m-1} + \mathcal{O}(||(\bar{q}, \bar{p})||^m) \quad (6)$$

where the Birkhoff normal form $\overline{H}$ is such that it admits as a symmetry the flow of the linear vector field X_{H_2}.

$\overline{H}$ can be computed explicitly and it is simpler than the original H as it has at least one extra symmetry, the linear flow of X_{H_2}. But in the absense of resonances, that is when apart from the identities $\omega_k = \omega_{n-k}$ there are not many rational relations in the eigenvalues, or if the original H has symmetries, the normal form $\overline{H}$ can be even more symmetric, see for instance theorem 4.1.

Studying $\overline{H}$ of course means making a small approximation error of order $\mathcal{O}(||(\bar{q}, \bar{p})||^m)$. But using for instance Gronwall's lemma, the Kolmogorov Arnol'd Moser theorem and Melnikov functions, one can obtain conclusions about X_H from studying $X_{\overline{H}}$ and thus the Birkhoff normal form is a powerful tool for examining low energy solutions and bifurcations of the perturbed harmonic oscillator H.

4. Example: the Fermi Pasta Ulam lattice

It was proven in [2] that apart from the standard 1 : 1-resonances, low order resonances in the eigenvalues (5) of the Fermi Pasta Ulam lattice are not present or at least in a certain sense harmless due to discrete symmetry. This has many consequences, among which the following:

Theorem 4.1. *Consider the Fermi Pasta Ulam lattice with even potential, i.e. $V(x) = 0$, $W(x) = \frac{1}{2}x^2 + \frac{\beta}{4}x^4 + \mathcal{O}(x^6)$. Then for every $n \in \mathbb{N}$, the Birkhoff normal form $H_2 + \overline{H}_4$ is Liouville integrable.*

This result was proved in [2]. As the normal form is integrable, the flows of the integrals are symmetries. The method of invariant theory allows for an explicit singular reduction of some of these symmetries. The reduced phase spaces are two-dimensional surfaces, some of which have singularities. For example the singular reduced phase space in Figure 1 which is a surface of revolution with the shape of a lemon.

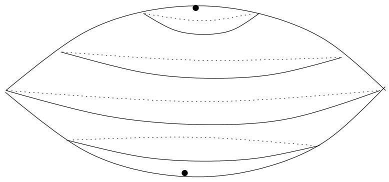

Figure 1. A lemon-shaped singular reduced phase space with a heteroclinic connection.

Figure 1 describes in a reduced setting the interaction between the normal modes $\bar{q}_k, \bar{q}_{n-k}, \bar{q}_{\frac{n}{2}-k}, \bar{q}_{\frac{n}{2}+k}$ and their momenta, which involve the cosine- and sine-waves with wavelengths n/k and $n/(\frac{n}{2}-k)$. Note that hence this situation can only exist if n is even. Every point in the reduced phase space represents a high-dimensional torus in the original phase space $T^*\mathbb{R}^n$ with a dynamical meaning.

The reduced phase space is foliated in level sets of the reduced Hamiltonian. We see two stable relative equilibria, indicated by black dots, surrounded by relative periodic orbits. The equilibria represent dynamically stable quasiperiodic solutions. More interesting are the two cone-like singularities which represent the superposition of two traveling waves with wavelengths n/k and $n/(\frac{n}{2}-k)$, equal energy and equal direction. But they are connected by a heteroclinic connection! Thus, a traveling wave can be destabilized by superposing to it another traveling wave. It turns out that this destabilisation occurs via a Hamiltonian Hopf bifurcation which can be studied explicitly in the reduced context. In Figure 1, the superposed traveling waves are connected by a heteroclinic cycle so that they can reverse directions. This interesting phenomenon can indeed be observed as a relaxation oscillation in numerical integrations of the original lattice equations X_H for various n, see [3].

Moreover, the heteroclinic connection in Figure 1 is reconstructed as a pinched torus in the original phase space. This implies that the integrable Birkhoff normal form has nontrivial monodromy and can not have global action-angle coordinates. It can be expected that this monodromy has impact on the global geometry of the KAM tori of X_H.

References

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