Geometry and dynamics in Hamiltonian lattices

Meetkunde en dynamica in Hamiltoniaanse roosters

(met een samenvatting in het Nederlands)

Proefschrift

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Introduction

Mais ce gentleman ne demandait rien. Il ne voyageait pas, il décrivait une circonférence. C'était un corps grave, parcourant une orbite autour du globe terrestre, suivant les lois de la mécanique rationnelle.

Jules Verne
in *Le tour du monde en quatre-vingts jours*

Physics gives us a number of principles for formulating the equations of motion for a classical mechanical system. There are Newton's laws, which result in a set of second order ordinary differential equations, and there is Hamilton's principle which gives us a variational problem. But classical mechanics does not stop when equations of motion have been written down. In fact, it is nowadays not so difficult to translate a classical mechanical system into a mathematical model or a set of equations. But it can be hard to analyse the model or to solve the equations, especially when they are nonlinear. This explains why our understanding of very simple mechanical systems is often far from complete. Usually we can not make good predictions for their behaviour.

This thesis intends to study some classical mechanical models mathematically, meaning that it tries to uncover the flow properties of certain ordinary differential equations and to give a physical interpretation of these mathematical results. This hopefully helps us to understand and predict the behaviour of some classical mechanical systems.

Classical mechanics

One of the first examples of a mathematical view on a mechanical system is Galilei's description of the motion of a falling object. In 1638, this famous astronomer and mathematical physicist claimed that the speed of a falling object increases every second by the same amount [**25**]. Galilei concludes this from observations and he even argues that this amount should be equal regardless of the mass of the object. Based on observations of Tycho Brahe, Kepler earlier had formulated a set of geometric rules for the motion of the planets [**35**], [**36**]. This is another important early example of a mathematical description of a physical system.

Isaac Newton was the first to write down equations of motion in the way we often meet them now: as a differential equation [**47**]. *Newton's equations* say that the acceleration of a physical object is proportional to the force exerted on that object. For the formulation of his equations, Newton needed the *differential calculus* that he developed at the same time as Leibniz.

Lagrange investigated how Newton's differential equations change under a coordinate transformation and he realised that one can write down the equations of motion in a coordinate invariant way [**39**]. In the modern setting, this means that the correct framework for classical mechanics is *differential geometry* [**62**]. His coordinate invariant equations are nowadays called the *Euler-Lagrange equations.* It turns out that Euler-Lagrange equations can also be found outside classical mechanics, for instance in variational problems. This shows that there is a link between classical mechanics and *variational calculus.*

Finally, Hamilton and Jacobi realised that there is sometimes yet another coordinate invariant way to write down the equations of classical mechanics [**33**]. These are now known as *Hamilton's equations.* The study of Hamiltonian systems is related to *symplectic geometry.*

We see that classical mechanics is closely tied to mathematics. For a long time, mathematical physics and classical mechanics were in fact more or less the same, but nowadays there are rather clear differences between classical and for instance relativistic and quantum mechanics. Throughout modern history, classical mechanics and mathematics have also heavily influenced each other. Fundamental physical questions have often led to the development of new mathematics and certain purely mathematical discoveries turned out to explain physical observations. This interplay has always been very fruitful. The strong relation between mathematics and classical mechanics is nicely illustrated in the standard texts [**1**] and [**42**].

At the end of the nineteenth century, scientists could translate an everyday physical system into a set of differential equations of Newtonian, Lagrangean or Hamiltonian type. But they were not very successful in extracting explicit information from these equations: in spite of their strong belief in mathematics, they could hardly ever write down the solutions to their equations of interest.

Poincaré adopted a new approach towards differential equations and can therefore be seen as the founder of modern dynamical systems theory. In [**51**] he develops several approximation methods, among which the technique of normal forms that is used abundantly in this thesis. He also proposed to study the *geometric* properties of solutions, as an alternative for finding explicit formulas. All this enabled him to draw approximate and qualitative conclusions when exact quantitative results were unattainable. But after Poincaré, the physics community lost its interest in classical mechanics for a while, as the theories of relativity and quantum mechanics seemed more relevant and promising.

Later in the twentieth century, dynamical systems theory rapidly developed after all and it is nowadays more alive than ever. Chaos theory [**76**] and bifurcation analysis [**38**], both already present in the work of Poincaré, are the backbones of this modern field of science. And for Hamiltonian systems, the inspiring Kolmogorov-Arnol'd-Moser (KAM) theorem [**5**] was proved.

Some classical mechanical models have a history which is literally interwoven with the developments in modern classical mechanical research. One of these models is the Fermi-Pasta-Ulam (FPU) lattice. The famous 'Fermi-Pasta-Ulam problem' has become a metaphor for many of our questions about classical and statistical mechanics [**75**].

The Fermi-Pasta-Ulam problem

In this thesis, we will pay much attention to the FPU lattice. This classical mechanical system consists of a one-dimensional chain of interacting particles. It can model a simple one-dimensional atomic structure such as a mono-atomic crystal, a long molecule or a nonlinear string. The lattice was introduced in the 1950s by E. Fermi, J. Pasta and S. Ulam [**21**], who had in mind

'a one-dimensional continuum ...
... with forces acting on the elements of this string.'

The FPU lattice models this string by a discrete number of equal point masses which represent the material elements of the string. Each of the point masses interacts with its nearest neighbours only.

When the forces between the particles of the lattice are linear, then the differential equations that describe their behaviour are also linear and these equations can be solved exactly. In fact, the Hamiltonian system is then Liouville integrable, which implies by the theorem of Liouville-Arnol'd [**2**] that the solutions are periodic or quasi-periodic and move on invariant Lagrangean tori. The model is of course much more interesting when the forces between the particles are nonlinear.

First of all, several authors have tried to find exact low-dimensional invariant manifolds in the nonlinear FPU lattice. These are important because they constitute families of solutions with interesting properties. Most of the invariant manifolds that are known for the FPU lattice were discovered more or less empirically. Fermi, Pasta and Ulam already presented some examples themselves [**21**]. Other invariant manifolds were discovered in [**3**] and [**50**], but these results are not very systematic. A better method should be based on the symmetries in the system. These symmetries are exploited in [**8**] and this leads to interesting conclusions about the FPU lattice, although they are still not complete.

Fermi, Pasta and Ulam were not only interested in exact solutions of the lattice equations, but primarily wanted to study its statistical properties. In fact, they expected that in the presence of nonlinear forces, the lattice would reach a thermal equilibrium, as was predicted by the laws of statistical mechanics [**32**]. In such a thermal equilibrium, the energy of all Fourier modes of the lattice should (averaged over time) be equal. A numerical experiment was performed in Los Alamos, to investigate how and at what time-scale a thermal equilibrium would be attained. The result was astonishing: the lattice did not even come close to thermal equilibrium, but behaved more or less quasi-periodically. Only when the initial energy was larger than a certain threshold, did the lattice indeed seem to 'thermalise'. This paradox is nowadays known as the 'Fermi-Pasta-Ulam problem'.

The computer experiment of Fermi, Pasta and Ulam is famous now and their stunning observations greatly stimulated the work in nonlinear dynamics after 1960 [**75**]. One possible explanation for the quasi-periodic behaviour of the FPU system, is based on the KAM theorem [**5**]. This theorem states that most of the invariant

Lagrangean tori of a Liouville integrable Hamiltonian system survive when this integrable system is perturbed a bit. It is required though for the KAM theorem that the integrable system satisfies a certain nondegeneracy condition, called *Kolmogorov's condition*.

Many authors, starting with Izrailev and Chirikov [**31**], have stated that the KAM theorem explains why the FPU lattice behaves quasi-periodically. This seems plausible, as the FPU system can be viewed as a small nonlinear perturbation of its integrable linearisation. But, as was clearly pointed out in [**22**] and [**75**], this linearisation does not satisfy Kolmogorov's nondegeneracy condition at all. It is hence completely unclear how the KAM theorem can be used.

Nishida, in 1971 [**48**], and Sanders, in 1977 [**61**], tried to overcome this problem by investigating a Birkhoff normal form for the FPU lattice. Under the assumption of a rather strong nonresonance condition on the linear frequencies of the lattice, they showed that this Birkhoff normal form is integrable and satisfies Kolmogorov's condition. This means that the KAM theorem can be applied. The problem is of course that the required nonresonance condition is actually not met in the generic situation. This leaves a large gap in their proofs.

Outline of this thesis

In Chapter 1 we describe the FPU lattice in more detail. Using symmetry methods we then start looking for invariant manifolds in the lattice. These invariant manifolds are the fixed point sets of the discrete symmetries of the lattice. We arrive at previously unknown results with a minimum of computational trouble. This chapter can therefore be considered as a continuation of [**8**]. Moreover, it is shown that the same invariant manifolds exist in the Klein-Gordon (KG) lattice and in thermodynamic and continuum limits of various lattices.

Chapter 2 forms the central part of this thesis. It starts with a discussion on the FPU problem. Then we adopt the approach of Nishida and Sanders and compute a Birkhoff normal form for the FPU lattice. A new idea is to incorporate symmetries in our arguments. This enables us to show that the nonresonance condition of Nishida and Sanders is not needed: every resonance is in some sense overruled by a symmetry. The Birkhoff normal form of the FPU lattice is hence integrable in many cases and often it also satisfies the nondegeneracy condition of Kolmogorov. According to the KAM theorem this proves the existence of many invariant tori on which the motion is quasi-periodic.

In Chapter 3 we perform a dynamical analysis of the lattice normal form and we give a physical interpretation of the results. A particularly nice phenomenon occurs in the quartic FPU lattice with periodic boundary conditions and an even number of particles. Its Birkhoff normal form is integrable and the integrable foliation of the phase space is singular. We can show that the singular objects are pinched tori and that the regular tori have nontrivial monodromy. The monodromy is an obstruction to the existence of global action-angle variables. The pinched tori are homoclinic and heteroclinic connections between travelling waves. Thus we discover a class of 'direction reversing travelling waves'. We observe these waves numerically in the original FPU system.

Having found pinched tori and monodromy in a Birkhoff normal form, we investigate in Chapter 4 how robust these phenomena are under Hamiltonian perturbations, as this may explain the numerical observations of Chapter 3. Not only can we prove that the Kolmogorov condition is always met near a pinched torus, but we also show that the monodromy of the integrable system can still be observed in the KAM tori of the nonintegrable perturbation.

Chapter 5 deals with a different problem, but shows that our methods also work in another setting. We analyse a parametrically forced spring-pendulum. Pendulums and spring-pendulums have always been popular objects of study in classical mechanics, see [**68**]. The spring-pendulum of Chapter 5 is parametrically excited by an external force. This parametric excitation can for instance be a crude model for a complicated dynamical system coupled to our spring-pendulum, such as a chain of spring-pendula. We design a time-dependent normal form theory for nonautonomous Hamiltonian systems and compute and analyse the normal form of our forced spring-pendulum. It turns out that the system can be full of interesting phenomena such as homoclinic orbits and multi-pulse solutions. But we can also find invariant tori again.

Several parts of this thesis have appeared previously as journal articles, in proceeding volumes or as a preprint. The references are:

B. Rink and F. Verhulst, *Near-integrability of periodic FPU-chains*, Physica A **285** (2000), 467-482.

B. Rink, *Symmetry and resonance in periodic FPU chains*, Commun. Math. Phys. **218** (2001), 665-685.

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B. Rink, *Symmetric invariant manifolds in the Fermi-Pasta-Ulam lattice*, Physica D **175** (2003), 31-42.

B. Rink, *A symmetric normal form for the Fermi Pasta Ulam chain* in the proceedings of the international conference SPT2001, D. Bambusi et al. (eds.), World Scientific, Singapore, 2001, pp. 175-182.

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CHAPTER 1

Symmetric invariant manifolds

We give a mathematical description of the Fermi-Pasta-Ulam (FPU) lattice and introduce the famous quasi-particles for this Hamiltonian system. After this introduction, we remark that the FPU lattice with periodic boundary conditions and n particles admits a large group of discrete symmetries. The fixed point sets of these symmetries naturally form invariant symplectic manifolds that are investigated in this chapter. For each m dividing n we find m degree of freedom invariant manifolds. They represent short wavelength solutions composed of m Fourier-modes and can be interpreted as embedded lattices with periodic boundary conditions and only m particles. Inside these invariant manifolds other invariant structures and exact solutions are found which represent for instance periodic and quasi-periodic solutions. Some of these results have been found previously by other authors via a study of mode coupling coefficients and recently also by investigating 'bushes of normal modes'. The method of this chapter is similar to the latter method and more systematic than the former. We arrive at previously unknown results without any difficult computations. It is shown moreover that similar invariant manifolds exist in the Klein-Gordon (KG) lattice and in the thermodynamic and continuum limits. This chapter is based on references [**56**] and [**57**].

1.1. Background

The Fermi-Pasta-Ulam (FPU) lattice is the famous discrete model for a continuous nonlinear string, introduced by E. Fermi, J. Pasta and S. Ulam [**21**]. It models the string by a finite number of equal point masses which represent the material elements of the string. Each of these point masses interacts with its nearest neighbours only. The physical variables of the lattice are the positions q_j of the particles, see Figure 1, and their conjugate momenta p_j.

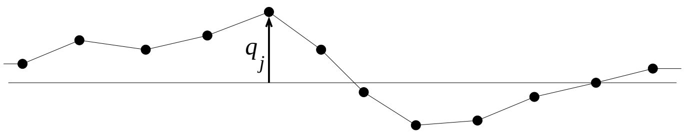

Figure 1: Schematic picture of the FPU lattice.

The FPU lattice may consist of a countable infinity of particles, but in this chapter we will mainly assume that there are only finitely many. We label them $j = 1, \ldots, n$.

We can distinguish different types of boundary conditions. We speak of fixed boundary conditions if the first and the last particle do not move, meaning that we have $q_0 = q_{n+1} = 0$ for all time. The FPU lattice with fixed boundary conditions models for instance a string with Dirichlet boundary conditions. It is also possible to choose periodic boundary conditions, in which case the first and the last particle are identified, that is $q_0 = q_n$ for all time. The FPU lattice with periodic boundary conditions can model for instance a spatially periodic molecule or mono-atomic structure. Both types of boundary conditions occur very often in the literature [**32**]. In this chapter we shall only consider lattices with periodic boundary conditions, as it will become clear that each lattice with fixed boundary conditions is naturally embedded as an invariant manifold of an appropriate periodic lattice. The particles of the periodic lattice are naturally labelled by elements of the cyclic group $\mathbb{Z}/_{n\mathbb{Z}}$.

The Hamiltonian equations of motion for the periodic FPU lattice are then formulated as follows. The space of positions $q = (q_1, \ldots, q_n)$ of the particles is $\mathbb{R}^n$ and the space of positions and conjugate momenta is the $2n$-dimensional cotangent bundle $T^*\mathbb{R}^n$ of $\mathbb{R}^n$ with coordinates $(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n)$. $T^*\mathbb{R}^n$ is a symplectic manifold with the canonical symplectic form $dq \wedge dp := \sum_{j=1}^n dq_j \wedge dp_j$. Given a Hamiltonian function $H : T^*\mathbb{R}^n \to \mathbb{R}$, the Hamiltonian vector field X_H on $T^*\mathbb{R}^n$ is defined by the relation $(dq \wedge dp)(X_H, \cdot) = dH$. In other words,

$$X_H = \sum_{j=1}^{n} \frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j}$$

The integral curves of X_H are hence the solutions of the ordinary differential equations

$$\dot{q}_j = \frac{\partial H}{\partial p_j}\ ,\ \dot{p}_j = -\frac{\partial H}{\partial q_j}$$

For the periodic FPU lattice, the Hamiltonian function is the sum of the kinetic energies of all the particles and the interparticle potential energies:

$$H = \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2}p_j^2 + W(q_{j+1} - q_j) \tag{1.1}$$

in which $W : \mathbb{R} \to \mathbb{R}$ is traditionally a potential energy density function of the form

$$W(x) = \frac{1}{2!}x^2 + \frac{\alpha}{3!}x^3 + \frac{\beta}{4!}x^4 \tag{1.2}$$

The parameters α and β measure the nonlinearities in the forces between the particles in the lattice. We also write

$$H = \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \left(\frac{1}{2}p_j^2 + \frac{1}{2}(q_{j+1} - q_j)^2\right) + \alpha H_3(q) + \beta H_4(q)$$

in which

$$H_r(q) = \frac{1}{r!}\sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} (q_{j+1} - q_j)^r$$

is a polynomial in q of degree r.

Several authors have tried to find exact low dimensional invariant manifolds for the FPU lattice. First of all because they represent interesting classes of solutions such as periodic and quasi-periodic solutions and standing and travelling waves. But also because it is believed by some authors, see for instance [**6**], that the destabilisation of invariant manifolds can lead to chaos and hence maybe to a sort of ergodicity that can lead to thermalisation of the lattice. As thermalisation has never been observed at low energies, this destabilisation should then of course occur above some energy threshold. The present chapter is inspired by the idea that the results of [**54**], which were primarily obtained for FPU lattices with periodic boundary conditions, will to a large extent also be applicable to subsystems of these periodic lattices. We will see for instance that every FPU lattice with fixed boundary conditions can be viewed as such a subsystem.

Most of the invariant manifolds that are known in the FPU lattice were discovered more or less empirically. In their original paper Fermi, Pasta and Ulam [**21**] already remarked that if the nonlinearity coefficient α in (1.2) vanishes and initially only waves with an odd wave number are excited, then waves with an even wave number will never gain energy. Later on, other invariant manifolds were discovered by studying mode coupling coefficients in detail, see for instance [**3**] and [**50**]. In these papers it is shown that certain sets of normal modes will not be excited if they initially have no energy.

As will be explained in Section 1.2, studying mode coupling coefficients can be quite unsatisfactory. A more systematic method for finding invariant manifolds in a physical system should be based on the symmetries of this system. The only reference that exploits these symmetries for the FPU lattice is [**8**] in which so-called 'bushes of normal modes' are computed. These 'bushes' are simply invariant manifolds of a certain type. Their definition and how to find them are discussed more elaborately in [**9**]. The basic idea is the well-known physical principle that the fixed point set of a symmetry forms an invariant manifold for the equations of motion. In [**8**], several previously unknown 'bushes' are classified. After computing the irreducible representations of the symmetry group of the FPU lattice and introducing appropriate 'symmetry-adapted coordinates', the computation of these 'bushes of normal modes' is fairly simple.

In this chapter it will be shown that the previously mentioned invariant manifolds and many others can be found even without introducing Fourier modes and studying mode coupling coefficients and without computing irreducible representations or symmetry-adapted coordinates. We only have to compute the fixed point sets of the various symmetries. As we incorporate more symmetries than [**8**] in our considerations, we find various invariant manifolds that were not discussed before, in particular for the so-called β-lattice. Moreover, our results are not only valid for the FPU lattice, but for any lattice with the same symmetries, such as the Klein-Gordon (KG) lattice [**46**]. They also apply in the thermodynamic limit as the number of particles grows large, and in the continuum limit: we can point out several infinite dimensional invariant manifolds for a rather broad class of nonlinear homogeneous partial differential equations.

1.2. Quasi-particles

Since we want to be able to compare our results with previous work, we introduce Fourier modes in this section. These Fourier modes are at the same time the 'symmetry-adapted coordinates' of [**8**]. It is natural to view the solutions of the FPU lattice as a superposition of waves and to make the following Fourier transformation:

$$q_j = \frac{1}{\sqrt{n}} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} e^{\frac{2\pi i j k}{n}} \bar{q}_k \quad , \quad p_j = \frac{1}{\sqrt{n}} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} e^{-\frac{2\pi i j k}{n}} \bar{p}_k \tag{1.3}$$

Using that

$$\frac{1}{n} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} e^{\frac{2\pi i j k}{n}} = \begin{cases} 1 & \text{if } j = 0 \bmod n \\ 0 & \text{if } j \neq 0 \bmod n \end{cases}$$

one easily calculates that the inverse mapping reads

$$\bar{q}_k = \frac{1}{\sqrt{n}} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} e^{-\frac{2\pi i j k}{n}} q_j \quad , \quad \bar{p}_k = \frac{1}{\sqrt{n}} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} e^{\frac{2\pi i j k}{n}} p_j \tag{1.4}$$

Moreover, it is readily seen that $\{\bar{q}_k, \bar{q}_{k'}\} = \{\bar{p}_k, \bar{p}_{k'}\} = 0$ and $\{\bar{q}_k, \bar{p}_{k'}\} = \delta_{kk'}$, the Kronecker delta. Hence, $(\bar{q}, \bar{p})$ are canonical coordinates. They are traditionally called *phonons* or *quasi-particles*. Written out in phonons, the FPU Hamiltonian (1.1) reads as follows. The kinetic energy becomes:

$$\sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2} p_j^2 = \frac{1}{2} \bar{p}_n^2 + \frac{1}{2} \bar{p}_{\frac{n}{2}}^2 + \sum_{1 \leq k < \frac{n}{2}} \bar{p}_k \bar{p}_{n-k}$$

where it is understood that the term $\frac{1}{2}\bar{p}_{\frac{n}{2}}^2$ occurs only if n is even. The potential energies H_r (for $r = 2, 3, 4$) become

$$\begin{aligned} H_r &= \frac{1}{r!} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} (q_{j+1} - q_j)^r \\ &= \frac{1}{r!} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \left(\frac{1}{\sqrt{n}} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} (e^{\frac{2\pi i (j+1) k}{n}} - e^{\frac{2\pi i j k}{n}}) \; \bar{q}_k \right)^r \\ &= \frac{1}{r! n^{\frac{r}{2}}} \sum_{\substack{j \in \mathbb{Z}/_{n\mathbb{Z}} \\ \theta : |\theta| = r}} \binom{r}{\theta} e^{\frac{2\pi i j (\Sigma_k k \theta_k)}{n}} \prod_{k \in \mathbb{Z}/_{n\mathbb{Z}}} (e^{\frac{2\pi i k}{n}} - 1)^{\theta_k} \; \bar{q}_k^{\;\theta_k} \\ &= n^{\frac{2-r}{2}} \sum_{\substack{\theta : |\theta| = r \\ \Sigma_k k \theta_k = 0 \bmod n}} \prod_{k \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{\theta_k!} (e^{\frac{2\pi i k}{n}} - 1)^{\theta_k} \; \bar{q}_k^{\;\theta_k} \end{aligned}$$

in which the sum is taken over those multi-indices $\theta \in \mathbb{Z}^n_{\geq 0}$ for which $|\theta| := \sum_k \theta_k = r$. We also used notation for the multinomial coefficient $\binom{r}{\theta} := \frac{r}{\Pi_k \theta_k!}$. We have obtained a rather compact and tractable formula for the Hamiltonian in phonon coordinates.

Let us also introduce real-valued phonons. For $1 \le k < \frac{n}{2}$ define

$$Q_k = (\bar{q}_k + \bar{q}_{n-k})/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \cos(\frac{2jk\pi}{n}) q_j$$

$$Q_{n-k} = i(\bar{q}_k - \bar{q}_{n-k})/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \sin(\frac{2jk\pi}{n}) q_j$$

$$P_k = (\bar{p}_k + \bar{p}_{n-k})/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \cos(\frac{2jk\pi}{n}) p_j$$

$$P_{n-k} = i(\bar{p}_{n-k} - \bar{p}_k)/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \sin(\frac{2jk\pi}{n}) p_j$$

and

$$Q_{\frac{n}{2}} = \bar{q}_{\frac{n}{2}} = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^j q_j \ , \ P_{\frac{n}{2}} = \bar{p}_{\frac{n}{2}} = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^j p_j$$

$$Q_n = \bar{q}_n = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} q_j \ , \ P_n = \bar{p}_n = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} p_j$$

The phonons (Q, P) are Fourier coefficients of sine and cosine wave-patterns in the lattice. For $1 \le k \le \frac{n}{2}$, the normal modes (Q_k, P_k) and (Q_{n-k}, P_{n-k}) both represents waves with wave number k.

The transformation $(q, p) \mapsto (Q, P)$ is again symplectic and one can express the Hamiltonian in terms of Q and P. In the case that $\alpha = \beta = 0$, that is for the harmonic lattice, one gets (see [**32**], [**50**] or [**59**])

$$H = \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2} p_j^2 + \frac{1}{2}(q_{j+1} - q_j)^2 = \sum_{k=1}^{n} \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2)$$

in which for $k = 1, \ldots, n$ the numbers ω_k are the well-known normal mode frequencies of the periodic FPU lattice:

$$\omega_k := 2 \sin(\frac{k\pi}{n})$$

Written down in real-valued phonon coordinates, the equations of motion of the harmonic lattice are simply the equations for $n - 1$ uncoupled harmonic oscillators and, as $\omega_n = 0$, one free particle. The situation is not so simple anymore if $\alpha, \beta \ne 0$.

Note however that whatever the values of α and β are, H is independent of $Q_n = \bar{q}_n = \frac{1}{\sqrt{n}} \sum_j q_j$. Hence the total momentum $P_n = \bar{p}_n = \frac{1}{\sqrt{n}} \sum_j p_j$ is a constant of motion and the equations for the remaining variables are completely independent of $(Q_n, P_n) = (\bar{p}_n, \bar{q}_n)$. It is common to set the latter coordinates equal to zero, or to neglect them completely. Thus one removes the total momentum from the equations of motion. Equivalently, one could also perform the Marsden-Weinstein reduction of the symmetry with infinitesimal generator $X_{P_n} = \frac{\partial}{\partial Q_n}$, cf. [**1**] or [**54**]. One remains with a system on $T^*\mathbb{R}^{n-1}$ with coordinates $(Q_1,\dots,Q_{n-1},P_1,\dots,P_{n-1})$. As $\omega_1,\dots,\omega_{n-1}>0$, we can conclude by the Morse-Lemma or Dirichlet's theorem [**1**], that the origin $(Q,P)=0$ is a dynamically stable equilibrium of this reduced system.

Nevertheless, in the nonlinear system the normal modes interact in a complicated manner that is governed by the Hamiltonians

$$H_r = \sum_{\theta:|\theta|=r} c_\theta \prod_{k=1}^{n-1} Q_k^{\theta_k}$$

in which the c_θ are certain coefficients. An expression for the c_θ can in principle be obtained from the formulas for the Hamiltonian $H_r(\bar{q})$ and the mapping $\bar{q}\mapsto Q$. For instance $H_4(Q)$ can explicitly be found in [**50**], although its computation is not given there. Luckily, not every possible coupling term occurs in the Hamiltonian equations of motion. Only those monomials $\bar{q}^{\,\theta}=\prod_k \bar{q}_k^{\,\theta_k}$ are present in $H_r(\bar{q})$ for which $\sum_k k\theta_k = 0 \bmod n$, whereas $H_r(Q)$ contains only the monomials $Q^\theta=\prod_k Q_k^{\theta_k}$ for which $c_\theta\neq 0$. In the next section we will see that this is a consequence of discrete symmetries in the system.

It is exactly the fact that not every coupling term occurs which accounts for the existence of various invariant manifolds, see [**3**] and [**50**]. Let $\mathcal{A}\subset \mathbb{Z}/_{n\mathbb{Z}}$. Then the manifold spanned by modes in $\mathcal{A}$ is

$$M_n^{\mathcal{A}} := \{(Q,P)\in T^*\mathbb{R}^n | Q_k = P_k = 0 \ \forall\ k\notin\mathcal{A}\}$$

In several cases, these $M_n^{\mathcal{A}}$ are invariant manifolds for the equations of motion. In [**8**] and [**9**] they are then called 'bushes of normal modes'. We will not use this terminology. One readily infers from the equations of motion $\dot{Q}_k=\frac{\partial H}{\partial P_k},\ \dot{P}_k=-\frac{\partial H}{\partial Q_k}$ that $M_n^{\mathcal{A}}$ is an invariant manifold (a 'bush') if and only if $c_\theta=0$ for all θ with the property that $\theta_k=1$ for some $k\notin\mathcal{A}$ and $\theta_{k'}=0$ for all $k'\notin\mathcal{A}\cup\{k\}$. Making use of this fact, several invariant manifolds have been discovered. If n is even, one can for instance choose $\mathcal{A}=\{\frac{n}{2}\}$. It is then obvious that $\mathcal{A}$ satisfies the required property since $k+(r-1)\frac{n}{2}\neq 0 \mod n$. The solutions in the invariant manifold $M_n^{\{\frac{n}{2}\}}$ are of the form $q_j(t)=\frac{(-1)^j}{\sqrt{n}}Q_{\frac{n}{2}}(t)$. This type of periodic solutions in which neighbouring particles are exactly out of phase, is well-known. In [**50**] a linear stability analysis is given for this solution in the β-lattice (i.e. $\alpha=0$) and in [**8**] a similar linear stability analysis is given for this solution in the α-lattice (i.e. $\beta=0$).

Studying mode coupling coefficients in this way, it was shown in [**3**] that if $\alpha=0$ and n is even, $M_n^{\{2,4,\dots,n\}}$ and $M_n^{\{1,3,\dots,n-1\}}$ are invariant. Poggi and Ruffo [**50**] show that $M_n^{\{\frac{n}{3},\frac{2n}{3}\}}$ and $M_n^{\{\frac{n}{4},\frac{3n}{4}\}}$ are invariant.

The above method is rather simple and easily understood but has the following limitations:

1. An explicit expression for the c_θ is required.
2. The method becomes more elaborate if one wants to find invariant manifolds of higher dimensions.

3. There is no a priori ‘physical’ reason why a certain $M_n^{\mathcal{A}}$ will be invariant.
4. Invariant manifolds might exist that are not of the form $M_n^{\mathcal{A}}$ for some $\mathcal{A} \subset \mathbb{Z}/_{n\mathbb{Z}}$.
5. It is not clear whether the discovered invariant manifolds will also be present in the continuum limit or in other one-dimensional lattice systems.

For these reasons, studying mode coupling coefficients is rather unsatisfactory. With the method presented in the following sections of this chapter it is possible to detect easily many more invariant manifolds. They arise in a natural way as fixed point sets of symmetries.

1.3. Symmetry

The Hamiltonian function (1.1) of the periodic FPU lattice has discrete symmetries with important dynamical consequences. Let us first discuss symmetries in general. Assume that $P : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ is a linear isomorphism with the following two properties:

1. P is symplectic, i.e. $P^*(dq \wedge dp) = dq \wedge dp$.
2. P leaves the Hamiltonian invariant, i.e. $P^*H := H \circ P = H$.

Under these assumptions, P is called a linear symmetry of H. The set of linear symmetries of H is a group under composition of functions. This group is denoted G_H.

For every symmetry $P \in G_H$ we find that the Hamiltonian vector field X_H induced by H is equivariant under P: $P^*X_H = X_{P^*H} = X_H$. For fixed but arbitrary $(q,p) \in T^*\mathbb{R}^n$, let $\gamma(t) = (P^{-1} \circ e^{tX_H} \circ P)(q,p)$. Then $\gamma(0) = (q,p)$ and $\gamma'(t) = P^*X_H(q,p) = X_H(q,p)$, so that also $\gamma(t) = e^{tX_H}(q,p)$. This implies that P commutes with the flow of X_H, that is $e^{tX_H} \circ P = P \circ e^{tX_H}$. Moreover, P sends integral curves of X_H to integral curves of X_H.

Of particular dynamical interest is the fixed point set of a symmetry P,

$$\mathrm{Fix}\, P = \{(q,p) \in T^*\mathbb{R}^n | P(q,p) = (q,p)\} \tag{1.5}$$

$\mathrm{Fix}\, P = \ker(P - \mathrm{Id})$ is a linear subspace of $T^*\mathbb{R}^n$. Let $(q,p) \in \mathrm{Fix}\, P$, then $P(e^{tX_H}(q,p)) = e^{tX_H}(P(q,p)) = e^{tX_H}(q,p)$. So Fix P is an invariant manifold for the flow of X_H. This explains why fixed point sets are so interesting.

When $G \subset G_H$ is a subgroup, then a fixed point set is also defined for it: Fix $G = \cap_{P \in G} \mathrm{Fix}\, P$. These are of course also invariant manifolds and they are commonly studied.

Fixed point sets of symmetries and fixed point sets of subgroups have a very simple relation. When $P_1, \ldots, P_m$ are symmetries, then $G = \langle P_1, \ldots, P_m \rangle \subset G_H$ is by definition the smallest subgroup of G_H containing $P_1, \ldots, P_m$. The symmetries $P_1, \ldots, P_m$ are called generators for this subgroup. One readily checks now that $\mathrm{Fix}\langle P_1, \ldots, P_m \rangle = \cap_j \mathrm{Fix}\, P_j$. It therefore suffices to study the fixed point sets of separate symmetries. If G is a subgroup of G_H that is generated by the symmetries $P_1, \ldots, P_m$, then the fixed point set of G is simply the intersection of the fixed point sets of the separate symmetries $P_1, \ldots, P_m$. As the number of elements of G can be considerably less then the number of subgroups of G, we prefer to study fixed point sets of separate symmetries first and take their intersections later.

If we assume that G is compact, then its elements are semi-simple (i.e. complex-diagonalisable) and therefore Fix G is a symplectic subspace of $T^*\mathbb{R}^n$. This implies that whenever H is symmetric under G, $X_{(H|_{\mathrm{Fix}\,G})} = (X_H)|_{\mathrm{Fix}\,G}$ on Fix G.

Let us discuss the symmetries of the FPU lattice now. Define the linear mappings $R, S, T : \mathbb{R}^n \to \mathbb{R}^n$ by

$$\begin{aligned} R &: (q_1, q_2, \ldots, q_{n-1}, q_n) \mapsto (q_2, q_3, \ldots, q_n, q_1) \\ S &: (q_1, q_2, \ldots, q_{n-1}, q_n) \mapsto (-q_{n-1}, -q_{n-2}, \ldots, -q_1, -q_n) \\ T &: (q_1, q_2, \ldots, q_{n-1}, q_n) \mapsto (-q_1, -q_2, \ldots, -q_{n-1}, -q_n) \end{aligned} \tag{1.6}$$

The mappings $(q,p) \mapsto (Rq, Rp)$, $(q,p) \mapsto (Sq, Sp)$ and $(q,p) \mapsto (Tq, Tp)$ from $T^*\mathbb{R}^n$ to $T^*\mathbb{R}^n$ are also denoted R, S and T respectively. They satisfy the multiplication relations $R^n = S^2 = T^2 = \mathrm{Id}$ and $RS = SR^{-1}$, while T commutes with everything. Hence the finite group $\langle R, S\rangle := \{\mathrm{Id}, R, R^2, \ldots, R^{n-1}, S, RS, \ldots, R^{n-1}S\}$ is a representation of the n-th dihedral group D_n, the symmetry group of the n-gon, whereas $\langle R, S, T\rangle$ is a representation of $D_n \times \mathbb{Z}/_{2\mathbb{Z}}$.

R, S and T are symplectic maps and R and S leave the Hamiltonian H invariant. T leaves H invariant only if the potential energy density function W is an even function, in other words if $\alpha = 0$. When $\alpha \neq 0$, then $\langle R, S\rangle$ is the symmetry group of H, whereas $\langle R, S, T\rangle$ is the symmetry group when W is even[1].

In the coming sections we shall investigate the various invariant manifolds Fix P for symmetries P. We shall describe them in terms of the original coordinates (q,p), but also in phonon-coordinates $(\bar{q}, \bar{p})$ and (Q, P). Therefore it is interesting to write down how R, S and T act in complex phonon coordinates:

$$\begin{aligned} R :&(\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_{n-1}, \bar{q}_n) \mapsto (e^{2\pi i/n}\bar{q}_1, e^{4\pi i/n}\bar{q}_2, \ldots, e^{2\pi i(n-1)/n}\bar{q}_{n-1}, e^{2\pi i n/n}\bar{q}_n) \\ &(\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_{n-1}, \bar{p}_n) \mapsto (e^{-2\pi i/n}\bar{p}_1, e^{-4\pi i/n}\bar{p}_2, \ldots, e^{-2\pi i(n-1)/n}\bar{p}_{n-1}, e^{-2\pi i n/n}\bar{p}_n) \\ S :&(\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_{n-1}, \bar{q}_n) \mapsto (-\bar{q}_{n-1}, -\bar{q}_{n-2}, \ldots, -\bar{q}_1, -\bar{q}_n) \\ &(\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_{n-1}, \bar{p}_n) \mapsto (-\bar{p}_{n-1}, -\bar{p}_{n-2}, \ldots, -\bar{p}_1, -\bar{p}_n) \\ T :&(\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_{n-1}, \bar{q}_n) \mapsto (-\bar{q}_1, -\bar{q}_2, \ldots, -\bar{q}_{n-1}, -\bar{q}_n) \\ &(\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_{n-1}, \bar{p}_n) \mapsto (-\bar{p}_1, -\bar{p}_2, \ldots, -\bar{p}_{n-1}, -\bar{p}_n) \end{aligned} \tag{1.8}$$

Note that by performing the transformation to complex phonons, R has been diagonalised whereas the actions of S and T have not at all changed. This means that

[1]The FPU Hamiltonian also has a reversing symmetry, namely the mapping

$$U : q \mapsto q \ , p \mapsto -p \tag{1.7}$$

U leaves the FPU Hamiltonian invariant, i.e. $U^*H = H$, and is anti-symplectic in the sense that $U^*(dq \wedge dp) = -dq \wedge dp$. This implies that the vector field X_H is anti-equivariant under U: $U^*X_H = -X_H$. In other words: if $t \mapsto \gamma(t)$ is an integral curve of X_H, then so is $t \mapsto U(\gamma(-t))$. More information on reversing symmetries can be found in [**40**].

$(\bar{q}, \bar{p})$ are what in [**8**] is called 'symmetry-adapted coordinates'. They are actually adapted to $\langle R \rangle$. The action of R on a monomial $\bar{q}^{\,\theta}$ is also very simple:

$$R^* \left(\prod_k \bar{q}_k^{\,\theta_k} \right) = e^{2\pi i \Sigma_k k\theta_k/n} \prod_k \bar{q}_k^{\,\theta_k}$$

In other words, the monomial $\bar{q}^{\,\theta}$ is R-symmetric if and only if $\sum_k k\theta_k = 0 \bmod n$. So R-symmetry is the reason why only these monomials occur in the FPU Hamiltonian.

1.4. Invariant manifolds for arbitrary potentials

In this section we study the invariant manifolds that are formed by the fixed point sets of elements of $\langle R, S\rangle \cong D_n$. So it is not yet assumed that the potential energy density function W is even.

For integers n and m, let $\gcd(n, m)$ be the greatest common divisor of n and m. For $m \in \mathbb{Z}$,

$$\mathrm{Fix}\, R^m = \{q_j = q_{j+\gcd(n,m)}, p_j = p_{j+\gcd(n,m)} \ \forall\ j\}$$

is an invariant $\gcd(n, m)$ degree of freedom symplectic submanifold of $T^*\mathbb{R}^n$. The Hamiltonian function $H|_{\mathrm{Fix}\, R^m}$ on the symplectic submanifold Fix R^m obviously simply models the periodic FPU lattice with $\gcd(n, m)$ particles. In this way, the periodic lattice with m particles is naturally embedded in the lattice with n particles if m divides n. In phonon coordinates,

$$\begin{aligned} \mathrm{Fix}\, R^m =& \{\bar{q}_k = \bar{p}_k = 0 \ \forall k \neq 0 \ \mathrm{mod}\ \frac{n}{\gcd(n,m)}\} \\ =& \{Q_k = P_k = 0 \ \forall k \neq 0 \ \mathrm{mod}\ \frac{n}{\gcd(n,m)}\} \end{aligned}$$

So if m divides n, then Fix $R^m = M_n^{\{\frac{n}{m}, \frac{2n}{m}, \ldots, \frac{(m-1)n}{m}, n\}}$ and is hence spanned by modes which represent a repeating spatial pattern with period m.

If for instance n is even, then Fix $R^2 = M_n^{\{\frac{n}{2}, n\}}$ is the two degree of freedom invariant manifold spanned by the $\frac{n}{2}$-th and the n-th normal modes. If we as usual neglect the n-th mode, which moves independently of all other modes, we find that $\mathrm{Fix}\, R^2$ consists of all solutions of the form $q_j(t) = \frac{(-1)^j}{\sqrt{n}} Q_{\frac{n}{2}}(t)$. These are the previously mentioned periodic solutions in which neighbouring particles are exactly out of phase. On the other hand one has for even n that $\mathrm{Fix}\, R^{\frac{n}{2}} = M_n^{\{2,4,\ldots,n\}}$. It consists of all even modes.

If 3 divides n, then $\mathrm{Fix}\, R^3 = M_n^{\{\frac{n}{3}, \frac{2n}{3}, n\}}$, whereas Fix $R^{\frac{n}{3}} = M_n^{\{3,6,\ldots,n-3,n\}}$. Etcetera. These invariant manifolds were discussed already extensively in [**8**].

The following invariant manifolds are only briefly discussed in [**8**]. For arbitrary $l \in \mathbb{Z}$ we can study

$$\begin{aligned} &\mathrm{Fix}\, R^l S = \{q_j = -q_{l-j}, p_j = -p_{l-j} \ \forall j\} = \{\bar{q}_k = -e^{-\frac{2\pi i k l}{n}} \bar{q}_{n-k} \ , \ \bar{p}_k = -e^{\frac{2\pi i k l}{n}} \bar{p}_{n-k} \ \forall k\} = \\ &\{Q_k \cos(\frac{lk\pi}{n}) + Q_{n-k} \sin(\frac{lk\pi}{n}) = P_k \cos(\frac{lk\pi}{n}) + P_{n-k} \sin(\frac{lk\pi}{n}) = 0 \ \forall\ 1 \leq k < \frac{n}{2} \ , \\ &Q_{\frac{n}{2}} = (-1)^{l+1} Q_{\frac{n}{2}} \ , \ P_{\frac{n}{2}} = (-1)^{l+1} P_{\frac{n}{2}} \ , \ Q_n = P_n = 0\} \end{aligned}$$

It is a $(2n-2-(-1)^l-(-1)^{n+l})/4$ degree of freedom symplectic subspace of $T^*\mathbb{R}^n$.

Note that $\mathrm{Fix}\, R^lS$ is not always of the form $M_n^{\mathcal{A}}$ for some $\mathcal{A}$. On the other hand, $\mathrm{Fix}\, S = M_n^{\{k|\frac{n}{2}<k<n\}}$ and if n is even, then $\mathrm{Fix}\, R^{\frac{n}{2}}S = M_n^{\{1,n-2,3,n-4,\ldots\}} = M_n^{\{k|2\le k\le \frac{n}{2},\ k=1 \bmod 2\}\cup\{k|\frac{n}{2}<k<n,\ k=0 \bmod 2\}}$. So for instance for $n=8$ these are $M_8^{\{5,6,7\}}$ and $M_8^{\{1,3,6\}}$.

If both n and l are even, then $\mathrm{Fix}\, R^lS$ has dimension $n/2-1$ and in $\mathrm{Fix}\, R^lS$ we have $q_{\frac{l}{2}} = q_{\frac{n+l}{2}} = 0$. In other words, if n is even, then for every even l the Hamiltonian function $H|_{\mathrm{Fix}\, R^lS}$ on the symplectic subspace $\mathrm{Fix}\, R^lS$ models the FPU lattice with fixed boundary conditions and $n/2-1$ moving particles. Hence, the FPU lattice with fixed boundary conditions and $n/2-1$ moving particles is naturally embedded in the periodic FPU lattice with n particles. This is the reason why we do not study FPU lattices with fixed boundary conditions separately.

1.5. Invariant manifolds for even potentials

If the potential energy density function W is even, then also T is a symmetry and the symmetry group of the FPU Hamiltonian is $\langle R,S,T\rangle \cong D_n \times \mathbb{Z}/_{2\mathbb{Z}}$. Let us study the fixed point sets of the symmetries R^mT and R^lST which have not yet been discussed in the previous section. Most results in this section are new, as the symmetry T was not considered in [**8**].

For $m \in \mathbb{Z}$,

$$\mathrm{Fix}\, R^mT = \{q_j = -q_{j+\gcd(n,m)}, p_j = -p_{j+\gcd(n,m)}\ \forall j\}$$

which is nontrivial only if $n/\gcd(n,m)$ is even -and hence n must be even. In this case it is a $\gcd(n,m)$ degree of freedom invariant symplectic manifold. In phonons,

$$\begin{aligned}\mathrm{Fix}\, R^mT =& \{\bar{q}_k = \bar{p}_k = 0\ \forall k \neq \frac{n}{2\gcd(n,m)} \bmod \frac{n}{\gcd(n,m)}\}\\ =& \{Q_k = P_k = 0\ \forall k \neq \frac{n}{2\gcd(n,m)} \bmod \frac{n}{\gcd(n,m)}\}\end{aligned}$$

So if $2m$ divides n, then $\mathrm{Fix}\, R^mT = M_n^{\{\frac{n}{2m},\frac{3n}{2m},\ldots,\frac{(2m-1)n}{2m}\}}$.

The special choice $m=\frac{n}{2}$ gives us the invariant manifold $\mathrm{Fix}\, R^{\frac{n}{2}}T = M_n^{\{1,3,5,\ldots,n-1\}}$ of all odd normal modes that was already discovered by Fermi, Pasta and Ulam [**21**]. The choice $m=1$ gives us $\mathrm{Fix}\, RT = M_n^{\{\frac{n}{2}\}}$, the well known $\frac{n}{2}$-th mode.

If n is divisible by 4, then $\mathrm{Fix}\, R^{\frac{n}{4}}T = M_n^{\{2,6,10,\ldots,n-2\}}$ is invariant. This is a new result. The invariant manifold $\mathrm{Fix}\, R^2T = M_n^{\{\frac{n}{4},\frac{3n}{4}\}}$ is discussed in [**50**]. It contains quasi-periodic solutions.

For an n divisible by 6 we find the invariant manifolds $M_n^{\{3,9,15,\ldots,n-3\}}$ and $M_n^{\{\frac{n}{6},\frac{n}{2},\frac{5n}{6}\}}$. Etcetera.

For $l \in \mathbb{Z}$,

$$\begin{aligned}&\operatorname{Fix} R^l ST = \{q_j = q_{l-j}, p_j = p_{l-j}\ \forall j\} = \{\bar{q}_k = e^{-\frac{2\pi i k l}{n}} \bar{q}_{n-k}\ ,\ \bar{p}_k = e^{\frac{2\pi i k l}{n}} \bar{p}_{n-k}\ \forall k\} = \\ &\{Q_k \sin(\frac{lk\pi}{n}) - Q_{n-k}\cos(\frac{lk\pi}{n}) = P_k \sin(\frac{lk\pi}{n}) - P_{n-k}\cos(\frac{lk\pi}{n}) = 0\ \forall\ 1 \le k < \frac{n}{2}\ , \\ &Q_{\frac{n}{2}} = (-1)^l Q_{\frac{n}{2}}\ ,\ P_{\frac{n}{2}} = (-1)^l P_{\frac{n}{2}}\}\end{aligned}$$

is a $(2n-2+(-1)^l+(-1)^{n+l})/4$ degree of freedom invariant symplectic manifold.

Note that again $\operatorname{Fix} R^l ST$ is not always of the form $M_n^{\mathcal{A}}$, but that on the other hand $\operatorname{Fix} ST = M_n^{\{k|0\le k\le \frac{n}{2}\}}$ and if n is even, $\operatorname{Fix} R^{\frac{n}{2}} ST = M_n^{\{0,n-1,2,n-3,4,\ldots\}} = M_n^{\{k|0\le k\le \frac{n}{2},\ k=0 \bmod 2\}\cup\{k|\frac{n}{2}<k<n,\ k=1 \bmod 2\}}$. So for instance for $n = 8$ these are $M_8^{\{1,2,3,4\}}$ and $M_8^{\{2,4,5,7\}}$.

1.6. Examples of intersections

We have studied the fixed point sets of the elements of the symmetry groups $\langle R, S\rangle$ and $\langle R, S, T\rangle$. They are equal to the fixed point sets of subgroups generated by one element. A fixed point set of a subgroup generated by more than one element must be the intersection of some of the fixed point sets that were already discussed. We will give just a few examples here.

If 3 divides n, then $\operatorname{Fix} R^3 \cap \operatorname{Fix} S = M_n^{\{\frac{2n}{3}\}}$, whereas $\operatorname{Fix} R^3 \cap \operatorname{Fix} ST = M_n^{\{\frac{n}{3}\}}$. The latter is only invariant if the potential W is even.

If 4 divides n, then $\operatorname{Fix} R^4 \cap \operatorname{Fix} S = M_n^{\{\frac{3n}{4}\}}$, $\operatorname{Fix} R^4 \cap \operatorname{Fix} ST = M_n^{\{\frac{n}{4},\frac{n}{2}\}}$ and $\operatorname{Fix} R^2 T \cap \operatorname{Fix} ST = M_n^{\{\frac{n}{4}\}}$.

If 5 divides n, then $\operatorname{Fix} R^5 \cap \operatorname{Fix} S = M_n^{\{\frac{3n}{5},\frac{4n}{5}\}}$, whereas $\operatorname{Fix} R^5 \cap \operatorname{Fix} ST = M_n^{\{\frac{n}{5},\frac{2n}{5}\}}$.

If 6 divides n, then $\operatorname{Fix} R^6 \cap \operatorname{Fix} S = M_n^{\{\frac{2n}{3},\frac{5n}{6}\}}$ and $\operatorname{Fix} R^6 \cap \operatorname{Fix} ST = M_n^{\{\frac{n}{6},\frac{n}{3},\frac{n}{2}\}}$. And we find that $\operatorname{Fix} R^3 T = M_n^{\{\frac{n}{6},\frac{n}{2},\frac{5n}{6}\}}$ can be split into $\operatorname{Fix} R^3 T \cap \operatorname{Fix} S = M_n^{\{\frac{5n}{6}\}}$ and $\operatorname{Fix} R^3 T \cap \operatorname{Fix} ST = M_n^{\{\frac{n}{6},\frac{n}{2}\}}$. The normal mode solutions for the β-lattice that lie in $M_n^{\{\frac{5n}{6}\}}$ have as far as I know never been discussed in the literature.

One can proceed and compute the intersections of the various fixed point sets of $R^k, S, R^{\frac{n}{2}} S, R^k T, ST$ and $R^{\frac{n}{2}} ST$ that can be described as an $M_n^{\mathcal{A}}$. We do not pursue this approach any further as most invariant manifolds in the FPU lattice that arise as an intersection of fixed point sets will not be of the form $M_n^{\mathcal{A}}$ for some $\mathcal{A}$.

1.7. Other lattices and the continuum limit

One-dimensional mono-atomic structures such as crystals and nonlinear strings are often modelled as an anharmonic lattice. Such a lattice consists of a finite or infinite row of point masses that each move in their own on site potential field and interact with neighbouring masses. The FPU lattice is just one example.

A major advantage of our symmetry method is that fixed point sets of symmetries are invariant manifolds in any Hamiltonian system admitting these symmetries. Hence we expect to find the invariant manifolds that we discovered in the FPU lattice with periodic boundary conditions also in other one-dimensional spatially homogeneous lattices, such as the Klein-Gordon (KG) lattice [**46**], which has often been used in the modelling of large molecules. The KG lattice with periodic boundary conditions has the Hamiltonian

$$H = \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2}p_j^2 + \frac{1}{2}(q_{j+1} - q_j)^2 + W(q_j)$$

in which W is a potential energy density function. The KG lattice models a one dimensional mono-atomic structure with small coupling between the atoms. The nonlinearities are now due to an on site potential field that influences the separate particles.

It is clear that the mappings R and ST, see formulas (1.6), again leave this Hamiltonian invariant, whereas R, S and T separately have this property if W is an even function. Thus we have again found symmetries and their fixed point sets are invariant manifolds. In particular, the invariant manifolds that we discovered in the FPU lattice with even potential are also present in the KG lattice with even potential.

In the thermodynamic limit it is assumed that a lattice consists of a countably infinite number of particles, labelled by $j \in \mathbb{Z}$. The equations of motion for the infinite FPU lattice are Hamiltonian equations on $T^*\mathbb{R}^{\mathbb{Z}}$ with Hamiltonian

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

The symmetries are now induced by

$$\begin{array}{ll} R & : (\ldots, q_{-1}; q_0, q_1, \ldots) \mapsto (\ldots, q_{-1}, q_0; q_1, \ldots) \\ S & : (\ldots, q_{-1}; q_0, q_1, \ldots) \mapsto (\ldots, -q_1, -q_0; -q_{-1}, \ldots) \\ T & : (\ldots, q_{-1}; q_0, q_1, \ldots) \mapsto (\ldots, -q_{-1}; -q_0, -q_1, \ldots) \end{array}$$

The finite dimensional manifold $\mathrm{Fix}\, R^n$ models an infinite lattice with a spatially repeating pattern of period n. Or, equivalently, the periodic lattice with n particles. Inside $\mathrm{Fix}\, R^n$ we find again the invariant structures that were discussed previously in this chapter. The invariant manifold $\mathrm{Fix}\, R^n S$ is an infinite dimensional one. It consists of solutions with $q_j = -q_{n-j}$ that are anti-symmetric around $j = n/2$. Etcetera. Similar conclusions hold of course for the thermodynamic limit of the KG lattice.

Our results are also valid in the continuum limit, when the discrete lattice equations are replaced by a homogeneous partial differential equation. Consider for example for $x \in \mathbb{R}/_{\mathbb{Z}}$ the equation

$$u_{tt} = u_{xx} + f(u)$$

for $f : \mathbb{R} \to \mathbb{R}$. This equation can also be written as the system of equations

$$u_t = v \ , \ v_t = u_{xx} + f(u)$$

which have the Hamiltonian

$$H = \int_{\mathbb{R}/_{\mathbb{Z}}} \frac{1}{2}v(x)^2 + \frac{1}{2}u_x(x)^2 - F(u(x))\ dx$$

in which $F' = f$. Define the symplectic operators

$$\begin{array}{ll} \mathcal{R}^a & : u(\cdot) \mapsto u(a+\cdot), \quad v(\cdot) \mapsto v(a+\cdot) \\ \mathcal{S} & : u(\cdot) \mapsto -u(-\ \cdot), \quad v(\cdot) \mapsto -v(-\ \cdot) \\ \mathcal{T} & : u(\cdot) \mapsto -u(\cdot), \quad\ \ v(\cdot) \mapsto -v(\cdot) \end{array}$$

The constant $a \in \mathbb{R}/_{\mathbb{Z}}$ is arbitrary. Clearly, H is invariant under $\mathcal{R}^a$ and $\mathcal{ST}$. H is invariant under $\mathcal{R}^a$, $\mathcal{S}$ and $\mathcal{T}$ separately if and only if F is even, that is if and only if f is odd.

The fixed point sets of these symmetries are invariant manifolds, possibly of infinite dimension. If $a \notin \mathbb{Q}$, then $\mathrm{Fix}\,\mathcal{R}^a$ consists of constant solutions only, but if $a = \frac{p}{q}$ is rational and $\gcd(p,q) = 1$, then $\mathrm{Fix}\,\mathcal{R}^{\frac{p}{q}}$ represents the solutions with $u(t,x) = u(t, x+\frac{1}{q})$. $\mathrm{Fix}\,\mathcal{R}^{\frac{1}{q}}\mathcal{T}$ consists of solutions with $u(x) = -u(x+\frac{1}{q})$. The latter is nontrivial only if q is even. For arbitrary a, $\mathrm{Fix}\,\mathcal{R}^a\mathcal{S}$ contains solutions with $u(x) = -u(a-x)$ and $\mathrm{Fix}\,\mathcal{R}^a\mathcal{ST}$ represents solutions with $u(x) = u(a-x)$.

It is natural to use the Fourier transformation

$$u(x,t) = \sum_{k\in\mathbb{Z}} u_k(t)e^{ik\pi x}\ ,\ v(x,t) = \sum_{k\in\mathbb{Z}} v_k(t)e^{ik\pi x}$$

and to express the fixed point sets in terms of the Fourier variables $(u_k, v_k)_{k\in\mathbb{Z}}$. We then find for instance the following invariant manifolds

$$\mathrm{Fix}\,\mathcal{R}^{\frac{p}{q}} = \{u_k = v_k = 0\ \forall k \neq 0 \mod q\} = M^{\{\ldots,-2q,-q,0,q,2q,\ldots\}}$$

$$\mathrm{Fix}\,\mathcal{R}^{\frac{p}{q}}\mathcal{T} = \{u_k = v_k = 0\ \forall k \neq q \mod 2q\} = M^{\{\ldots,-3q,-q,q,3q,\ldots\}}$$

Etcetera.

[**37**], [**64**] and [**71**] study the equation $u_{tt} = u_{xx} + u^3$ by the Galerkin-averaging method. By an analysis of mode coupling coefficients it is discovered in these articles that the manifolds $M^{\{\ldots,-2q,-q,0,q,2q,\ldots\}}$ and $M^{\{\ldots,-3q,-q,q,3q,\ldots\}}$ are invariant in a certain finite dimensional system of differential equations, the Galerkin-averaging approximation, which approximates the original partial differential equation. We arrive here at the much stronger result that these conclusions hold for any odd nonlinearity f and in the *original* partial differential equation.

1.8. Discussion

In a systematic way we found various invariant manifolds for the FPU oscillator lattice with periodic boundary conditions. These invariant manifolds represent interesting classes of solutions such as periodic and quasi-periodic solutions, standing and travelling waves and embedded lower dimensional FPU lattices with periodic or fixed boundary conditions. They are moreover interesting since it is believed by some authors [**6**] that destabilisation of these invariant manifolds can lead to chaos.

Some of the invariant structures that we found have previously been discovered by other authors by an analysis of mode coupling coefficients. Our method on the contrary is similar to the method of 'bushes of normal modes' and looks for fixed point sets of symmetries which are natural invariant manifolds. We can derive our results without knowing the mode coupling coefficients explicitly. In fact, it is not even necessary to introduce normal modes at all as an expression for the invariant manifolds can simply be obtained in terms of the original physical variables, the positions and momenta of the particles in the lattice. In this way, we find several previously undiscussed invariant manifolds in the FPU lattice.

Among others, we have shown that an FPU lattice with fixed endpoints is always embedded in another FPU lattice with periodic boundaries. This will imply that the results of the coming chapters, which are proved for periodic lattices, also have implications for lattices with fixed endpoints.

The invariant manifolds that are found for the FPU lattice, are also present in other homogeneous Hamiltonian lattices such as the KG lattice and even in lattices with an infinity of particles. In the continuum limit, when the lattice equations are replaced by a homogeneous partial differential equation, we point out analogous infinite dimensional invariant structures.

CHAPTER 2

Symmetry and resonance

The symmetry and resonance properties of the Fermi-Pasta-Ulam lattice are exploited to prove that the Birkhoff normal form of the lattice is nondegenerately integrable in many cases. For a lower-order resonant Hamiltonian system this is exceptional and the result is caused by the special combination of resonances and symmetries in the lattice. The FPU Hamiltonian can therefore be seen as a perturbation of a nondegenerate Liouville integrable Hamiltonian, which according to the KAM theorem proves the existence of many invariant tori on which the motion is quasi-periodic. This chapter is based on references [**53**], [**54**] and [**59**].

2.1. Introduction

We consider again the n particles FPU lattice with periodic boundary conditions. This is the Hamiltonian system on $T^*\mathbb{R}^n$ with Hamiltonian function

$$H = \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2}p_j^2 + W(q_{j+1} - q_j) \tag{2.1}$$

in which $W(x) = \frac{1}{2!}x^2 + \frac{\alpha}{3!}x^3 + \frac{\beta}{4!}x^4$ is a potential energy function. As in the previous chapter, we can make the symplectic transformation to phonons $(q, p) \mapsto (Q, P)$, which after ignoring the total momentum results in a new Hamiltonian on $T^*\mathbb{R}^{n-1}$:

$$H = \sum_{k=1}^{n-1} \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2) + \alpha H_3(Q) + \beta H_4(Q) \tag{2.2}$$

The linear frequencies ω_k are given by

$$\omega_k = 2\sin\left(\frac{k\pi}{n}\right)$$

When the forces between all the particles are linear, i.e. when $\alpha = \beta = 0$, then the equations of motion are also linear and they can be solved exactly. The solutions are actually superposed goniometric functions with frequencies ω_k. In fact, the Hamiltonian system is Liouville integrable in this situation. Integrals are for instance the linear energies

$$E_k := \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2)$$

As the level sets of these integrals are compact, by the theorem of Liouville-Arnol'd [**2**] the solutions are periodic or quasi-periodic and move on invariant Lagrangean tori.

The FPU model is of course much more interesting when the forces between the particles are nonlinear, i.e. when α or β is nonzero. In this anharmonic case, the E_k are no longer constants of motion and the solutions will in general not be goniometric functions, although some normal mode solutions may continue to exist, as was shown in the previous chapter.

Fermi, Pasta and Ulam were particularly interested in the statistical properties of the nonlinear FPU lattice. In fact, they expected that the nonlinear lattice would attain a thermal equilibrium, as was predicted by the laws of statistical mechanics. This means that averaged over time, the initial energy of the lattice would automatically be redistributed and equipartitioned among all the Fourier modes of the lattice. On almost every solution curve $(Q(t), P(t))$, the quantities

$$\overline{E_k} = \lim_{T\to\infty} \frac{1}{T} \int_0^T E_k(Q(t), P(t))dt$$

should hence be equal, i.e. independent of k. The process of relaxation to thermal equilibrium is called *thermalisation*, see [**32**]. Fermi, Pasta and Ulam performed a numerical experiment to investigate how and at what time-scale this thermalisation would take place. The result was astonishing, see [**21**] and [**32**]: there was no sign of thermalisation at all. The energy that was initially put in the first Fourier mode, was shared by only a few other modes; the remaining modes were hardly excited. Moreover, within a rather short time the system returned close to its initial state. Other authors later observed that this recurrent behaviour was structural and even found the phenomenon of superrecurrence, see [**32**]. It turned out that the lattice did not reach a thermal equilibrium, but behaved more or less quasi-periodically. On the other hand, when the initial energy was larger then a certain threshold, the lattice indeed seemed to thermalise.

The computer experiment of Fermi, Pasta and Ulam is famous now and their stunning observations greatly stimulated the work in nonlinear dynamics after 1960. People tend to explain the FPU experiment in two ways now. In their 1965 article [**77**], Zabuski and Kruskal considered the Korteweg-de Vries equation as a continuum limit of the FPU lattice and numerically found the first indications for the stable behaviour of solitary waves. We now know that the Korteweg-de Vries equation is integrable [**49**]. This clearly suggests an explanation for FPU's observations, although the relation between the FPU lattice and its infinite dimensional limits has never been completely understood.

Another possibly correct explanation for the quasi-periodic behaviour of the FPU system, is based on the Kolmogorov-Arnol'd-Moser (KAM) theorem [**2**], [**5**]. As is well-known [**2**], the solutions of an n degree of freedom Liouville integrable Hamiltonian system move on n-dimensional tori and are periodic or quasi-periodic. The KAM theorem ensures that most of these invariant tori survive when the integrable system is perturbed a bit. But for the KAM theorem to hold, it is required that a certain nondegeneracy condition, called *Kolmogorov's condition*, is satisfied. Kolmogorov's condition requires that the frequency map, which assigns to each Liouville torus of the integrable system the frequencies of the (quasi-)periodic motion on this torus, is a local diffeomorphism.

Many authors, starting with Izrailev and Chirikov [**31**], have stated that the KAM theorem explains the observation of quasi-periodic motion in the FPU experiment. This seems plausible, as the FPU system can be viewed as a small nonlinear perturbation of its integrable linearisation. But, as was clearly pointed out by Ford in [**22**], this linearisation does not satisfy Kolmogorov's nondegeneracy condition at all, as its frequency map is constant. It is hence completely unclear how the KAM-theorem can be used. This gap in the theory was recently mentioned again in the book of Weissert [**75**]. Only a few authors have made a serious attempt to overcome this problem, making use of the Birkhoff normal form.

First of all, T. Nishida [**48**] in 1971 published a paper that considers the FPU lattice with fixed endpoints and $\alpha = 0$. He explains that, under the assumption that the linear frequencies of this lattice are nonresonant, there is a nonlinear symplectic near-identity transformation in an open subset of the phase space, called the Birkhoff transformation, with the following property: written out in the new coordinates, the Hamiltonian function is a quadratic function of the normal mode energies E_k plus a higher order perturbation. The lattice Hamiltonian can thus be seen as a perturbation of a Liouville integrable Hamiltonian depending quadratically on its integrals. Nishida's article consists mainly of a computation of the Birkhoff normal form. Moreover, he verifies the Kolmogorov condition for this normal form and thus proves that most solution curves of low energy are quasi-periodic. But this is all under the assumption that the frequencies are nonresonant! Generically, this is not the case. Nishida refers to an unpublished result of Izumi in which the frequencies are proven to be nonresonant if the number of particles in the lattice is prime or a power of 2. I was not able to trace back Izumi's proof of this statement, but note that the same result had already been obtained by Hemmer [**28**] in 1959. In any case, Nishida's argument is not valid if n is not prime or no power of two and hence it is rather poor.

Another normal form result for the FPU lattice was obtained by Sanders [**61**]. This author computes the normal form of the periodic lattice with $\alpha = 0$ and n odd. Again under a nonresonance condition that can not be verified, he shows that the Birkhoff normal form is Liouville integrable.

The aim of this chapter is to prove the conjectures of Nishida and Sanders. Of course we will focus on the periodic lattice: we will show that with the results of the previous section, we obtain immediate consequences for the lattice with fixed endpoints as it is embedded in the lattice with periodic boundary conditions.

The periodic lattice has some important properties with implications for its normal form. First of all, its eigenvalues display resonances, among which obvious ones: $\omega_k = \omega_{n-k}$. This is usually bad if we want to have an integrable normal form. But on the other hand, the periodic lattice has nice symmetry properties and it turns out that these symmetry properties overrule all the problematic lower order resonances in the eigenvalues. The conclusion is that independent of the number of particles in the lattice, we can find a near-identity transformation of the phase-space that brings the FPU Hamiltonian approximately into a very simple form, the so-called Birkhoff normal form. This normal form is nondegenerately integrable in many cases. It must be stressed that it is highly exceptional that one can find such a transformation for a resonant Hamiltonian system. This chapter will make clear that the special symmetry, eigenvalue and resonance characteristics of the periodic FPU Hamiltonian play a crucial role in the construction of the Birkhoff normal form. It turns out that these characteristics cause the nondegenerate near-integrability of the lattice. The conclusion is that the KAM theorem applies because of these resonance and symmetry properties: the quasi-periodic behaviour that Fermi, Pasta and Ulam observed is in some sense an exceptional feature of the FPU system.

2.2. Normal forms

We shall study the FPU Hamiltonian using Birkhoff normalisation. This is a variant of Poincaré normalisation designed specifically for Hamiltonian systems. Birkhoff normalisation is a way of constructing a symplectic near-identity transformation of the phase-space with the purpose of approximating the original Hamiltonian system by a simpler one. The study of this 'Birkhoff normal form' can lead to important conclusions about the original system. First of all, the solutions of the normal form approximate the low-energy solutions of the original system on a long time-scale and integrals of the normal form are near-integrals of the original system, see [**70**]. Furthermore, normalisation is an important tool for studying local bifurcation phenomena [**38**]. And last but not least, if the normal form of the FPU lattice is integrable in a nondegenerate way, then the FPU lattice can be viewed as a perturbation of a nondegenerate integrable system. We may apply the KAM-theorem then and conclude that almost all low-energy solutions of (2.2) are quasi-periodic and move on tori. This will then prove the various statements in [**48**], [**59**] and [**61**].

The setting of Birkhoff normalisation is the following:

Let $\mathcal{F}_k$ be the finite-dimensional space of homogeneous k-th degree polynomials in the phase space variables $(Q_1, \ldots, Q_{n-1}, P_1, \ldots, P_{n-1})$. The set of all power series without linear part, $\mathcal{F} := \bigoplus_{k\geq 2} \mathcal{F}_k$, is a Lie-algebra with the Poisson bracket

$$\{F, G\} := dF \cdot X_G = -dG \cdot X_F = \sum_{k=1}^{n-1} \frac{\partial F}{\partial Q_k}\frac{\partial G}{\partial P_k} - \frac{\partial F}{\partial P_k}\frac{\partial G}{\partial Q_k}$$

One checks that $\{\mathcal{F}_k, \mathcal{F}_l\} \subset \mathcal{F}_{k+l-2}$. This means that $\mathcal{F}$ is a graded Lie-algebra.

For each $h \in \mathcal{F}$ the adjoint operator $\mathrm{ad}_h : \mathcal{F} \to \mathcal{F}$ is the linear map defined by $\mathrm{ad}_h(H) = \{h, H\}$. When $h \in \mathcal{F}_k$, then $\mathrm{ad}_h : \mathcal{F}_l \to \mathcal{F}_{k+l-2}$.

The flow e^{tX_h} of a Hamiltonian vector field X_h is a symplectic transformation in $T^*\mathbb{R}^{n-1}$. We can pull back a Hamiltonian function $H \in \mathcal{F}$ under this flow. The curve $t \mapsto (e^{tX_h})^* H$ then satisfies the linear differential equation $\frac{d}{dt}(e^{tX_h})^* H = -\mathrm{ad}_h((e^{tX_h})^* H)$. The solution reads $(e^{tX_h})^* H = e^{-t\mathrm{ad}_h} H$ and in particular

$$(e^{-X_h})^* H = e^{\mathrm{ad}_h} H = H + \{h, H\} + \frac{1}{2}\{h, \{h, H\}\} + \ldots$$

Let us now write $H \in \mathcal{F}$ as

$$H = H_2 + H_3 + H_4 + \ldots$$

for $H_k \in \mathcal{F}_k$. And assume that $h_3 \in \mathcal{F}_3$. Then the near-identity 'Lie-transformation' $e^{-X_{h_3}} = \mathrm{Id} - X_{h_3} + \ldots$ transforms H into

$$H' := (e^{-X_{h_3}})^* H = e^{\mathrm{ad}_{h_3}} H = \underbrace{H_2}_{\in \mathcal{F}_2} + \underbrace{H_3 + \{h_3, H_2\}}_{\in \mathcal{F}_3} + \ldots \tag{2.3}$$

The dots represent terms in $\mathcal{F}_k$ with $k \geq 4$. Assume now, as is the case for the FPU Hamiltonian (2.2), that $\mathrm{ad}_{H_2} : \mathcal{F}_k \to \mathcal{F}_k$ is semi-simple (i.e. complex-diagonalisable) for every $k \geq 2$. Then $\mathcal{F}_k = \ker \mathrm{ad}_{H_2} \oplus \mathrm{im}\, \mathrm{ad}_{H_2}$. In particular H_3 is uniquely decomposed as $H_3 = f_3 + g_3$, with $f_3 \in \ker \mathrm{ad}_{H_2}$, $g_3 \in \mathrm{im}\, \mathrm{ad}_{H_2}$. Now choose a $h_3 \in \mathcal{F}_3$ such that $\mathrm{ad}_{H_2}(h_3) = g_3$. One could for example choose $h_3 = \tilde{g}_3 := (\mathrm{ad}_{H_2}|_{\mathrm{im}\, \mathrm{ad}_{H_2}})^{-1}(g_3)$. This choice makes the Birkhoff normal form unique. But clearly, one has the freedom to choose $h_3 = \tilde{g}_3 + p_3$ for any $p_3 \in \ker \mathrm{ad}_{H_2} \cap \mathcal{F}_3$. For the new Hamiltonian H' we calculate from (2.3) that $H_2' = H_2$, $H_3' = f_3 \in \ker \mathrm{ad}_{H_2}$, $H_4' = H_4 + \{h_3, H_3 - \frac{1}{2} g_3\}$, etc.

But now we can again write $H_4' = f_4 + g_4$ with $f_4 \in \ker \mathrm{ad}_{H_2}$, $g_4 \in \mathrm{im}\, \mathrm{ad}_{H_2}$ and it is clear that by a suitable choice of $h_4 \in \mathcal{F}_4$ the Lie-transformation $e^{-X_{h_4}}$ transforms our H' into H'' for which $H_2'' = H_2$, $H_3'' = f_3 \in \ker \mathrm{ad}_{H_2}$ and $H_4'' = f_4 \in \ker \mathrm{ad}_{H_2}$. Continuing in this way, we can for any finite $r \geq 3$ find a sequence of symplectic near-identity transformations $e^{-X_{h_3}}, \ldots, e^{-X_{h_r}}$ with the property that $e^{-X_{h_k}}$ only changes the H_l with $l \geq k$ and 'normalises' H_k. We summarise the result as follows:

Theorem 2.1 (Birkhoff normal form theorem)**.** *Let $H = H_2 + H_3 + \ldots \in \mathcal{F}$ be a Hamiltonian on $T^*\mathbb{R}^{n-1}$ such that $H_k \in \mathcal{F}_k$ for each k and $ad_{H_2} : \mathcal{F} \to \mathcal{F}$ is semi-simple. Then for every finite $r \geq 3$ there is an open neighbourhood $0 \in U \subset T^*\mathbb{R}^{n-1}$ and a symplectic diffeomorphism $\Phi : U \to T^*\mathbb{R}^{n-1}$ with the properties that $\Phi(0) = 0$, $D\Phi(0) = \mathrm{Id}$ and*

$$\Phi^* H = H_2 + \overline{H}_3 + \ldots + \overline{H}_r + \mathcal{O}(||(Q,P)||^{r+1})$$

where $\{H_2, \overline{H}_k\} = 0$ for every $3 \leq k \leq r$. The transformed and truncated Hamiltonian $\overline{H} := H_2 + \overline{H}_3 + \ldots + \overline{H}_r$ is called a Birkhoff normal form of H of order r.

It is clear from the argument of this section how $\overline{H}$ can be constructed. More information about the procedure of normalisation can be found in [**10**], [**11**] and [**24**].

The normal form $\overline{H}$ is usually simpler than the original H because it Poisson commutes with the quadratic Hamiltonian H_2. This firstly means that H_2 is a constant of motion for $\overline{H}$ and secondly that the flow $e^{tX_{H_2}}$ is a symmetry of $\overline{H}$.

H and $\overline{H}$ are symplectically equivalent modulo a small perturbation of order $\mathcal{O}(||(Q,P)||^{r+1})$. Studying $\overline{H}$ instead of H thus means neglecting this perturbation term. So we make an approximation error, but this error is very small in the low energy domain, that is for small $||(Q,P)||$.

Using Gronwall's lemma, it is easy to show that the low energy solutions of the Birkhoff normal form $X_{\overline{H}}$ approximate the low energy solutions of the original Hamiltonian system X_H. One readily proves for instance the following result, which says that solutions with small energy stay very close on a long time-scale. It is formulated a bit heuristically here:

Proposition 2.2. *Let H_2 be positive definite and let $x(t)$ and $y(t)$ be solution curves of X_H and $X_{\overline{H}}$ respectively such that $x(0) = y(0)$ and $||x(0)||$ and $||y(0)||$ are of order ε $(0 < \varepsilon \ll 1)$. Then $||x(t) - y(t)||$ is of order ε^2 on the time-scale $1/\varepsilon$.*

Also, any integral of $\overline{H}$ is nearly preserved by X_H for a long time. See [**70**] for other and stronger approximation results.

2.3. Normal forms and symmetry

In Section 1.3 we saw that the periodic FPU Hamiltonian has several discrete linear symmetries. We will now show that one can construct normal forms of the FPU Hamiltonian that have the same symmetry properties as the FPU Hamiltonian itself. The author acknowledges Hans Duistermaat for bringing this crucial point to his attention and for stressing that it could lead to interesting conclusions.

The symmetries R, S and T of the FPU Hamiltonian are given in (1.6). From (1.8) we see that all these symmetries leave invariant the space spanned by the variables $(Q_1, \ldots, Q_{n-1}, P_1, \ldots, P_{n-1})$. Hamiltonian (2.2), which gives the FPU Hamiltonian in phonon coordinates and which is defined on $T^*\mathbb{R}^{n-1}$, is hence naturally invariant under the same symmetries.

The symmetry properties of a Hamiltonian are captured in the definition of the symmetric subspace of $\mathcal{F}$. When G is a group of symplectic linear isomorphisms $P : T^*\mathbb{R}^{n-1} \to T^*\mathbb{R}^{n-1}$, then we define

$$\mathcal{F}^G := \{H \in \mathcal{F} \mid P^*H = H \ \forall \ P \in G\}$$

Note that the FPU Hamiltonian is in $\mathcal{F}^{\langle R,S \rangle}$ and sometimes in $\mathcal{F}^{\langle R,S,T \rangle}$.

The next observation is that every symplectic symmetry $P \in G$ is a Lie-algebra automorphism of $\mathcal{F}$:

$$P^*\{f, g\} = \{P^*f, P^*g\} \tag{2.4}$$

simply because P is symplectic. Now take f and g in $\mathcal{F}^G$. Then from (2.4) it follows that $P^*\{f, g\} = \{P^*f, P^*g\} = \{f, g\}$. This means that $\mathcal{F}^G$ is a Lie-subalgebra of $\mathcal{F}$: if $f, g \in \mathcal{F}^G$, then so is $\{f, g\}$. Alternatively stated: if $h \in \mathcal{F}^G$, then $\mathrm{ad}_h : \mathcal{F}^G \to \mathcal{F}^G$. In particular, $e^{\mathrm{ad}_h} : \mathcal{F}^G \to \mathcal{F}^G$.

What does this imply for the normal form of a symmetric Hamiltonian? Suppose that $H = H_2 + H_3 + \ldots$ is invariant under a group of linear symmetries G. This implies that every H_k is invariant under G.

As H_2 is symmetric under $P \in G$, we have

$$P^*\mathrm{ad}_{H_2}(f) = P^*\{H_2, f\} = \{P^*H_2, P^*f\} = \{H_2, P^*f\} = \mathrm{ad}_{H_2} P^*f$$

so P^* and ad_{H_2} commute on $\mathcal{F}$. In particular, this implies that ad_{H_2} leaves $\mathcal{F}^G$ invariant. So $\mathcal{F}^G = (\ker \mathrm{ad}_{H_2} \cap \mathcal{F}^G) \oplus (\mathrm{im}\ \mathrm{ad}_{H_2} \cap \mathcal{F}^G)$ and if we decompose H_3 as $H_3 = f_3 + g_3$ with $f_3 \in \ker \mathrm{ad}_{H_2}$, $g_3 \in \mathrm{im}\ \mathrm{ad}_{H_2}$, then f_3, $g_3 \in \mathcal{F}_3^G$ automatically. $h_3 = \tilde{g}_3 = (\mathrm{ad}_{H_2}|_{\mathrm{im}\ \mathrm{ad}_{H_2}})^{-1}(g_3)$ is the unique element of $\mathrm{im}\ \mathrm{ad}_{H_2} \cap \mathcal{F}_3^G$ for which

$\mathrm{ad}_{H_2}(h_3) = g_3$. But since $\tilde{g}_3 \in \mathcal{F}_3^G$, we find that $H' = (e^{-X_{\tilde{g}_3}})^* H = e^{\mathrm{ad}_{\tilde{g}_3}} H \in \mathcal{F}^G$. Of course the choice $h_3 = \tilde{g}_3 + p_3$ also suffices for any $p_3 \in \ker \mathrm{ad}_{H_2} \cap \mathcal{F}_3^G$.

It should be clear that continuing this procedure, we can produce normal forms $\overline{H} \in \mathcal{F}^G$ of H up to any finite order. We summarise:

Theorem 2.3. [1] *Let $H = H_2 + H_3 + \ldots \in \mathcal{F}$ with $H_k \in \mathcal{F}_k$ for each k and suppose that $H \in \mathcal{F}^G$ for some group G of linear symplectic symmetries. Then a normal form $\overline{H} = H_2 + \overline{H}_3 + \ldots + \overline{H}_r$ for H can be constructed such that $\overline{H} \in \mathcal{F}^G$.*

The following result is also interesting. When H is a Hamiltonian function with compact linear symmetry group G, then $\mathrm{Fix}\, G$ is symplectic and invariant under the flow of X_H. Moreover, $X_{(H|_{\mathrm{Fix}\, G})} = (X_H)|_{\mathrm{Fix}\, G}$ on $\mathrm{Fix}\, G$. For its normal form, we have the following convenient corollary:

Corollary 2.4. *Let H be a Hamiltonian function with compact linear symmetry group G. Then the normal form of $H|_{\mathrm{Fix}\, G}$ is simply the restriction of the symmetric normal form $\overline{H}$ of H to $\mathrm{Fix}\, G$, i.e.*

$$\overline{H|_{\mathrm{Fix}\, G}} = \overline{H}|_{\mathrm{Fix}\, G}$$

Proof: This simply follows from the fact that every near-identity transformation $e^{-X_{h_k}}$ appearing in the construction of the symmetric normal form leaves $\mathrm{Fix}\, G$ invariant. □

This corollary tells us that it is sufficient to compute the normal form of the full system to know the normal forms of its subsystems. In particular, when we know the normal forms of the periodic FPU lattices, then it is very simple to compute the normal forms of the many subsystems described in Chapter 1, among which are the lattices with fixed endpoints.

2.4. Simultaneous diagonalisation

We proved that it is possible to construct a Birkhoff normal form $\overline{H}$ for the FPU Hamiltonian H given in (2.2) that has the same symmetry properties as the FPU Hamiltonian itself. We shall investigate the implications of this result.

First of all, we know that as R is a symmetry of the FPU Hamiltonian, R^* commutes with ad_{H_2}, where H_2 is the quadratic part of the FPU Hamiltonian. Therefore ad_{H_2} leaves the eigenspaces of R^* invariant and we can diagonalise ad_{H_2} and R^* simultaneously. This allows us to calculate the subspace $\mathcal{F}_k^{\langle R \rangle} \cap \ker \mathrm{ad}_{H_2} \subset \mathcal{F}_k$ in which $\overline{H}_k$ is contained and helps us formulating some important restrictions on the normal form of the FPU Hamiltonian.

[1] Although the bookkeeping is a bit harder, one can also prove that normal forms can be made invariant under reversing symmetries. For definitions and a proof, see [**10**].

In order to perform this simultaneous diagonalisation, we introduce the *'superphonons'* (z, ζ). For $1 \leq k < \frac{n}{2}$, define:

$$\begin{aligned}
z_k &:= \frac{1}{\sqrt{2}}\bar{p}_{n-k} + \frac{i\omega_k}{\sqrt{2}}\bar{q}_k = \frac{1}{\sqrt{2n}}\sum_{j=1}^{n} e^{-\frac{2\pi ijk}{n}}(p_j + i\omega_k q_j) \\
\zeta_k &:= \frac{1}{i\sqrt{2}\omega_k}\bar{p}_k - \frac{1}{\sqrt{2}}\bar{q}_{n-k} = \frac{1}{i\omega_k\sqrt{2n}}\sum_{j=1}^{n} e^{\frac{2\pi ijk}{n}}(p_j - i\omega_k q_j) \qquad (2.5) \\
z_{n-k} &:= -\frac{1}{\sqrt{2}}\bar{p}_{n-k} + \frac{i\omega_k}{\sqrt{2}}\bar{q}_k = -\frac{1}{\sqrt{2n}}\sum_{j=1}^{n} e^{-\frac{2\pi ijk}{n}}(p_j - i\omega_k q_j) \\
\zeta_{n-k} &:= \frac{1}{i\sqrt{2}\omega_k}\bar{p}_k + \frac{1}{\sqrt{2}}\bar{q}_{n-k} = \frac{1}{i\omega_k\sqrt{2n}}\sum_{j=1}^{n} e^{\frac{2\pi ijk}{n}}(p_j + i\omega_k q_j)
\end{aligned}$$

and if n is even:

$$\begin{aligned}
z_{\frac{n}{2}} &:= \frac{1}{\sqrt{2}i\omega_{\frac{n}{2}}}(\bar{p}_{\frac{n}{2}} + i\omega_{\frac{n}{2}}\bar{q}_{\frac{n}{2}}) = \frac{1}{i\omega_{\frac{n}{2}}\sqrt{2n}}\sum_{j=1}^{n}(-1)^j(p_j + i\omega_{\frac{n}{2}}q_j) \qquad (2.6) \\
\zeta_{\frac{n}{2}} &:= \frac{1}{\sqrt{2}}(\bar{p}_{\frac{n}{2}} - i\omega_{\frac{n}{2}}\bar{q}_{\frac{n}{2}}) = \frac{1}{\sqrt{2n}}\sum_{j=1}^{n}(-1)^j(p_j - i\omega_{\frac{n}{2}}q_j)
\end{aligned}$$

One checks that $\{z_k, z_{k'}\} = \{\zeta_k, \zeta_{k'}\} = 0$ and $\{z_k, \zeta_{k'}\} = \delta_{kk'}$, the Kronecker delta. So our superphonons define canonical coordinates, i.e. $dQ \wedge dP = dz \wedge d\zeta$.

From (1.6) we infer that $R^*q_j = q_{j+1}$ and $R^*p_j = p_{j+1}$, where $q_j, p_j : T^*\mathbb{R}^n \to \mathbb{R}$ are the original coordinate functions. So from (2.5) we see that

$$\begin{aligned}
R^*: \quad z_k \mapsto e^{\frac{2\pi ik}{n}}z_k, \quad \zeta_k \mapsto e^{-\frac{2\pi ik}{n}}\zeta_k, \quad z_{n-k} \mapsto e^{\frac{2\pi ik}{n}}z_{n-k}, \quad \zeta_{n-k} \mapsto e^{-\frac{2\pi ik}{n}}\zeta_{n-k} \\
z_{\frac{n}{2}} \mapsto -z_{\frac{n}{2}} \text{ and } \zeta_{\frac{n}{2}} \mapsto -\zeta_{\frac{n}{2}} \qquad (2.7)
\end{aligned}$$

We conclude that R^* acts diagonally on (z, ζ)-coordinates. And it acts diagonally on monomials in (z, ζ): if $\Theta, \theta \in \mathbb{Z}^n_{\geq 0}$ are multi-indices, then

$$R^*: \ z^\Theta\zeta^\theta \mapsto e^{\frac{2\pi i\mu(\Theta,\theta)}{n}} \ z^\Theta\zeta^\theta \qquad (2.8)$$

μ being defined as:

$$\mu(\Theta, \theta) := \sum_{1 \leq k < \frac{n}{2}} k(\Theta_k + \Theta_{n-k} - \theta_k - \theta_{n-k}) + \frac{n}{2}(\Theta_{\frac{n}{2}} - \theta_{\frac{n}{2}}) \mod n \qquad (2.9)$$

On the other hand one calculates:

$$H_2 = \sum_{1 \leq k < \frac{n}{2}} i\omega_k(z_k\zeta_k - z_{n-k}\zeta_{n-k}) + i\omega_{\frac{n}{2}}z_{\frac{n}{2}}\zeta_{\frac{n}{2}} \qquad (2.10)$$

So we also diagonalised ad_{H_2} with respect to monomials:

$$\mathrm{ad}_{H_2}:\ z^{\Theta}\zeta^{\theta} \mapsto \nu(\Theta,\theta) z^{\Theta}\zeta^{\theta} \tag{2.11}$$

in which $\nu(\Theta,\theta)$ is defined as

$$\nu(\Theta,\theta) := \sum_{1\le k<\frac{n}{2}} i\omega_k(\theta_k - \theta_{n-k} - \Theta_k + \Theta_{n-k}) \ + i\omega_{\frac{n}{2}}(\theta_{\frac{n}{2}} - \Theta_{\frac{n}{2}}) \tag{2.12}$$

Note that this proves that ad_{H_2} is indeed semi-simple for the FPU lattice. Monomials $z^{\Theta}\zeta^{\theta}$ commuting with H_2 (the ones for which $\nu(\Theta,\theta) = 0$) are called *resonant* monomials. They are particularly important because they cannot be normalised away.

2.5. Restrictions for symmetric normal forms

From Section 2.3 we know that we can compute a symmetric normal form for the periodic FPU Hamiltonian of any desired order. Suppose we did so up to order r. Then $\overline{H}_k \in \mathcal{F}_k^{\langle R\rangle} \cap \ker \mathrm{ad}_{H_2}$ for any $2 \le k \le r$. But since both R^* and ad_{H_2} act diagonally in (z,ζ)-coordinates, we know that this $\overline{H}_k$ must be a linear combination of monomials $z^{\Theta}\zeta^{\theta}$ for which

$$|\Theta| + |\theta| = k\ ,\ \ \mu(\Theta,\theta) = 0 \bmod n \ \text{ and } \ \nu(\Theta,\theta) = 0 \tag{2.13}$$

We shall later formulate extra restrictions on $\overline{H}_k$, which arise because $\overline{H}_k$ can even be chosen in the smaller space $\mathcal{F}_k^{\langle R,S\rangle} \cap \ker \mathrm{ad}_{H_2}$. But first we investigate which Θ and θ satisfy (2.13). Because the ω_k in (2.12) are of the form $2\sin(\frac{k\pi}{n})$, this is actually a number-theoretic question that we shall solve for $|\Theta| + |\theta| = 2,\ 3,\ 4$.

The quadratic case - i.e. $|\Theta| + |\theta| = 2$ - is easy: since all the ω_k are different, we find from $\nu(\Theta,\theta) = 0$ that the Lie-subalgebra $\mathcal{F}_2\ \cap\ \ker \mathrm{ad}_{H_2} \subset \mathcal{F}_2$ is spanned by the monomials

$$z_k\zeta_k,\ z_{n-k}\zeta_{n-k},\ z_k z_{n-k},\ \zeta_k\zeta_{n-k}\ (1 \le k < \frac{n}{2}) \text{ and } z_{\frac{n}{2}}\zeta_{\frac{n}{2}} \tag{2.14}$$

R acts diagonally on these basis-elements as follows:

$$\begin{gathered} R^*: z_k\zeta_k \mapsto z_k\zeta_k,\ z_{n-k}\zeta_{n-k} \mapsto z_{n-k}\zeta_{n-k},\ z_{\frac{n}{2}}\zeta_{\frac{n}{2}} \mapsto z_{\frac{n}{2}}\zeta_{\frac{n}{2}} \\ z_k z_{n-k} \mapsto e^{\frac{4\pi i k}{n}} z_k z_{n-k},\ \zeta_k\zeta_{n-k} \mapsto e^{-\frac{4\pi i k}{n}}\zeta_k\zeta_{n-k} \end{gathered} \tag{2.15}$$

The symmetric Lie-subalgebra $\mathcal{F}_2^{\langle R\rangle} \cap \ker \mathrm{ad}_{H_2} = \mathrm{span}\{z_k\zeta_k, z_{n-k}\zeta_{n-k}, z_{\frac{n}{2}}\zeta_{\frac{n}{2}}\}$ is Abelian.

From (1.6) and (2.5) we calculate the action of S on the coordinate-functions:

$$\begin{gathered} S^*: z_k \mapsto -i\omega_k\zeta_{n-k},\ \zeta_k \mapsto \frac{1}{i\omega_k} z_{n-k},\ z_{n-k} \mapsto i\omega_k\zeta_k,\ \zeta_{n-k} \mapsto \frac{-1}{i\omega_k} z_k \\ z_{\frac{n}{2}} \mapsto -z_{\frac{n}{2}},\ \zeta_{\frac{n}{2}} \mapsto -\zeta_{\frac{n}{2}} \end{gathered} \tag{2.16}$$

So the action of S on the basis-elements of $\mathcal{F}_2^{\langle R\rangle} \cap \ker \mathrm{ad}_{H_2}$ reads:

$$S^* : z_k\zeta_k \mapsto -z_{n-k}\zeta_{n-k},\ z_{n-k}\zeta_{n-k} \mapsto -z_k\zeta_k,\ z_{\frac{n}{2}}\zeta_{\frac{n}{2}} \mapsto z_{\frac{n}{2}}\zeta_{\frac{n}{2}} \qquad (2.17)$$
$$z_k z_{n-k} \mapsto \omega_k^2 \zeta_k\zeta_{n-k},\ \zeta_k\zeta_{n-k} \mapsto \frac{1}{\omega_k^2} z_k z_{n-k}$$

We conclude that the Lie-subalgebra $\mathcal{F}_2^{\langle R,S\rangle} \cap \ker \mathrm{ad}_{H_2}$ is spanned by the quadratics $z_k\zeta_k - z_{n-k}\zeta_{n-k}$ and $z_{\frac{n}{2}}\zeta_{\frac{n}{2}}$. Note that H_2 itself is indeed a linear combination of these quadratic monomials.

The analysis is less trivial if we consider the cases $|\Theta| + |\theta| = 3,\ 4$. We can prove the following result about monomials that are both symmetric and resonant:

Theorem 2.5.

i) The set of multi-indices $(\Theta, \theta) \in \mathbb{Z}_{\geq 0}^{2n-2}$ for which $|\Theta|+|\theta| = 3,\ \mu(\Theta,\theta) = 0 \bmod n$ and $\nu(\Theta,\theta) = 0$ is empty.

ii) The set of multi-indices $(\Theta, \theta) \in \mathbb{Z}_{\geq 0}^{2n-2}$ for which $|\Theta|+|\theta| = 4,\ \mu(\Theta,\theta) = 0 \bmod n$ and $\nu(\Theta,\theta) = 0$ is contained in the set defined by the relations $\theta_k - \theta_{n-k} - \Theta_k + \Theta_{n-k} = \theta_{\frac{n}{2}} - \Theta_{\frac{n}{2}} = 0$.

Proof:

i) Suppose that $|\Theta| + |\theta| = 3$ and $\mu(\Theta, \theta) = 0 \mod n$. Then we can conclude from looking closely at (2.9) and (2.12) that there must be integers $k, l, m \neq 0 \mod n$ with $k+l+m = 0 \mod n$ for which $\nu(\Theta,\theta) = 2i\sin(\frac{k\pi}{n}) + 2i\sin(\frac{l\pi}{n}) + 2i\sin(\frac{m\pi}{n}) = 2i\sin(\frac{k\pi}{n}) + 2i\sin(\frac{l\pi}{n}) - 2i\sin(\frac{k\pi}{n} + \frac{l\pi}{n})$. Now I learnt the following trick from Frits Beukers: write $2i\sin(\frac{k\pi}{n}) = x - 1/x$ and $2i\sin(\frac{l\pi}{n}) = y - 1/y$ for some x, y on the complex unit circle. Then $\nu(\Theta,\theta) = x - 1/x + y - 1/y - xy + 1/xy = (1-x)(1-y)(1-xy)/xy$. This is zero only in the trivial cases that $x = 1$ ($k = 0 \mod n$), $y = 1$ ($l = 0 \mod n$) or $xy = 1$ ($m = 0 \mod n$). But we already knew that $k, l, m \neq 0 \mod n$. The result also follows from the convexity of the sine function.

ii) The proof of the second statement is similar and based on the fact that $2i\sin\alpha + 2i\sin\beta + 2i\sin\gamma - 2i\sin(\alpha+\beta+\gamma) = x - 1/x + y - 1/y + z - 1/z - xyz + 1/xyz = (1-xy)(1-xz)(1-yz)/xyz$, which again is zero in trivial cases only. □

From Theorem 2.5 we know that the only monomials of order 3 or 4 that are both symmetric and resonant, are the trivial ones, i.e. the ones for which $\nu(\Theta,\theta)$ in (2.12) is trivially zero.

This is an unexpected and nontrivial result, as in Appendix 2.9 it is shown that lower order resonances do indeed occur. The appendix can be considered as a continuation of the work by Izumi and Hemmer [**28**] as it gives a list of all the solutions of

$$|\Theta| + |\theta| = 3, 4\ ,\ \nu(\Theta,\theta) = 0$$

We find for instance that

$$\sin(\pi/6) + \sin(\pi/10) - \sin(3\pi/10) = 0$$

and

$$\sin(\pi/6) + \sin(3\pi/14) - \sin(\pi/14) - \sin(5\pi/14) = 0$$

These relations lead to several nontrivial resonant monomials. But Theorem 2.5 tells us that these monomials are not symmetric and hence cannot occur in the normal form. So the results of the appendix show that Theorem 2.5 is nontrivial. Moreover, the nontrivial resonance relations in the appendix are important for the study of nonsymmetric nonlinear perturbations of the FPU Hamiltonian.

We will now investigate the exact implications of Theorem 2.5 for the normal form of the FPU lattice. The results are summarised in Theorem 2.6.

From *i)* we see that $\{0\} = \mathcal{F}_3^{\langle R\rangle} \cap \ker \mathrm{ad}_{H_2} \subset \mathcal{F}_3 \cap \ker \mathrm{ad}_{H_2}$. First of all, this implies that we can always transform away H_3 from the periodic FPU Hamiltonian: $\overline{H}_3 = 0$. For systems with a third order resonance relation one can generally not expect $\overline{H}_3$ to be trivial, so this is an unexpected result: consider for example the periodic lattice with 6 particles for which $\omega_1 : \omega_3 : \omega_5 = 1 : 2 : 1$. For Hamiltonian systems in $1:2:1$-resonance the normal form is usually highly nontrivial, see [**17**]. But in [**59**] it was already observed that the $1:2:1$-resonance is not 'active' in the periodic lattice with 6 particles. We have now proved that no resonance will ever be active at H_3-level in the periodic FPU lattice . This simplification is caused by the symmetry R of the FPU system.

Secondly, we conclude from *i)* that the h_3 of Section 2.3 is uniquely determined by the requirement that it is in $\mathcal{F}_3^{\langle R\rangle}$. This in turn uniquely determines $\overline{H}_4$.

From *ii)* we infer that any element of $\mathcal{F}_4^{\langle R\rangle} \cap \ker \mathrm{ad}_{H_2}$ must be a linear combination of products of two of the basis-elements in (2.14). Note however that not all these products are really R-invariant and that the full normal form is even invariant under S and sometimes T. We work out these extra restrictions now in a few short computations.

The question which products of the basis-elements (2.14) are invariant under R is easy to answer with help of the formulas (2.15). Clearly, all products of $z_k\zeta_k$, $z_{n-k}\zeta_{n-k}$ and $z_{\frac{n}{2}}\zeta_{\frac{n}{2}}$ are. R acts on the terms $(z_k\zeta_k)(z_{k'}z_{n-k'})$, $(z_k\zeta_k)(\zeta_{k'}\zeta_{n-k'})$, $(z_{n-k}\zeta_{n-k})(z_{k'}z_{n-k'})$, $(z_{n-k}\zeta_{n-k})(\zeta_{k'}\zeta_{n-k'})$, $(z_{\frac{n}{2}}\zeta_{\frac{n}{2}})(z_{k'}z_{n-k'})$ and $(z_{\frac{n}{2}}\zeta_{\frac{n}{2}})(\zeta_{k'}\zeta_{n-k'})$ as multiplication with a factor $e^{\pm\frac{4\pi i k'}{n}} \neq 1$, so these terms are not invariant under R. R^* multiplies $(z_k z_{n-k})(\zeta_{k'}\zeta_{n-k'})$ by $e^{\frac{4\pi i(k-k')}{n}}$ which is 1 if and only if $2(k-k') = 0$ mod n. But because $1 \le k, k' < \frac{n}{2}$, the condition is $2(k-k') = 0$, i.e. $k = k'$. Thus we end up with a term that we already had: $(z_k z_{n-k})(\zeta_k\zeta_{n-k}) = (z_k\zeta_k)(z_{n-k}\zeta_{n-k})$. Finally, the terms $(z_k z_{n-k})(z_{k'}z_{n-k'})$ and $(\zeta_k\zeta_{n-k})(\zeta_{k'}\zeta_{n-k'})$ are multiplied by a factor $e^{\pm\frac{4\pi i(k+k')}{n}}$ which is 1 if and only if $2(k+k') = 0$ mod n. But since $1 \le k, k' < \frac{n}{2}$, the only possibility is that $2(k+k') = n$, that is n must be even and $k+k' = \frac{n}{2}$. This concludes our search for quartic monomials that are invariant under R and Poisson commute with H_2.

We shall check now which combinations of these terms are also invariant under S. The action of S on $\mathcal{F}_2 \cap \ker \mathrm{ad}_{H_2}$ can be diagonalised in real coordinates. For this purpose, besides our familiar complex basis, we also define the following real basis-elements for $\mathcal{F}_2 \cap \ker \mathrm{ad}_{H_2}$, which are also called *Hopf-variables.* For $1 \leq k < \frac{n}{2}$, let

$$\begin{aligned} a_k :=& i(z_k\zeta_k - z_{n-k}\zeta_{n-k}) = \frac{1}{2\omega_k}(P_k^2 + P_{n-k}^2 + \omega_k^2 Q_k^2 + \omega_k^2 Q_{n-k}^2) \\ b_k :=& i(z_k\zeta_k + z_{n-k}\zeta_{n-k}) = P_k Q_{n-k} - P_{n-k}Q_k \\ c_k :=& \frac{1}{\omega_k}(\omega_k^2\zeta_k\zeta_{n-k} + z_k z_{n-k}) = \frac{1}{2\omega_k}(P_{n-k}^2 - P_k^2 + \omega_k^2 Q_{n-k}^2 - \omega_k^2 Q_k^2) \\ d_k :=& \frac{i}{\omega_k}(\omega_k^2\zeta_k\zeta_{n-k} - z_k z_{n-k}) = \frac{1}{\omega_k}(P_k P_{n-k} + \omega_k^2 Q_k Q_{n-k}) \end{aligned} \tag{2.18}$$

and if n is even

$$a_{\frac{n}{2}} := i z_{\frac{n}{2}}\zeta_{\frac{n}{2}} = \frac{1}{2\omega_{\frac{n}{2}}}(P_{\frac{n}{2}}^2 + \omega_{\frac{n}{2}}^2 Q_{\frac{n}{2}}^2)$$

Note that these basis-elements are subject to the relation

$$a_k^2 = b_k^2 + c_k^2 + d_k^2 \tag{2.19}$$

and that H_2 can be expressed as

$$H_2 = \sum_{1\leq k\leq \frac{n}{2}} \omega_k a_k \tag{2.20}$$

Our definitions diagonalise the action of S:

$$S^* : a_k \mapsto a_k,\ a_{\frac{n}{2}} \mapsto a_{\frac{n}{2}},\ b_k \mapsto -b_k,\ c_k \mapsto c_k,\ d_k \mapsto -d_k \tag{2.21}$$

The products $a_k a_{k'}$, $a_{\frac{n}{2}} a_k$ and $b_k b_{k'}$ are invariant under both R and S. The products $a_k b_{k'}$ and $a_{\frac{n}{2}} b_k$ are not invariant under S, although they are under R. The reader can easily check that the only other term that can appear is $d_k d_{\frac{n}{2}-k} - c_k c_{\frac{n}{2}-k}$.

We summarise the results of this section in the following theorem:

Theorem 2.6. *Let $H = H_2 + \alpha H_3 + \beta H_4$ be the periodic FPU Hamiltonian (2.2). Then there is a unique quartic Birkhoff normal form $\overline{H}$ of H which is invariant under R and S. For this normal form we have $\overline{H}_3 = 0$, whereas $\overline{H}_4$ is a linear combination of the quartic terms $a_k a_{k'}$, $b_k b_{k'}$ $(1 \leq k, k' < \frac{n}{2})$ and if n is even also $a_{\frac{n}{2}} a_k$ $(1 \leq k \leq \frac{n}{2})$ and $d_k d_{\frac{n}{2}-k} - c_k c_{\frac{n}{2}-k}$ $(1 \leq k \leq \frac{n}{4})$.*

2.6. Near-integrals

Because the Birkhoff normal form of the periodic FPU Hamiltonian is subject to many restrictions, as indicated in Theorem 2.6, we can point out some integrals for the normal form. These are near-integrals of the periodic FPU lattice: quantities that are nearly conserved by the flow of the original lattice (2.2) for a long time, cf. [**70**].

In order to compute these integrals, we first write down the Poisson relations between the Hopf-variables (2.18). They read, as can readily be computed:

$$\{b_k, c_k\} = 2d_k\ ,\quad \{b_k, d_k\} = -2c_k\ ,\quad \{c_k, d_k\} = 2b_k \tag{2.22}$$

All the other Poisson brackets between the various Hopf-variables are zero. Knowing these Poisson relations, we can draw the conclusions described in the following sections:

2.6.1. The lattice with fixed endpoints. From Chapter 1 we know that the Hamiltonian of the lattice with fixed endpoints and n moving particles is the Hamiltonian of the periodic lattice with $2n+2$ particles, restricted to the fixed point set of the symmetry S. The phase space of the periodic lattice with $2n+2$ particles is, after neglecting the total momentum, $T^*\mathbb{R}^{2n+1}$ with variables (Q, P). From the definition of the real phonons in Chapter 2 and the definition of S, we conclude that

$$S: \ (Q_1, \ldots, Q_{2n+1}, P_1, \ldots, P_{2n+1}) \mapsto \\ (-Q_1, \ldots, -Q_{n+1}, Q_{n+2}, \ldots, Q_{2n+1}, -P_1, \ldots, -P_{n+1}, P_{n+2}, \ldots, P_{2n})$$

So that

$$\text{Fix } S = \{(Q,P) \in T^*\mathbb{R}^{2n+1} \mid Q_k = P_k = 0 \ \forall \ 1 \leq k \leq n+1 \ \} \cong T^*\mathbb{R}^n$$

The Hamiltonian of the fixed endpoint lattice is simply the restriction of the periodic Hamiltonian (2.2) to this fixed point set. So after choosing canonical coordinates $\mathcal{Q}_k := Q_{n+k+1}, \mathcal{P}_k := P_{n+k+1}$ on Fix $S \subset T^*\mathbb{R}^{2n+1}$, the Hamiltonian of the fixed endpoint lattice becomes

$$H = \sum_{k=1}^{n} \frac{1}{2}(\mathcal{P}_k^2 + \Omega_k^2 \mathcal{Q}_k^2) + \alpha H_3(\mathcal{Q}) + \beta H_4(\mathcal{Q}) \tag{2.23}$$

which is defined on $T^*\mathbb{R}^n$ with coordinates $(\mathcal{Q}, \mathcal{P})$ and symplectic form $d\mathcal{Q} \wedge d\mathcal{P}$. The linear frequencies of the fixed endpoint lattice are $\Omega_k := 2\sin(\frac{k\pi}{2n+2})$. The integrals of the linearised system are the normal mode energies $E_k := \frac{1}{2}(\mathcal{P}_k^2 + \Omega_k^2\mathcal{Q}_k^2)$ $(1 \leq k \leq n)$.

Corollary 2.7 (Conjectured by Nishida in [**48**]). *The quartic Birkhoff normal form of the FPU lattice with fixed endpoints (2.23) is integrable with integrals E_k.*

Proof: By Corollary 2.4, the Birkhoff normal form of (2.23) is the restriction of the Birkhoff normal form of the periodic lattice with $2n+2$ particles, to Fix S. But on Fix S, we have that $b_k = c_k = d_k = 0$ and $a_k = E_k/\Omega_k$. So according to Theorem 2.6, $\overline{H}_4$ is a quadratic function of the Poisson commuting E_k. So, clearly, is H_2. □

The integral map $E: T^*\mathbb{R}^n \to \mathbb{R}^n$ that maps $(\mathcal{Q}, \mathcal{P}) \mapsto (E_1, \ldots, E_n)$ is regular when $E_k > 0$ for every k. This means that the derivatives $DE_k(\mathcal{Q}, \mathcal{P})$ are all linearly independent. As the level sets of E are compact, the theorem of Liouville-Arnol'd ensures that for each $e_1, \ldots, e_n > 0$, the level set $\{E = e\}$ is a smooth n-dimensional torus.

To compute the flow on these tori, we transform to action-angle coordinates $(\mathcal{Q}, \mathcal{P}) \mapsto (a, \varphi)$ as follows. Let arg : $\mathbb{R}^2 \backslash \{(0,0)\} \to \mathbb{R}/_{2\pi\mathbb{Z}}$ be the argument function, arg : $(r\cos\Phi, r\sin\Phi) \mapsto \Phi$ and define $a_k = E_k/\Omega_k$, $\varphi_k = \arg(\mathcal{P}_k, \Omega_k\mathcal{Q}_k)$. With the formula $d\ \arg(x,y) = \frac{xdy-ydx}{x^2+y^2}$, one can verify that (a,φ) are canonical coordinates: $dQ\wedge dP = d\varphi\wedge da$. So in these coordinates the equations of motion read $\dot a_k = 0, \dot\varphi_k = \Omega_k + \partial\overline{H}_4/\partial a_k(a)$. This simply defines periodic or quasi-periodic motion. To verify that the normal form $\overline{H}$ is nondegenerate, we examine the frequency map Ω which adds to each invariant torus the frequencies of the flow on it:

$$\Omega : a \ \mapsto \left(\Omega_1 + \frac{\partial\overline{H}_4}{\partial a_1}(a), \ldots, \Omega_n + \frac{\partial\overline{H}_4}{\partial a_n}(a)\right)$$

Ω is a local diffeomorphism if and only if the constant derivative matrix $\frac{\partial^2\overline{H}_4}{\partial a_k\partial a_{k'}}$ is invertible. To check this, we need to compute the normal form explicitly, see Section 2.7.

2.6.2. The odd periodic lattice. Under a nonresonance condition, the following result was shown by Sanders [**61**] for the periodic odd FPU lattice in the case that $\alpha = 0$. But the corollary is also true if $\alpha\neq 0$, and a nonresonance condition is not needed:

Corollary 2.8. *If n is odd, then the quartic Birkhoff normal form of the periodic FPU Hamiltonian (2.2) is Liouville integrable with the quadratic integrals* a_k, b_k $(1\le k\le \frac{n-1}{2})$.

Proof: H_2 is a linear combination of the quadratics a_k and $\overline{H}_4$ is a linear combination of the quartic terms $a_ka_{k'}$ and $b_kb_{k'}$. The a_k and b_k Poisson commute with all these terms and with each other. □

It is not difficult to check that the integral map $F : T^*\mathbb{R}^{n-1}\to\mathbb{R}^{n-1}$ that maps $(Q,P)\mapsto(a,b)$ has image

$$\text{im } F = \{(a,b)\in\mathbb{R}^{n-1} | a_k\ge 0, |b_k|\le a_k\} \tag{2.24}$$

F is regular in the interior of im F, that is when $0<|b_k|<a_k$ for every k. As the level sets of F are moreover clearly compact, the theorem of Liouville-Arnol'd ensures that for each (a,b) with $0<|b_k|<a_k$, the level set $F^{-1}(a,b)$ is a smooth $n-1$-dimensional torus.

To compute the flow on these tori, we make the transformation to action-angle coordinates $(Q,P)\mapsto(a,b,\phi,\psi)$ as follows. For $1\le k\le\frac{n-1}{2}$, define

$$\begin{aligned}
a_k &:= \frac{1}{2\omega_k}(P_k^2 + P_{n-k}^2 + \omega_k^2Q_k^2 + \omega_k^2Q_{n-k}^2)\\
b_k &:= P_kQ_{n-k} - P_{n-k}Q_k \qquad\qquad (2.25)\\
\phi_k &:= \frac{1}{2}\arg(-P_{n-k}-\omega_kQ_k, P_k-\omega_kQ_{n-k}) + \frac{1}{2}\arg(P_{n-k}-\omega_kQ_k, P_k+\omega_kQ_{n-k})\\
\psi_k &:= \frac{1}{2}\arg(-P_{n-k}-\omega_kQ_k, P_k-\omega_kQ_{n-k}) - \frac{1}{2}\arg(P_{n-k}-\omega_kQ_k, P_k+\omega_kQ_{n-k})
\end{aligned}$$

Note that this is a well-defined smooth transformation as long as $0<|b_k|<a_k$ for each k. One verifies that the (a,b,ϕ,ψ) are canonical coordinates: $dQ\wedge dP = \sum_{1\le k\le\frac{n-1}{2}} d\phi_k\wedge da_k + d\psi_k\wedge db_k$.

The normal form $\overline{H}$ is a function of the actions a_k, b_k. Hence (a, b, ϕ, ψ) are action-angle variables, [**2**], [**11**]. The induced equations of motion read:

$$\dot{a}_k = \dot{b}_k = 0 \tag{2.26}$$
$$\dot{\phi}_k = \omega_k + \frac{\partial \overline{H}_4}{\partial a_k}(a) \ , \quad \dot{\psi}_k = \frac{\partial \overline{H}_4}{\partial b_k}(b)$$

which simply define periodic or quasi-periodic motion. To verify that the normal form $\overline{H}$ is nondegenerate, we need to check that the frequency map

$$\omega : (a,b) \ \mapsto \left(\omega_1 + \frac{\partial \overline{H}_4}{\partial a_1}(a), \ldots, \omega_{\frac{n-1}{2}} + \frac{\partial \overline{H}_4}{\partial a_{\frac{n-1}{2}}}(a), \frac{\partial \overline{H}_4}{\partial b_1}(b), \ldots, \frac{\partial \overline{H}_4}{\partial b_{\frac{n-1}{2}}}(b)\right)$$

is a local diffeomorphism. This is true if and only if both the constant derivative matrices $\frac{\partial^2 \overline{H}_4}{\partial a_k \partial a_{k'}}$ and $\frac{\partial^2 \overline{H}_4}{\partial b_k \partial b_{k'}}$ are invertible. To check this, we need to compute the normal form explicitly, see Section 2.7.

The situation is more difficult in the case of

2.6.3. The even periodic lattice.

Corollary 2.9. *If n is even, then the Birkhoff normal form of the periodic FPU lattice (2.2) has the quadratic integrals a_k $(1 \leq k \leq \frac{n}{2})$ and $b_k - b_{\frac{n}{2}-k}$ $(1 \leq k < \frac{n}{4})$.*

Proof: H_2 is a linear combination of the quadratics a_k $(1 \leq k \leq \frac{n}{2})$, whereas $\overline{H}_4$ is a linear combination of the fourth order terms $a_k a_{k'}$ $(1 \leq k, k' \leq \frac{n}{2})$, $b_k b_{k'}$ $(1 \leq k, k' < \frac{n}{2})$ and $d_k d_{\frac{n}{2}-k} - c_k c_{\frac{n}{2}-k}$ $(1 \leq k \leq \frac{n}{4})$. The a_k clearly commute with all these terms. So do the terms $b_k - b_{\frac{n}{2}-k}$: $\{b_k - b_{\frac{n}{2}-k}, b_{k'}\} = \{b_k - b_{\frac{n}{2}-k}, a_{k'}\}$ $= \{b_k - b_{\frac{n}{2}-k}, a_{\frac{n}{2}}\} = 0$. But one also verifies from (2.22) that $\{b_k - b_{\frac{n}{2}-k}, c_k c_{\frac{n}{2}-k} - d_k d_{\frac{n}{2}-k}\} = c_{\frac{n}{2}-k}\{b_k, c_k\} - c_k\{b_{\frac{n}{2}-k}, c_{\frac{n}{2}-k}\} - d_{\frac{n}{2}-k}\{b_k, d_k\} + d_k\{b_{\frac{n}{2}-k}, d_{\frac{n}{2}-k}\} = 2c_{\frac{n}{2}-k}d_k - 2c_k d_{\frac{n}{2}-k} + 2d_{\frac{n}{2}-k}c_k - 2d_k c_{\frac{n}{2}-k} = 0$. □

If n is even, then the $n-1$-degree of freedom Hamiltonian normal form has at least $\frac{3n-4}{4}$ (if 4 divides n) or $\frac{3n-2}{4}$ (if 4 does not divide n) quadratic integrals. These are near-integrals for the original Hamiltonian. We have not yet found a complete system of integrals for the Birkhoff normal form. But in Section 2.7.3, we will meet this set of integrals for the even β-lattice.

2.7. Explicit results for the β-lattice

Until now we could present near-integrability results without computing the Birkhoff normal form of the FPU lattice explicitly, but using only the symmetry and resonance properties of the lattice. This means that our results are not only valid for the FPU lattice, but for every Hamiltonian system with the same symmetries and resonances. In this section we present the explicit normal form of the periodic FPU Hamiltonian in the case that $H_3 = 0$, i.e. $\alpha = 0$ in (2.1). This lattice, that has no cubic terms, is usually referred to as the β-lattice. A calculation of the normal form of order 4 is relatively easy in this case, because one does not have to transform away H_3 first. The calculation is still rather cumbersome though and that is why we present it only partially. The reader can find similar computations in [**48**], [**59**] and [**61**].

Theorem 2.10. *If $\alpha = 0$, then a quartic Birkhoff normal form for the periodic FPU lattice (2.2) is given by $\overline{H} = H_2 + \beta\overline{H}_4$, where*

$$\overline{H}_4 = \frac{1}{n}\left\{ \sum_{0<k<l<\frac{n}{2}} \frac{\omega_k\omega_l}{4} a_k a_l + \sum_{0<k<\frac{n}{2}} \frac{\omega_k^2}{32}(3a_k^2 - b_k^2) + \frac{1}{4}a_{\frac{n}{2}}^2 + \frac{1}{2}a_{\frac{n}{2}} \sum_{0<k<\frac{n}{2}} \omega_k a_k \right.$$
$$\left. + \frac{1}{8}\sum_{0<k<\frac{n}{4}} \omega_k\omega_{\frac{n}{2}-k}(d_k d_{\frac{n}{2}-k} - c_k c_{\frac{n}{2}-k}) + \frac{1}{16}(d_{\frac{n}{4}}^2 - c_{\frac{n}{4}}^2) \right\} \tag{2.27}$$

In formula (2.27) it is understood that terms with the subscript $\frac{n}{2}$ and $\frac{n}{4}$ only appear if 2 respectively 4 divides n.

Sketch of proof: In complex phonon-coordinates H_4 reads

$$H_4 = \frac{1}{n} \sum_{\substack{\theta:|\theta|=4 \\ \Sigma_k k\theta_k = 0 \bmod n}} \prod_{k\in\mathbb{Z}/n\mathbb{Z}} \frac{1}{\theta_k!}(e^{\frac{2\pi i k}{n}} - 1)^{\theta_k}\ \bar{q}_k^{\ \theta_k} \tag{2.28}$$

Because of the nonresonance properties in Theorem 2.5, the terms $\bar{q}^{\ \theta}$ can all be transformed away completely by normalisation, except for those of the form $\bar{q}_k^4$, $\bar{q}_k^2\bar{q}_{n-k}^2$, $\bar{q}_k\bar{q}_{n-k}\bar{q}_{k'}^2$ and $\bar{q}_k\bar{q}_{n-k}\bar{q}_{k'}\bar{q}_{n-k'}$. Thus we end up with a partially normalised H_4 which is a linear combination of these terms. Each of these terms is expressed in (z,ζ)-coordinates and thereafter normalised. We end up with (2.27). □

The described method of computation resembles very much the normal form computations of Nishida [**48**] and Sanders [**61**] but is in our case easier due to the compact formula (2.28) for the Hamiltonian in complex phonon coordinates. Furthermore, we did not make any nonresonance assumptions.

Theorem 2.10 allows us to formulate various interesting KAM-statements about the FPU lattice.

2.7.1. The β-lattice with fixed endpoints.

Theorem 2.11 (Conjectured by Nishida in [**48**]). *If $\alpha = 0$ and $\beta \neq 0$, then the integrable quartic Birkhoff normal form $\overline{H} = H_2 + \beta\overline{H}_4$ of the FPU lattice with fixed endpoints (2.23) satisfies the Kolmogorov nondegeneracy condition. Hence almost all low-energy solutions of the FPU lattice with fixed endpoints are quasi-periodic and move on invariant tori. In fact, the relative measure of all these tori lying inside the small ball $\{0 \leq H \leq \varepsilon\}$, goes to 1 as ε goes to 0.*

Proof: From (2.27) we compute that the Birkhoff normal form of the β-lattice with n moving particles and fixed endpoints is $\overline{H} = H_2 + \beta \overline{H}_4$ where

$$\overline{H}_4 = \frac{1}{n} \left(\sum_{1 \le k < l \le n} \frac{\Omega_k \Omega_l}{4} a_k a_l + \sum_{1 \le k \le n} \frac{3\Omega_k^2}{32} a_k^2 \right)$$

where $a_k = E_k/\Omega_k$. This result agrees completely with the conjectured normal form of Nishida in [**48**]. To check Kolmogorov's condition, we have to compute the second order derivative matrix of $\overline{H}_4$ with respect to the actions a_k. The nondegeneracy of this matrix was already checked by Nishida himself. □

After a long computation, it should also be possible to write down an expression for the fixed endpoints normal form if $\alpha \neq 0$. We know a priori that this normal form is integrable and depends quadratically on the E_k. For checking Kolmogorov's condition, one has to compute this normal form explicitly. But this computation is not easy: after transforming away H_3 we obtain the transformed $H_4' = \beta H_4 + \frac{\alpha^2}{2}\{(\mathrm{ad}_{H_2}|_{\mathrm{im\ ad}_{H_2}})^{-1}(H_3), H_3\}$ which thereafter has to be normalised to produce $\overline{H}_4$. The result is most likely that for a large open set of α and β the nondegeneracy condition holds and the KAM theorem applies. Without computation this is clear for $|\alpha| \ll |\beta|$, because then the coefficients of the normal form (2.27) can change only slightly.

2.7.2. The odd periodic β-lattice. In formula (2.27) we see again what was already predicted in Theorem 2.6, namely that $\overline{H}_4$ is a linear combination of the terms $a_k a_{k'}$ and $b_k b_{k'}$ $(1 \le k, k' \le \frac{n-1}{2})$. According to Corollary 2.8 this normal form is integrable, the a_k and b_k being the quadratic integrals. To check the nondegeneracy condition, we compute the second order derivative matrices of $\overline{H}_4$ with respect to the action variables a_k and b_k:

$$\frac{\partial^2 \overline{H}_4}{\partial a_k \partial a_{k'}} = \frac{1}{16\ n} \begin{pmatrix} 3\omega_1^2 & 4\omega_1\omega_2 & \cdots & 4\omega_1\omega_{\frac{n-1}{2}} \\ 4\omega_2\omega_1 & 3\omega_2^2 & \cdots & 4\omega_2\omega_{\frac{n-1}{2}} \\ \vdots & & \ddots & \vdots \\ 4\omega_{\frac{n-1}{2}}\omega_1 & 4\omega_{\frac{n-1}{2}}\omega_2 & \cdots & 3\omega_{\frac{n-1}{2}}^2 \end{pmatrix} \tag{2.29}$$

$$\frac{\partial^2 \overline{H}_4}{\partial b_k \partial b_{k'}} = -\frac{1}{16\ n} \begin{pmatrix} \omega_1^2 & & & \\ & \omega_2^2 & & \\ & & \ddots & \\ & & & \omega_{\frac{n-1}{2}}^2 \end{pmatrix} \tag{2.30}$$

$\frac{\partial^2 \overline{H}_4}{\partial b_k \partial b_{k'}}$ is clearly nondegenerate. But so is $\frac{\partial^2 \overline{H}_4}{\partial a_k \partial a_{k'}}$. This can be proved by applying elementary row and column operations to (2.29), thus reducing it to upper diagonal form. This yields an expression for the determinant that is unequal to 0. We conclude that the periodic β-lattice with an odd number of particles can, after a near-identity transformation, be written as a perturbation of a nondegenerate integrable Hamiltonian system. Therefore, the KAM theorem applies:

Theorem 2.12. *If n is odd, $\alpha = 0$ and $\beta \neq 0$, then the integrable quartic Birkhoff normal form $\overline{H} = H_2 + \beta\overline{H}_4$ of the periodic FPU Hamiltonian (2.2) is integrable and satisfies the Kolmogorov nondegeneracy condition. Hence almost all low-energy solutions of this lattice are periodic or quasi-periodic and move on invariant tori. In fact, the relative measure of all these tori lying inside the small ball $\{0 \leq H \leq \varepsilon\}$, goes to 1 as ε goes to 0.*

We know that the normal form is also integrable if $\alpha \neq 0$ and that it depends quadratically on the actions (a, b). But for checking Kolmogorov's condition, one has to compute this normal form explicitly. As for the fixed endpoint lattice, this is a hard computation.

2.7.3. The even periodic β-lattice. It is a surprise that in the normal form of the even β-lattice no terms $b_k b_{k'}$ $(k \neq k')$ arise, see formula (2.27). This leads to the following remarkable conclusion:

Corollary 2.13. *If n is even, $\alpha = 0$ and $\beta \neq 0$, then the normal form $\overline{H} = H_2 + \beta\overline{H}_4$ of the periodic FPU lattice (2.2) is Liouville integrable. The integrals are the quadratics a_k $(1 \leq k \leq \frac{n}{2})$, $b_k - b_{\frac{n}{2}-k}$ $(1 \leq k < \frac{n}{4})$ and $d_{\frac{n}{4}}$ (if n is a multiple of 4) and the quartic terms $\omega_k^2 b_k^2 + \omega_{\frac{n}{2}-k}^2 b_{\frac{n}{2}-k}^2 + 4\omega_k\omega_{\frac{n}{2}-k}(c_k c_{\frac{n}{2}-k} - d_k d_{\frac{n}{2}-k})$ $(1 \leq k < \frac{n}{4})$.*

Proof: This follows from simply computing all the Poisson brackets, using (2.22) and the fact that the Poisson brackets form a derivation. □

Only the $a_k, b_k - b_{\frac{n}{2}-k}$ and $d_{\frac{n}{4}}$ induce a 2π-periodic flow and can therefore be seen as actions after some symplectic action-angle transformation. It is at this moment not clear how to practically construct the remaining action variables or to check Kolmogorov's condition.

One exceptional case is easier: the β-problem with 4 particles. Its Birkhoff normal form reads:

$$\overline{H} = H_2 + \beta\overline{H}_4 = \sqrt{2}a_1 + 2a_2 + \frac{\beta}{4}\left(\frac{1}{8}a_1^2 + \frac{1}{4}a_2^2 + \frac{\sqrt{2}}{2}a_1a_2 + \frac{1}{8}d_1^2\right) \tag{2.31}$$

which has the commuting integrals a_1, a_2 and d_1. The frequency map is

$$\omega : (a_1, a_2, d_1) \mapsto (\sqrt{2} + \frac{\beta}{16}a_1 + \frac{\sqrt{2}\beta}{8}a_2, 2 + \frac{\beta}{8}a_2 + \frac{\sqrt{2}\beta}{8}a_1, \frac{\beta}{16}d_1) \tag{2.32}$$

ω is nondegenerate, since

$$\frac{\partial\omega}{\partial(a_1, a_2, d_1)} = \frac{\beta}{4}\begin{pmatrix} \frac{1}{4} & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{4} \end{pmatrix} \tag{2.33}$$

is invertible. So a similar theorem as 2.12 holds for the β-lattice with 4 particles.

It is unclear what happens for the even lattice if $\alpha \neq 0$. The normal form might not be integrable. On the other hand we already found about $\frac{3n}{4}$ integrals. And in [**59**] it was shown that the normal forms of the α-β-lattices with up to 6 particles are all Liouville integrable.

2.8. Discussion

The characteristic features of the FPU lattice such as quasi-periodicity are seldomly found in the low-energy domain of high-dimensional resonant Hamiltonian systems. But the FPU lattice is exceptional due to its particular symmetries and eigenvalues which cause or may cause nondegenerate integrability of the Birkhoff normal form. This in turn implies that the KAM theorem can be used to explain the quasi-periodic motion in the lattice. Nevertheless, the following questions remain unanswered:

1. From Corollaries 2.7 and 2.8 we know that the normal forms of the lattice with fixed endpoints and the odd periodic lattice are always integrable. We checked a nondegeneracy condition for the corresponding β-lattices and were able to apply the KAM theorem. Can we also compute the integrable normal forms if $\alpha \neq 0$? Are they really nondegenerate? This is likely to be a tough computation.
2. What is the reason that the normal form of the even β-lattice is integrable as we know from Corollary 2.9? Is there some hidden symmetry in the lattice that prevents terms $b_k b_k'$ $(k \neq k')$ from appearing in the normal form, thus enforcing the integrability? One can check that R, S, T and U do not cause this degeneration.
3. We saw that the solutions of the Birkhoff normal form can explicitly be written down for the odd β-lattice. Can we also say something about the dynamics of the even β-problem? This question will be treated in Chapter 3. Is it possible to explicitly construct action-angle coordinates for the normal form of the even β-problem, globally or locally, and verify the Kolmogorov nondegeneracy condition? A partial answer to this problem will be given in Chapter 4.
4. What about the even α-β-lattice? As indicated in Corollary 2.9, its normal form has a lot of conserved quantities. But is it also really Liouville integrable? If yes, then there is a big chance for the KAM theorem to work. Otherwise: can we find a counterexample of an even α-β-lattice with a nonintegrable normal form?

2.9. Appendix: computation of exact resonances

This appendix contains a computation of all possible nontrivial low order resonances in the eigenvalues of the FPU lattice. So it lists all the possible relations of the form

$$\sum_{j=1}^{N} \sin(k_j \pi / n) = 0$$

for n arbitrary, $N = 3, 4$ and $1 \leq k_j \leq \frac{n}{2}$. Due to symmetry, these resonances have no impact on the normal form of the lattice equations (2.2), as was shown in this chapter. But it is very interesting to see which resonances exactly are overruled by symmetry. This appendix can therefore be considered as an addition to the work of Izumi and Hemmer [**28**]. The nontrivial resonances are moreover of interest for the study of nonsymmetric nonlinear perturbations of the FPU lattice.

This appendix is based on notes of Frits Beukers. In the computations, some algebra will be used that might be uncommon to the reader.

2.9.1. Sums of roots of unity. We are interested in solving the resonance equation $\nu(\Theta, \theta) = 0$, that is we want to find vanishing sums of the eigenvalues $i\omega_j = 2i\sin(\frac{j\pi}{n})$. A study of these sums is possible if we first consider sums of roots of unity.

Fix $N \in \mathbb{N}$. We study the equation

$$\zeta_1 + \zeta_2 + \cdots + \zeta_N = 0 \tag{P}$$

in the unknown roots of unity ζ_i. The solutions will be determined modulo permutation of the terms and multiplication by a common root of unity. We also assume that there are *no vanishing subsums*, that is $\sum_{i \in I} \zeta_i \neq 0$ for all $I \subset \{1, \ldots, N\}, \#I < N$. We first state our basic tool. Let K be a field generated over $\mathbb{Q}$ by some roots of unity. Let p^k be a prime power and let $\zeta := e^{2\pi i/p^k}$. Suppose $\zeta \notin K$ and $\zeta^p \in K$.

Proposition 2.14. *The minimal polynomial of ζ over the field K is given by $X^p - \zeta^p$ if $k \geq 2$ and $X^{p-1} + X^{p-2} + \cdots + X + 1$ if $k = 1$.*

For the proof of this proposition we refer to [**74**], §60-61.

To return to our problem (P) let us choose $M \in \mathbb{N}$ minimal so that $(\zeta_i/\zeta_j)^M = 1$ for all $i, j = 1, 2, \cdots, N$. Since we can multiply every term of our relation with ζ_1^{-1} and put $\zeta_i = \zeta_i/\zeta_1$ we may as well assume that all ζ_i are M-th roots of unity. Let p^k be a primary factor of M. Set $M' = M/p$ and write $\zeta_i = \tilde{\zeta}_i \zeta^{n_i}$ where $\tilde{\zeta}_i \in K := \mathbb{Q}(e^{2\pi i/M'})$ and $n_i \in \{0, 1, 2, \ldots, p-1\}$. Then, according to proposition 2.14, the minimal polynomial of ζ over K is $X^p - \zeta^p$ if $k \geq 2$ and $X^{p-1} + X^{p-2} + \cdots + X + 1$ if $k = 1$.

We now rewrite our relation in the following form

$$\sum_{s=0}^{p-1} \zeta^s \sum_{n_i = s} \tilde{\zeta}_i = 0 \tag{Q}$$

If $k \geq 2$ the minimal polynomial of ζ over K is $X^p - \zeta^p$. In particular this means that there exists no nontrivial K-linear relation between $1, \zeta, \ldots, \zeta^{p-1}$. So equation (R) implies that all coefficients are zero, hence $\zeta^s \sum_{n_i = s} \tilde{\zeta}_i = 0$ for all $s = 0, 1, 2, \ldots, p-1$. By the minimal choice of M, at least two of the exponents n_i, n_j should be different. Hence the assumption $k \geq 2$ leads automatically to vanishing subsums.

Let us now assume $k = 1$. Then the minimal polynomial of ζ over K is $X^{p-1} + X^{p-2} + \cdots + X + 1$. This means that any K-linear relation between $1, \zeta, \ldots, \zeta^{p-1}$

must have all of its coefficients equal. Hence, (R) implies that all sums

$$\sum_{n_i=s} \tilde{\zeta}_i \tag{R}$$

have the same value σ. Since we do not want vanishing subsums we necessarily have $\sigma \neq 0$. This in its turn implies that each of the summations contains at least one term and so $p \leq N$. This puts a bound on our search range.

2.9.2. Explicit computations. In this section we compute vanishing sums of roots of unity having no vanishing subsums. It should be noted that the solutions are given modulo permutation of terms and multiplication by a common root of unity.

For each of the specific values of N we shall be considering, we denote by M the smallest number such that $(\zeta_i/\zeta_j)^M = 1$ for i, j. From the previous section we know that M is square free and that $p \leq N$ for all prime divisors of M. Furthermore, we also note that if M divides 6, then it is easy to see that the only possible relations without vanishing subsums are $1 - 1 = 0$ and $1 + \delta + \delta^2 = 0$ where $\delta = e^{2\pi i/3}$. So we shall assume that there is a prime ≥ 5 dividing M. By $N \geq p \geq 5$ the first interesting case to be considered is $N = 5$.

$N = 5$. We have $5|M$. Then (P) partitions our sum in precisely five parts, each with equal sum. Hence $1+\eta+\eta^2+\eta^3+\eta^4 = 0$ where $\eta = e^{2\pi i/5}$.

$N = 6$. Then $p \leq 5$, hence $5|M$. Then (P) partitions our sum in four parts of length 1 and one with length 2. Hence we see that $-\delta - \delta^2 + \eta + \eta^2 + \eta^3 + \eta^4 = 0$ is the solution.

$N = 7$. Then $p \leq 7$. If $7|M$ then necessarily, $1 + \epsilon + \epsilon^2 + \epsilon^3 + \epsilon^4 + \epsilon^5 + \epsilon^6 = 0$ where $\epsilon = e^{2\pi i/7}$.

Suppose 5 is the largest prime dividing M. Then (P) gives a partitioning in 31111 or 22111. The first gives rise to solutions with zero subsums. The second gives rise to the solutions $(-\delta-\delta^2)(1+\eta)+\eta^2 + \eta^3 + \eta^4 = 0$ and $(-\delta - \delta^2)(1 + \eta^2) + \eta + \eta^3 + \eta^4 = 0$.

$N = 8$. Then $p \leq 7$. If $7|M$ then (P) implies that we have a partitioning 2111111 and $-\delta - \delta^2 + \epsilon + \epsilon^2 + \epsilon^3 + \epsilon^4 + \epsilon^5 + \epsilon^6 = 0$.

Suppose 5 is the largest prime dividing M. Then (P) gives a partitioning 41111, 32111 or 22211. The first two give rise only to vanishing subsums. The last solution gives rise to $(-\delta - \delta^2)(1 + \eta^i + \eta^j) + \eta^k + \eta^l = 0$ where $\{i, j, k, l\} = \{1, 2, 3, 4\}$.

2.9.3. Resonances. We are interested in vanishing sums of the eigenvalues $2i\omega_k = 2i\sin(\frac{k\pi}{n})$. So we look for all solutions of $\zeta_1+\cdots+\zeta_N = 0$ such that together with each ζ_i, minus its complex conjugate $-\zeta_i^{-1}$ also occurs. Since we shall only be interested in sums of 3 or 4 eigenvalues $i\omega_k$, we restrict ourselves to $N = 6, 8$. We include sums with vanishing subsums, except vanishing subsums of the form $\zeta - \zeta = 0$, since these give rise to vanishing subsums of $i\omega_k$'s. So all vanishing subsums of roots of unity must have length at least three.

$N = 6$. To bring our relation without zero subsums in the desired form, we have to multiply it by $\pm i$ and we derive

$$2i \sin(\pi/6) + 2i \sin(\pi/10) - 2i \sin(3\pi/10) = 0 \ .$$

Now we look at relations with vanishing subsums. There can only be two vanishing subsums of length three. Hence $(\zeta_1 + \zeta_2)(1 + \delta + \delta^2) = 0$ with ζ_1, ζ_2 arbitrary. It is necessary and sufficient to assume that $\zeta_1\zeta_2 = -1$. This means $(\zeta - \zeta^{-1})(1 + \delta + \delta^2)$ where ζ is arbitrary. Hence,

$$2i \sin(\pi r) + 2i \sin(\pi(r + 2/3)) + 2i \sin(\pi(r + 4/3)) = 0 \ ,$$

where r is an arbitrary rational number.

$N = 8$. Let us first see what we get from our relations without zero subsums. We find

$$2i \sin(\pi/6) + 2i \sin(3\pi/14) - 2i \sin(\pi/14) - 2i \sin(5\pi/14) = 0$$
$$2i \sin(\pi/6) + 2i \sin(13\pi/30) - 2i \sin(7\pi/30) - 2i \sin(3\pi/10) = 0$$
$$2i \sin(\pi/6) + 2i \sin(\pi/30) - 2i \sin(11\pi/30) + 2i \sin(\pi/10) = 0$$

Any relation with vanishing subsums must have subsums both of length 4, or subsums of lengths 3 and 5. The first case cannot occur, but the second yields $\zeta_1(1 + \delta + \delta^2) + \zeta_2(1 + \eta + \cdots + \eta^4) = 0$. Both ζ_1, ζ_2 must be purely imaginary and have opposite sign. So we can take $\zeta_1 = -\zeta_2 = i$, hence

$$2i \sin(\pi/2) - 2i \sin(\pi/6) + 2i \sin(\pi/10) - 2i \sin(3\pi/10) = 0$$

This lists all possible nontrivial low order resonance relations for the eigenvalues of the FPU lattice.

CHAPTER 3

Direction reversing waves and monodromy

In this chapter we consider the FPU β-lattice with periodic boundary conditions. Due to special resonances and discrete symmetries, the Birkhoff normal form of this Hamiltonian system is Liouville integrable as was shown in the previous chapter. The normal form equations of motion could quite easily be solved for lattices with an odd number of particles. In this chapter we analyse the normal form of the lattice with an even number of particles and we observe that several nontrivial phenomena occur. First of all, the phase space of the normal form is decomposed in invariant subspaces that describe the interaction between the Fourier modes with wave number k and the Fourier modes with wave number $\frac{n}{2} - k$. We study how the level sets of the integrals of the normal form foliate these invariant subspaces. The integrable foliations turn out to be singular and the method of singular reduction shows that the normal form has invariant pinched tori and monodromy, see [**16**]. Monodromy is an obstruction to the existence of global action-angle variables. The pinched tori are interpreted as homoclinic and heteroclinic connections between travelling waves. Thus we discover a class of solutions of the normal form which can be described as direction reversing travelling waves. The relation between the FPU lattice and its Birkhoff normal form can be understood from KAM theory and approximation theory. This explains why we observe the impact of the direction reversing travelling waves numerically as a relaxation oscillation in the original FPU system. This chapter is based on references [**56**] and [**57**].

3.1. Introduction

Once more, we look at the n particle FPU lattice with periodic boundary conditions, which is the Hamiltonian system on $T^*\mathbb{R}^n$ with Hamiltonian function

$$H = \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2} p_j^2 + W(q_{j+1} - q_j) \tag{3.1}$$

where $W(x) = \frac{1}{2!}x^2 + \frac{\beta}{4!}x^4$ is this time an even potential energy function. In this case we speak of the 'β-lattice', as we have assumed that the nonlinearity coefficient α is zero.

The familiar symplectic linear transformation to phonons $(q,p) \mapsto (Q,P)$ results in a new Hamiltonian on $T^*\mathbb{R}^{n-1}$:

$$H = \sum_{k=1}^{n-1} \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2) + \beta H_4(Q) \tag{3.2}$$

Of course we have neglected the total momentum, which accounts for the dimension reduction.

The FPU lattice is well-known for its unexpected statistical properties, which can to some extent be explained by computing a Birkhoff normal form for it and using the KAM theorem. In the previous chapter of this thesis, we discussed this normalisation and obtained some useful approximation results. For the β-lattice we were able to compute the Birkhoff normal form explicitly in Theorem 2.10. In Corollaries 2.8 and 2.13 it was shown that the normal form is Liouville integrable. This is caused by special resonances and discrete symmetries in the FPU Hamiltonian. But apart from the integrability, many properties of the Birkhoff normal form remained unstudied. Therefore it will be the topic of one more chapter of this thesis.

It turned out that the structure of the integrable normal form of the periodic β-lattice depends strongly on the parity of the number of particles n in this lattice. When n is odd, then all the integrals of the Birkhoff normal form are quadratic functions of the phase space variables (Q, P), as was shown in Corollary 2.8. These quadratics form a set of global action variables which can be augmented to a set of global action-angle variables. The foliation of the phase space into invariant tori is trivial in the sense that the set of Liouville tori is a trivial torus bundle over the set of regular values of the integrals. Moreover, the equations of motion can be solved explicitly. The normal form turns out to be even nondegenerate in the sense of the KAM theorem, which proves the abundance of quasi-periodic solutions in the low energy domain of the original system (3.2). Thus, for odd n the normal form is quite tractable.

But the situation is not so easy when n is even and hence in this chapter we shall study the dynamics and bifurcations of the integrable Birkhoff normal form (3.2) of the periodic β-lattice in the case that n is even. The difficulty is that some of the integrals of the even normal form are not quadratic but quartic functions of the phase space variables (Q, P). It turns out that this leads to various nontrivial phenomena. The foliation of the phase space in Liouville tori is not trivial. Moreover, several dynamically interesting global and local bifurcations occur. Among others, we find 'direction reversing travelling waves' in the even β-lattice. This means that there is an enormous qualitative difference between the Birkhoff normal forms of the odd and the even lattices, which can also be observed numerically in the original FPU lattice.

3.2. Outline of this chapter

In Chapter 1 we encountered some interesting invariant submanifolds for the anharmonic FPU lattice. The first important remark of the present chapter will be that the phase space of the even Birkhoff normal form can be decomposed in even more invariant symplectic subspaces: the phase space of the normal form is a direct sum

$$T^*\mathbb{R}^{n-1} = \bigoplus_{0 \le k \le \frac{n}{4}} \mathcal{A}_k$$

of invariant symplectic subspaces

$$\mathcal{A}_k = \{(Q,P) \in T^*\mathbb{R}^{n-1} \mid Q_{k'} = P_{k'} = 0 \ \forall \ k' \notin \{k, n-k, \frac{n}{2}-k, \frac{n}{2}+k\} \ \}$$

$\mathcal{A}_k$ describes the interaction of the modes with wave numbers k and $\frac{n}{2}-k$. It also turns out that the foliation of $T^*\mathbb{R}^{n-1}$ by the level sets of the integrals of the even normal form is simply the Cartesian product of the foliations of the various $\mathcal{A}_k$.

Of particular interest are the $\mathcal{A}_k$ with $1 \leq k < \frac{n}{4}$. These are symplectic subspaces with four degrees of freedom that exist when n is even and $n \geq 6$. They describe the interaction between the two modes with wave number k and the two modes with wave number $\frac{n}{2}-k$. We study the foliations of these subspaces using geometric arguments based on invariant theory and the method of singular reduction, see [**11**]. This geometric approach reveals all the integrable structure that is present in the normal form.

In the reduced system we find four relative equilibria that can undergo a Hamiltonian Hopf bifurcation [**44**] if one varies certain energies. We also see that there can be homoclinic or heteroclinic connections between the relative equilibria and we derive under which conditions these connections exist. It turns out that the singular fibers over the homoclinic and heteroclinic connections are pinched tori: whiskered tori with coinciding stable and unstable manifolds.

It is well-known [**43**], [**66**] that the presence of a pinched torus results in nontrivial monodromy: the foliation of $\mathcal{A}_k$ in Liouville tori is not trivial. Nontrivial monodromy is an important obstruction to the existence of global action-angle variables, see [**16**].

On the other hand, our analysis yields interesting dynamical information. The relative equilibria can be interpreted as waves in the periodic FPU lattice that travel clockwise and counterclockwise. Thus it turns out that in the normal form there are homoclinic and heteroclinic connections between these travelling waves. Although the pinched tori themselves might not really be present in the original FPU system, we expect from [**65**] that many of the Liouville tori close to a pinched torus survive as KAM tori in the original FPU lattice. These KAM tori constitute a large collection of interesting new solutions of the periodic FPU lattice, showing a relaxation oscillation between travelling waves in opposite directions. We indeed detect this relaxation oscillation numerically in the original equations induced by (3.1). This type of solution has the remarkable property that it displays an interesting interaction of the normal modes with wave numbers k and $\frac{n}{2}-k$ without transferring energy between modes with different wave numbers.

3.3. Phase space splitting and regular reduction

Let us recall a few facts from Chapter 2. For $1 \leq k < \frac{n}{2}$ we had defined the Hopf-variables

$$\begin{aligned} a_k &:= \frac{1}{2\omega_k}(P_k^2 + P_{n-k}^2 + \omega_k^2 Q_k^2 + \omega_k^2 Q_{n-k}^2) \\ b_k &:= P_k Q_{n-k} - P_{n-k} Q_k \end{aligned} \tag{3.3}$$

$$\begin{aligned} c_k :=& \frac{1}{2\omega_k}(P_{n-k}^2 - P_k^2 + \omega_k^2 Q_{n-k}^2 - \omega_k^2 Q_k^2) \\ d_k :=& \frac{1}{\omega_k}(P_k P_{n-k} + \omega_k^2 Q_k Q_{n-k}) \end{aligned} \tag{3.4}$$

and if n is even

$$a_{\frac{n}{2}} := \frac{1}{2\omega_{\frac{n}{2}}}(P_{\frac{n}{2}}^2 + \omega_{\frac{n}{2}}^2 Q_{\frac{n}{2}}^2)$$

In Theorem 2.10 we computed that the Birkhoff normal form of the periodic FPU Hamiltonian (3.2) with quartic nonlinearities and n particles is $\overline{H} = H_2 + \beta \overline{H}_4$, where $H_2 = \sum_{1\le k \le \frac{n}{2}} \omega_k a_k$ and

$$\begin{aligned} \overline{H}_4 = \frac{1}{n} \Bigg\{ & \sum_{0<k<l<\frac{n}{2}} \frac{\omega_k \omega_l}{4} a_k a_l + \sum_{0<k<\frac{n}{2}} \frac{\omega_k^2}{32}(3a_k^2 - b_k^2) + \frac{1}{4} a_{\frac{n}{2}}^2 + \frac{1}{2} a_{\frac{n}{2}} \sum_{0<k<\frac{n}{2}} \omega_k a_k \\ & + \frac{1}{8} \sum_{0<k<\frac{n}{4}} \omega_k \omega_{\frac{n}{2}-k}(d_k d_{\frac{n}{2}-k} - c_k c_{\frac{n}{2}-k}) + \frac{1}{16}(d_{\frac{n}{4}}^2 - c_{\frac{n}{4}}^2) \Bigg\} \end{aligned} \tag{3.5}$$

For even n this has resulted in the following proposition:

Proposition 3.1. *If the number of particles n is* even, *then the Birkhoff normal form (3.5) is Liouville integrable. The integrals are the quadratics $\mathcal{H}_k := a_k$ $(1 \le k \le \frac{n}{2})$, $\mathcal{I}_k := b_k - b_{\frac{n}{2}-k}$ $(1 \le k < \frac{n}{4})$ and $\mathcal{J} := \frac{1}{2\sqrt{2n}} d_{\frac{n}{4}}$ (if n is a multiple of 4) and the quartics $\mathcal{K}_k := \frac{1}{32n}(4\omega_k\omega_{\frac{n}{2}-k}(d_k d_{\frac{n}{2}-k} - c_k c_{\frac{n}{2}-k}) - \omega_k^2 b_k^2 - \omega_{\frac{n}{2}-k}^2 b_{\frac{n}{2}-k}^2)$ $(1 \le k < \frac{n}{4})$.*

We shall now use the short-hand notation $\tilde{k} = \frac{n}{2} - k$. We want to study how the level sets of the integrals of Proposition 3.1 foliate the phase space $T^*\mathbb{R}^{n-1}$. Therefore it is very useful to note that these integrals are uncoupled in the following sense: the integral $\mathcal{H}_{\frac{n}{2}}$ depends only on the phase space variables $(Q_{\frac{n}{2}}, P_{\frac{n}{2}})$. The integrals $\mathcal{H}_{\frac{n}{4}}$ and $\mathcal{J}$ depend only on the variables $(Q_{\frac{n}{4}}, Q_{\frac{3n}{4}}, P_{\frac{n}{4}}, P_{\frac{3n}{4}})$. The integrals $\mathcal{H}_k, \mathcal{H}_{\tilde{k}}, \mathcal{I}_k$ and $\mathcal{K}_k$ depend only on the variables $(Q_k, Q_{\tilde{k}}, Q_{n-k}, Q_{n-\tilde{k}}, P_k, P_{\tilde{k}}, P_{n-k}, P_{n-\tilde{k}})$. So we have the following:

Theorem 3.2. *For even n, the phase space of the Birkhoff normal form (3.5) is the direct sum of invariant symplectic subspaces*

$$T^*\mathbb{R}^{n-1} = \bigoplus_{0\le k\le \frac{n}{4}} \mathcal{A}_k$$

in which

$$\mathcal{A}_k = \{(Q,P) \in T^*\mathbb{R}^{n-1} \mid Q_{k'} = P_{k'} = 0 \ \forall \ k' \notin \{k, n-k, \tilde{k}, n-\tilde{k}\} \ \}$$

Moreover, the foliation of $T^*\mathbb{R}^{n-1}$ is the Cartesian product of the foliations of the $\mathcal{A}_k$.

Note that with the terminology of Chapter 1, $\mathcal{A}_k = M_n^{\{k,\tilde{k},n-k,n-\tilde{k}\}}$. By Theorem 3.2 it is sufficient to know how $\mathcal{H}_{\frac{n}{2}}$ foliates $\mathcal{A}_0 \cong T^*\mathbb{R}$, how $\mathcal{H}_{\frac{n}{4}}$ and $\mathcal{J}$ foliate $\mathcal{A}_{\frac{n}{4}} \cong T^*\mathbb{R}^2$ and how $\mathcal{H}_k, \mathcal{H}_{\tilde{k}}, \mathcal{I}_k$ and $\mathcal{K}_k$ foliate $\mathcal{A}_k \cong T^*\mathbb{R}^4$. The foliation of $T^*\mathbb{R}^{n-1}$ by all integrals is the Cartesian product of these foliations.

3.3.1. The foliation of $\mathcal{A}_0$. This subspace describes the behaviour of the normal mode $(Q_{\frac{n}{2}}, P_{\frac{n}{2}})$. It is clear that $\mathcal{H}_{\frac{n}{2}} = \frac{1}{4}(P_{\frac{n}{2}}^2 + 4Q_{\frac{n}{2}}^2)$ foliates $\mathcal{A}_0 \cong T^*\mathbb{R}$ in ellipses. In other words, the Fourier mode with the highest wave number ($\frac{n}{2}$ waves in the lattice) and the highest vibrational frequency ($\omega_{\frac{n}{2}} = 2$) has constant energy in the normal form.

3.3.2. The foliation of $\mathcal{A}_{\frac{n}{4}}$. The system on $\mathcal{A}_{\frac{n}{4}} \cong T^*\mathbb{R}^2$ with integrals $\mathcal{H}_{\frac{n}{4}}$ and $\mathcal{J}$ describes the interaction of the $\frac{n}{4}$-th and $\frac{3n}{4}$-th normal mode. These modes have equal wave number $\frac{n}{4}$ and equal vibrational frequency $\sqrt{2}$, but are out of phase, as one describes a cosine wave in the FPU lattice and the other a sine wave.

The foliation of $\mathcal{A}_{\frac{n}{4}}$ can be described in the following standard way. It is clear that im $\mathcal{H}_{\frac{n}{4}} = \mathbb{R}_{\geq 0}$ and that for $h_{\frac{n}{4}} \in \mathbb{R}_{\geq 0}$, the inverse image $\mathcal{H}_{\frac{n}{4}}^{-1}(h_{\frac{n}{4}}) \subset \mathcal{A}_{\frac{n}{4}}$ is a three-dimensional ellipsoid. The flow of $X_{\mathcal{H}_{\frac{n}{4}}}$ induces an S^1-symmetry on this ellipsoid given by

$$(\phi_{\frac{n}{4}}, \begin{pmatrix} Q_{\frac{n}{4}} \\ Q_{\frac{3n}{4}} \\ P_{\frac{n}{4}} \\ P_{\frac{3n}{4}} \end{pmatrix}) \mapsto \begin{pmatrix} Q_{\frac{n}{4}} \cos\phi_{\frac{n}{4}} + \frac{1}{\sqrt{2}} P_{\frac{n}{4}} \sin\phi_{\frac{n}{4}} \\ Q_{\frac{3n}{4}} \cos\phi_{\frac{n}{4}} + \frac{1}{\sqrt{2}} P_{\frac{3n}{4}} \sin\phi_{\frac{n}{4}} \\ P_{\frac{n}{4}} \cos\phi_{\frac{n}{4}} - \sqrt{2} Q_{\frac{n}{4}} \sin\phi_{\frac{n}{4}} \\ P_{\frac{3n}{4}} \cos\phi_{\frac{n}{4}} - \sqrt{2} Q_{\frac{3n}{4}} \sin\phi_{\frac{n}{4}} \end{pmatrix} \tag{3.6}$$

The orbits of this circle action have dimension one if $h_{\frac{n}{4}} > 0$ and dimension zero otherwise. The reduced phase space $\mathcal{H}_{\frac{n}{4}}^{-1}(h_{\frac{n}{4}})/_{S^1}$ can be found by applying the Hopf map $\mathcal{F}^{(1)} : \mathcal{H}_{\frac{n}{4}}^{-1}(h_{\frac{n}{4}}) \to S^2_{h_{\frac{n}{4}}}$ which is defined by

$$\mathcal{F}^{(1)} : (Q, P) \mapsto (b_{\frac{n}{4}}, c_{\frac{n}{4}}, d_{\frac{n}{4}})$$

see [**11**]. The fibers of $\mathcal{F}^{(1)}$ are exactly the orbits of the S^1-action, so $S^2_{h_{\frac{n}{4}}}$ constitutes the reduced phase space. Every Hamiltonian function on $\mathcal{A}_{\frac{n}{4}}$ that commutes with $\mathcal{H}_{\frac{n}{4}}$ reduces to a Hamiltonian on $S^2_{h_{\frac{n}{4}}}$ because it is constant on the orbits of the S^1-action. In particular, $\mathcal{J} = \frac{1}{2\sqrt{2n}} d_{\frac{n}{4}}$. The foliation of $S^2_{h_{\frac{n}{4}}}$ in level sets of $\mathcal{J}$ is trivial: the level sets are the circles of constant $d_{\frac{n}{4}}$ and there are two stable relative equilibria. They are depicted in Figure 1. Reconstructing this picture by the Hopf map, we get the desired foliation of $\mathcal{A}_{\frac{n}{4}}$.

3.3.3. The foliations of the $\mathcal{A}_k$. If $n \geq 6$ is even, then for each $1 \leq k < \frac{n}{4}$, we have the four commuting integrals $\mathcal{H}_k, \mathcal{H}_{\tilde{k}}, \mathcal{I}_k$ and $\mathcal{K}_k$ on $\mathcal{A}_k \cong T^*\mathbb{R}^4$. They describe the interaction between the two modes with wave number k and the two modes with wave number $\tilde{k}$. Note that these two pairs of modes do not exchange energy, since $\mathcal{H}_k$ and $\mathcal{H}_{\tilde{k}}$ are constants. Still it turns out that their interaction is very interesting. We shall see that the foliations of the $\mathcal{A}_k$ contain singularities.

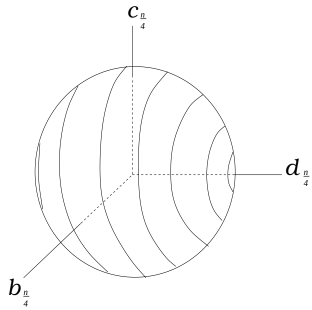

Figure 1: The reduced space $S^2_{h_{\frac{n}{4}}}$ and the level sets of $\mathcal{J}$.

On $\mathcal{A}_k$, consider the commuting Hamiltonians $\mathcal{H}_k$ and $\mathcal{H}_{\tilde{k}}$. They define a mapping $\mathcal{H}_{k,\tilde{k}} := (\mathcal{H}_k, \mathcal{H}_{\tilde{k}})$. It is easy to see that im $\mathcal{H}_{k,\tilde{k}} = (\mathbb{R}_{\geq 0})^2$, whereas the level sets $\mathcal{H}^{-1}_{k,\tilde{k}}(h_k, h_{\tilde{k}})$ are Cartesian products of ellipsoids.

Because the flows of the Hamiltonian vector fields of $\mathcal{H}_k$ and $\mathcal{H}_{\tilde{k}}$ commute and are periodic with period 2π, they define a linear symplectic T^2-action on $\mathcal{H}^{-1}_{k,\tilde{k}}(h_k, h_{\tilde{k}}) \subset \mathcal{A}_k$ given by

$$\left(\begin{pmatrix} \phi_k \\ \phi_{\tilde{k}} \end{pmatrix}, \begin{pmatrix} Q_k \\ Q_{\tilde{k}} \\ Q_{n-\tilde{k}} \\ Q_{n-k} \\ P_k \\ P_{\tilde{k}} \\ P_{n-\tilde{k}} \\ P_{n-k} \end{pmatrix} \right) \mapsto \begin{pmatrix} Q_k \cos\phi_k + \frac{1}{\omega_k} P_k \sin\phi_k \\ Q_{\tilde{k}} \cos\phi_{\tilde{k}} + \frac{1}{\omega_{\tilde{k}}} P_{\tilde{k}} \sin\phi_{\tilde{k}} \\ Q_{n-\tilde{k}} \cos\phi_{\tilde{k}} + \frac{1}{\omega_{\tilde{k}}} P_{n-\tilde{k}} \sin\phi_{\tilde{k}} \\ Q_{n-k} \cos\phi_k + \frac{1}{\omega_k} P_{n-k} \sin\phi_k \\ P_k \cos\phi_k - \omega_k Q_k \sin\phi_k \\ P_{\tilde{k}} \cos\phi_{\tilde{k}} - \omega_{\tilde{k}} Q_{\tilde{k}} \sin\phi_{\tilde{k}} \\ P_{n-\tilde{k}} \cos\phi_{\tilde{k}} - \omega_{\tilde{k}} Q_{n-\tilde{k}} \sin\phi_{\tilde{k}} \\ P_{n-k} \cos\phi_k - \omega_k Q_{n-k} \sin\phi_k \end{pmatrix} \tag{3.7}$$

The orbits of this T^2-action are all tori of dimension $\#\{k' \in \{k, \tilde{k}\} \mid h_{k'} \neq 0\}$.

We want to study the reduced phase-space $\mathcal{H}^{-1}_{k,\tilde{k}}(h_k, h_{\tilde{k}})/_{T^2}$. We do this by applying the reduction map $\mathcal{F}^{(2)} : \mathcal{H}^{-1}_{k,\tilde{k}}(h_k, h_{\tilde{k}}) \to S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ defined by

$$\mathcal{F}^{(2)} : (Q, P) \mapsto (b_k, c_k, d_k, b_{\tilde{k}}, c_{\tilde{k}}, d_{\tilde{k}})$$

$\mathcal{F}^{(2)}$ is the Cartesian product of two Hopf mappings. The fibers of $\mathcal{F}^{(2)}$ are exactly the orbits of the T^2-action, so $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ constitutes the reduced phase space. Every Hamiltonian function on $\mathcal{A}_k$ that commutes with $\mathcal{H}_k$ and $\mathcal{H}_{\tilde{k}}$ reduces to a Hamiltonian function on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ because it is constant on the orbits of the T^2-action. In particular $\mathcal{I}_k$ and $\mathcal{K}_k$. The Hamiltonian equations of motion induced by such a Hamiltonian reduce to Hamiltonian equations on the orbit space $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$. For a

Hamiltonian function H, these reduced equations read

$$\frac{d}{dt}\begin{pmatrix} b_{k'} \\ c_{k'} \\ d_{k'} \end{pmatrix} = 2 \begin{pmatrix} \partial_{b_{k'}} H \\ \partial_{c_{k'}} H \\ \partial_{d_{k'}} H \end{pmatrix} \times \begin{pmatrix} b_{k'} \\ c_{k'} \\ d_{k'} \end{pmatrix}$$

for $k' = k, \tilde{k}$. Thus we obtain a two degree of freedom integrable Hamiltonian system on the product of two spheres. We will now study this reduced integrable system, which describes the interaction of wave patterns with wave numbers k and $\tilde{k}$.

3.4. Travelling waves

Let us now consider the reduced integrable system on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ with Hamiltonian $\mathcal{K}_k$ and momentum $\mathcal{I}_k = b_k - b_{\tilde{k}}$. The flow of $X_{\mathcal{I}_k}$ induces a Hamiltonian S^1-action on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ given by

$$(t, \begin{pmatrix} b_k \\ c_k \\ d_k \\ b_{\tilde{k}} \\ c_{\tilde{k}} \\ d_{\tilde{k}} \end{pmatrix}) \mapsto \begin{pmatrix} b_k \\ c_k \cos 2t - d_k \sin 2t \\ d_k \cos 2t + c_k \sin 2t \\ b_{\tilde{k}} \\ c_{\tilde{k}} \cos 2t + d_{\tilde{k}} \sin 2t \\ d_{\tilde{k}} \cos 2t - c_{\tilde{k}} \sin 2t \end{pmatrix} \tag{3.8}$$

This action has four isolated fixed points, namely the points $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$. But because the Hamiltonian $\mathcal{K}_k$ is invariant under the action (3.8), this implies that the derivative of $\mathcal{K}_k$ also vanishes at these points. In other words, the points $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$ constitute the set of joint critical points of $\mathcal{I}_k$ and $\mathcal{K}_k$.

Critical points of the reduced system on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ are called relative equilibria, because in the reconstructed system on $\mathcal{A}_k \cong T^*\mathbb{R}^4$ (or $T^*\mathbb{R}^{n-1}$ if you like) their fibers represent invariant sets, see [**1**]. It follows from (3.7) that in $\mathcal{A}_k$ the critical fiber $(\mathcal{F}^{(2)})^{-1}(\pm_k h_k, 0, 0, \pm_{\tilde{k}} h_{\tilde{k}}, 0, 0)$ is the following parameterised torus

$$\begin{aligned} \{\ (&\sqrt{h_k}\cos\phi_k, \sqrt{h_{\tilde{k}}}\cos\phi_{\tilde{k}}, \sqrt{h_{\tilde{k}}}\sin\phi_{\tilde{k}}, \sqrt{h_k}\sin\phi_k, \\ &\mp_k \sqrt{h_k}\sin\phi_k, \mp_{\tilde{k}}\sqrt{h_{\tilde{k}}}\sin\phi_{\tilde{k}}, \pm_{\tilde{k}}\sqrt{h_{\tilde{k}}}\cos\phi_{\tilde{k}}, \pm_k\sqrt{h_k}\cos\phi_k) \mid (\phi_k, \phi_{\tilde{k}}) \in T^2\ \} \end{aligned} \tag{3.9}$$

It has dimension $\#\{k' \in \{k, \tilde{k}\} | h_{k'} \neq 0\}$. This torus is invariant under the flow of $X_{\overline{H}}$ so one can write the equations induced by $\overline{H}$ as equations for $\phi \in T^2$. Using expression (3.5) it is not hard to compute that they read:

$$\frac{d\phi_k}{dt} = \pm_k\left(\frac{\partial \overline{H}}{\partial \mathcal{H}_k}\,|_{\mathcal{H}=h} - \frac{\omega_k^2 h_k}{16}\right) \tag{3.10}$$

$$\frac{d\phi_{\tilde{k}}}{dt} = \pm_{\tilde{k}}\left(\frac{\partial \overline{H}}{\partial \mathcal{H}_{\tilde{k}}}\,|_{\mathcal{H}=h} - \frac{\omega_{\tilde{k}}^2 h_{\tilde{k}}}{16}\right) \tag{3.11}$$

Hence the motion in the critical fibers is uniform. The corresponding solutions have a clear physical interpretation: we can transform back to the original position coordinates to obtain that

$$q_j = \sqrt{\frac{2h_k}{n\omega_k}}\cos(\frac{2\pi jk}{n} - \phi_k) + \sqrt{\frac{2h_{\tilde{k}}}{n\omega_{\tilde{k}}}}\cos(\frac{2\pi j\tilde{k}}{n} - \phi_{\tilde{k}})$$

in the critical fibers. The constants h_k and $h_{\tilde{k}}$ are supposed to be small, since otherwise the normal form approximation has no validity. So a solution that lies in a critical fiber is a superposition of

1. a small amplitude travelling wave with wave number k and speed approximately $\pm_k\omega_k$.
2. a small amplitude travelling wave with wave number $\tilde{k}$ and speed approximately $\pm_{\tilde{k}}\omega_{\tilde{k}}$.

If $\pm_k = \pm_{\tilde{k}}$ then these waves move in the same direction. Otherwise one moves clockwise and the other moves counterclockwise.

Travelling waves, superposed travelling waves and solitary waves have previously been studied in the infinite FPU lattice [**23**], [**30**]. But they can obviously also occur in a finite periodic lattice, as was already remarked in [**61**]. Travelling waves in the periodic lattice can also be interpreted as spatially periodic travelling waves in the infinite lattice, as each periodic lattice is naturally embedded as a symmetric invariant manifold in the infinite lattice, see Chapter 1.

We shall study the stability of the travelling wave solutions and homoclinic and heteroclinic connections between them. We do this of course in the reduced context, that is we consider them as critical points in the reduced phase space $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$.

3.5. Stability of the relative equilibria

We want to determine the stability type of the superposed travelling wave solutions in the Birkhoff normal form, that is the stability type of the relative equilibria $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$ on the reduced phase space $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$. We will assume from now on that the linear energies h_k and $h_{\tilde{k}}$ are both strictly positive, so that our reduced phase space has dimension four. (The analysis is trivial if one of these energies is zero.) We perform our stability analysis in local coordinates on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ near $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$ by simply projecting $(b_k, c_k, d_k, b_{\tilde{k}}, c_{\tilde{k}}, d_{\tilde{k}}) \mapsto (c_k, d_k, c_{\tilde{k}}, d_{\tilde{k}})$. Note that these are not Darboux coordinates. The critical points themselves are all mapped to $(0, 0, 0, 0)$.

3.5.1. A Lyapunov function. One way of proving stability is by pointing out a Lyapunov function. The Hamiltonian $\mathcal{K}_k$ is the first candidate since it is an a priori constant of motion. But it turns out that $\mathcal{K}_k$ is not definite at any of the relative equilibria. Luckily, we have another constant of motion, namely $\mathcal{I}_k$. We now use that at $(\pm_k h_k, 0, 0, \pm_{\tilde{k}} h_{\tilde{k}}, 0, 0)$ one may write $b_k = \pm_k\sqrt{h_k^2 - c_k^2 - d_k^2} = \pm_k(h_k - \frac{1}{2h_k}(c_k^2 + d_k^2) + \ldots)$ and $b_{\tilde{k}} = \pm_{\tilde{k}}\sqrt{h_{\tilde{k}}^2 - c_{\tilde{k}}^2 - d_{\tilde{k}}^2} = \pm_{\tilde{k}}(h_{\tilde{k}} - \frac{1}{2h_{\tilde{k}}}(c_{\tilde{k}}^2 + d_{\tilde{k}}^2) + \ldots)$. So

$$\mathcal{I}_k = b_k - b_{\tilde{k}} = \pm_k h_k \mp_{\tilde{k}} h_{\tilde{k}} \mp_k \frac{1}{2h_k}(c_k^2 + d_k^2) \pm_{\tilde{k}} \frac{1}{2h_{\tilde{k}}}(c_{\tilde{k}}^2 + d_{\tilde{k}}^2) + \ldots$$

which is definite at $(0,0,0,0)$ if and only if $\pm_k \neq \pm_{\tilde{k}}$. We conclude that the relative equilibria $\pm(h_k, 0, 0, -h_{\tilde{k}}, 0, 0)$ are stable.

Near the relative equilibria $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ we will try to make linear combinations of $\mathcal{K}_k$ and $\mathcal{I}_k$ that are definite. It is easily computed that in local coordinates $(c_k, d_k, c_{\tilde{k}}, d_{\tilde{k}})$

$$(32n\mathcal{K}_k \pm 2\lambda h_k h_{\tilde{k}} \mathcal{I}_k) = (\omega_k^2 + \lambda h_{\tilde{k}})(c_k^2 + d_k^2) + (\omega_{\tilde{k}}^2 - \lambda h_k)(c_{\tilde{k}}^2 + d_{\tilde{k}}^2) + 4\omega_k \omega_{\tilde{k}}(d_k d_{\tilde{k}} - c_k c_{\tilde{k}}) + \dots$$

modulo constants. Using that $|c_k c_{\tilde{k}} - d_k d_{\tilde{k}}| \leq ||(c_k, d_k)|| \cdot ||(c_{\tilde{k}}, d_{\tilde{k}})||$, one sees that this expression is definite if and only if

$$\det \begin{pmatrix} \omega_k^2 + \lambda h_{\tilde{k}} & 2\omega_k \omega_{\tilde{k}} \\ 2\omega_k \omega_{\tilde{k}} & \omega_{\tilde{k}}^2 - \lambda h_k \end{pmatrix} = -\lambda^2 h_k h_{\tilde{k}} + \lambda(\omega_{\tilde{k}}^2 h_{\tilde{k}} - \omega_k^2 h_k) - 3\omega_k^2 \omega_{\tilde{k}}^2 > 0$$

The preceding inequality has real solutions λ if the discriminant

$$r := \omega_k^4 h_k^2 - 14\omega_k^2 \omega_{\tilde{k}}^2 h_k h_{\tilde{k}} + \omega_{\tilde{k}}^4 h_{\tilde{k}}^2 \tag{3.12}$$

is positive. So if $r > 0$ then the relative equilibria $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ are stable.

3.5.2. Linearisation. Because we still don't know anything about stability if $r < 0$, an alternative is to study the linearisation of the vector field $X_{\mathcal{K}_k}$ at $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$. Again in local coordinates, it reads

$$X_{\mathcal{K}_k} \begin{pmatrix} c_k \\ d_k \\ c_{\tilde{k}} \\ d_{\tilde{k}} \end{pmatrix} = \pm \frac{1}{8n} \begin{pmatrix} 0 & \omega_k^2 h_k & 0 & 2\omega_k \omega_{\tilde{k}} h_k \\ -\omega_k^2 h_k & 0 & 2\omega_k \omega_{\tilde{k}} h_k & 0 \\ 0 & 2\omega_k \omega_{\tilde{k}} h_{\tilde{k}} & 0 & \omega_{\tilde{k}}^2 h_{\tilde{k}} \\ 2\omega_k \omega_{\tilde{k}} h_{\tilde{k}} & 0 & -\omega_{\tilde{k}}^2 h_{\tilde{k}} & 0 \end{pmatrix} \begin{pmatrix} c_k \\ d_k \\ c_{\tilde{k}} \\ d_{\tilde{k}} \end{pmatrix} + \text{h.o.t.}$$

'h.o.t.' stands of course for 'higher order terms'. One calculates that the characteristic polynomial of the above matrix reads

$$C(\lambda) = \lambda^4 + \lambda^2(\omega_k^4 h_k^2 + \omega_{\tilde{k}}^4 h_{\tilde{k}}^2 - 8\omega_k^2 \omega_{\tilde{k}}^2 h_k h_{\tilde{k}})/(8n)^2 + 9(\omega_k^4 \omega_{\tilde{k}}^4 h_k^2 h_{\tilde{k}}^2)/(8n)^4$$

so the eigenvalues are the numbers

$$\lambda = \pm \frac{1}{16n} \sqrt{p \pm q\sqrt{r}}$$

where

$$p := 16\omega_k^2 \omega_{\tilde{k}}^2 h_k h_{\tilde{k}} - 2\omega_k^4 h_k^2 - 2\omega_{\tilde{k}}^4 h_{\tilde{k}}^2 \quad , \quad q := 2\omega_k^2 h_k - 2\omega_{\tilde{k}}^2 h_{\tilde{k}}$$

and r as defined previously in (3.12). Note that $C(\lambda) = C(-\lambda)$, so if λ is an eigenvalue of (3.13), then so are $-\lambda, \bar{\lambda}$ and $-\bar{\lambda}$. The reason is of course that our matrix is conjugate to an infinitesimally symplectic matrix.

The next observation is that if $r \geq 0$ or $q = 0$ then $p \pm q\sqrt{r} \in \mathbb{R}$ so the eigenvalues are purely real or purely imaginary, dependent on the signs of $p \pm q\sqrt{r}$. On the other hand, if $r < 0$ and $q \neq 0$ then none of the eigenvalues lies on the real or the imaginary axis. A simple analysis now leads to the following results:

1. If $r > 0$ then there are four distinct purely imaginary eigenvalues. We have a double center point.
2. If $r = 0$, we find double imaginary eigenvalues. The linearisation matrix is not semi-simple.

3. If $r < 0$ then none of the eigenvalues lies on the imaginary axis. We have a double focus equilibrium point (focus-focus point).

This is illustrated in the bifurcation diagram in Figure 2.

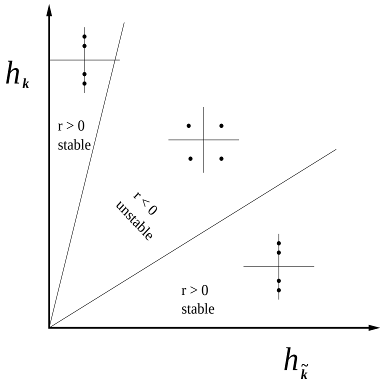

Figure 2: Bifurcation diagram of the linear stability of the relative equilibria.

The set of $h_k, h_{\tilde{k}}$ for which $r = 0$ consists of two half lines in the positive quadrant. At each of these half lines, the relative equilibria undergo a linear Hamiltonian Hopf bifurcation [**44**]: two pairs of imaginary eigenvalues come together and split into a quadruple of non-imaginary eigenvalues, where at the bifurcation value the linearisation matrix has a nilpotent part. So the linear stability of the relative equilibria $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ changes from neutrally stable to unstable. The linear instability implies of course that the equilibria are unstable also in the nonlinear system. This concludes the stability analysis of the relative equilibria. In Section 3.6 we shall investigate the Hamiltonian Hopf bifurcation in more detail as we will also incorporate the nonlinear terms of the Hamiltonian in our analysis of the bifurcation.

3.5.3. Stability results. We investigated the relative equilibria and their stability with respect to perturbations in the initial data. The results are summarised in the following corollary:

Corollary 3.3. *The relative equilibria* $\pm(h_k, 0, 0, -h_{\tilde{k}}, 0, 0)$ *are stable. The stability of the relative equilibria* $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ *depends on the bifurcation parameter*

$$r = \omega_k^4 h_k^2 - 14\omega_k^2 \omega_{\tilde{k}}^2 h_k h_{\tilde{k}} + \omega_{\tilde{k}}^4 h_{\tilde{k}}^2$$

They are stable for $r > 0$ *and unstable for* $r < 0$.

In terms of travelling wave solutions, one may interpret Corollary 3.3 as follows:

The superposition of two travelling waves with wave numbers k *and* $n/2 - k$ *is stable if the two waves move in opposite directions. A superposition of waves in equal directions can be both stable and unstable. It is stable only if one of the waves is relatively small with respect to the other. Otherwise it is unstable.*

3.6. Singular reduction

In the next sections we shall try to understand the Hamiltonian Hopf bifurcation of the previous paragraph geometrically. For this purpose, we shall make a reduction of the S^1-symmetry (3.8) on the four dimensional reduced phase space $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ to obtain another reduced phase space of still lower dimension. However, the S^1-action (3.8) on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ has isotropy: four of its orbits are not circles, but the equilibrium points $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$. Therefore the regular Marsden-Weinstein reduction [**1**] is not sufficient and we have to use the methods of invariant theory and singular reduction, see [**11**]. From the singularly reduced system on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}/_{S^1}$ we can study the Hamiltonian Hopf bifurcation geometrically and in more detail. Moreover, in Section 3.7 we will show that if the relative equilibria $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ are unstable, then there are homoclinic and heteroclinic connections connecting them: pinched tori. In the original foliation of $\mathcal{A}_k \subset T^*\mathbb{R}^{n-1}$ these pinched tori are whiskered tori with coinciding stable and unstable manifolds.

The flow of $X_{\mathcal{I}_k}$ induces a Hamiltonian S^1-action on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ given by (3.8). The orbits of this S^1-action are all circles, except for exactly the relative equilibria $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$.

The following quantities are invariant under this action:

$$a_k,\ a_{\tilde{k}},\ \pi_k := b_k,\ \rho_k := b_{\tilde{k}},\ \sigma_k := d_k d_{\tilde{k}} - c_k c_{\tilde{k}},\ \tau_k := d_k c_{\tilde{k}} + d_{\tilde{k}} c_k$$

In fact, every other invariant can be expressed as a function of $a_k, a_{\tilde{k}}, \pi_k, \rho_k, \sigma_k$ and τ_k: they form a Hilbert basis of the ring of invariant functions. The invariants satisfy the relations

$$\sigma_k^2 + \tau_k^2 = (a_k^2 - \pi_k^2)(a_{\tilde{k}}^2 - \rho_k^2)$$

Having fixed $a_k = h_k$, $a_{\tilde{k}} = h_{\tilde{k}}$, this reduces to

$$\sigma_k^2 + \tau_k^2 = (h_k^2 - \pi_k^2)(h_{\tilde{k}}^2 - \rho_k^2)$$

Therefore, the set

$$P_{h_k, h_{\tilde{k}}} := \{(\pi_k, \rho_k, \sigma_k, \tau_k) \in \mathbb{R}^4 | \sigma_k^2 + \tau_k^2 = (h_k^2 - \pi_k^2)(h_{\tilde{k}}^2 - \rho_k^2),\ |\pi_k| \leq h_k,\ |\rho_k| \leq h_{\tilde{k}}\}$$

constitutes the orbit space $S^2_{h_k} \times S^2_{h_{\tilde{k}}}/_{S^1}$ Note that we did not yet restrict ourselves to a level of constant $\mathcal{I}_k$: this will come later.

Every function on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ that commutes with $\mathcal{I}_k$, reduces to a function on $P_{h_k, h_{\tilde{k}}}$ since it is constant on orbits. In particular,

$$\mathcal{I}_k = \pi_k - \rho_k \text{ and } \mathcal{K}_k := \frac{1}{32n}(4\omega_k \omega_{\tilde{k}} \sigma_k - \omega_k^2 \pi_k^2 - \omega_{\tilde{k}}^2 \rho_k^2)$$

The reduction map is the map

$$\mathcal{F}^{(3)} : (b_k, c_k, d_k, b_{\tilde{k}}, c_{\tilde{k}}, d_{\tilde{k}}) \mapsto (\pi_k, \rho_k, \sigma_k, \tau_k)$$

which goes from $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ to $P_{h_k, h_{\tilde{k}}}$. The reduction map is a submersion everywhere, except of course at the relative equilibria. Unfortunately it is not possible yet to make a drawing of $P_{h_k, h_{\tilde{k}}}$ since it can not be embedded in $\mathbb{R}^3$. But there is an elegant way to overcome this problem.

One sees that both $\mathcal{I}_k$ and $\mathcal{K}_k$ are independent of τ_k, that is these Hamiltonians are invariant under the $\mathbb{Z}_2$-action generated by the time reversal symmetry $\tau_k \mapsto -\tau_k$. The orbits of the $\mathbb{Z}_2$-action consist of one point if $\tau_k = 0$ and otherwise of two points. The $\mathbb{Z}_2$-action is reduced by simply forgetting about τ_k: the reduction map is $(\pi_k, \rho_k, \sigma_k, \tau_k) \mapsto (\pi_k, \rho_k, \sigma_k)$. The reduced space is the set

$$P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2 = \{(\pi_k, \rho_k, \sigma_k) \in \mathbb{R}^3 | \sigma_k^2 \leq (h_k^2 - \pi_k^2)(h_{\tilde{k}}^2 - \rho_k^2),\ |\pi_k| \leq h_k,\ |\rho_k| \leq h_{\tilde{k}}\}$$

In Figure 3 we draw $P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2$ for $h_k, h_{\tilde{k}} > 0$.

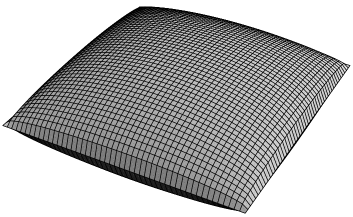

Figure 3: The solid pillow or reduced space $P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2$.

$P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2 = S^2_{h_k} \times S^2_{h_{\tilde{k}}}/_{S^1 \times \mathbb{Z}_2}$ has the shape of a solid pillow. The surface of the pillow is everywhere smooth, except at the four corner points, which are cone-like singularities that represent the relative equilibria $(\pm h_k, 0, 0, \pm h_{\tilde{k}}, 0, 0)$.

The level sets of $\mathcal{I}_k = \pi_k - \rho_k$ are two dimensional planes. The intersection of such a plane with the pillow is a topological disk, a point or empty. Near the singularities $(\pi_k, \rho_k, \sigma_k) = \pm(h_k, -h_{\tilde{k}}, 0)$ the disks are very small, indicating that $\mathcal{I}_k$ is definite at these points as a function on the pillow and hence that the relative equilibria $\pm(h_k, 0, 0, -h_{\tilde{k}}, 0, 0)$ are stable, see Figure 4. But near the other two corners of the pillow, the singularities $\pm(h_k, h_{\tilde{k}}, 0)$, the level set of $\mathcal{I}_k$ intersects the pillow in a very large set, see Figure 5, meaning that $\mathcal{I}_k$ is not definite.

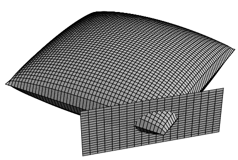

Figure 4: $\mathcal{I}_k$ near $h_k + h_{\tilde{k}}$.

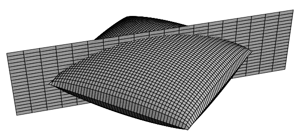

Figure 5: $\mathcal{I}_k$ near $h_k - h_{\tilde{k}}$.

Let us consider the level set of $\mathcal{I}_k$ that passes exactly through the singularity $(h_k, h_{\tilde{k}}, 0)$. It is the plane $\mathcal{I}_k = \pi_k - \rho_k = h_k - h_{\tilde{k}}$. The intersection of this plane with the pillow is the topological disk

$$\{(\pi_k, \rho_k, \sigma_k) \in \mathbb{R}^3 | \sigma_k^2 \leq (h_k^2 - \pi_k^2)(h_{\tilde{k}}^2 - (\pi_k + h_{\tilde{k}} - h_k)^2) \ , \rho_k = \pi_k + h_{\tilde{k}} - h_k\}$$

If $h_k = h_{\tilde{k}}$, then this disk has two singular points. It has one singular point if $h_k \neq h_{\tilde{k}}$. The intersection of a level set of $\mathcal{K}_k$ with this plane is a parabola. The parabola that contains the singularity $(h_k, h_{\tilde{k}}, 0)$ is given by the formulas

$$\sigma_k = \alpha(\pi_k) := \frac{1}{4\omega_k \omega_{\tilde{k}}}(\omega_k^2 \pi_k^2 + \omega_{\tilde{k}}^2(\pi_k + h_{\tilde{k}} - h_k)^2 - \omega_k^2 h_k^2 - \omega_{\tilde{k}}^2 h_{\tilde{k}}^2) \ , \ \rho_k = \pi_k + h_{\tilde{k}} - h_k$$

We now make a linear approximation to both this parabola and the singular disk at the singular point $(h_k, h_{\tilde{k}}, 0)$. So we calculate the derivative $\frac{d\alpha}{d\pi_k}|_{\pi_k = h_k} = \frac{1}{2\omega_k \omega_{\tilde{k}}}$ $(\omega_k^2 h_k + \omega_{\tilde{k}}^2 h_{\tilde{k}})$. On the other hand, the tangent cone that approximates the cone-like singularity of the singular disk at the singular point is given by

$$\{|\sigma_k| \leq 2\sqrt{h_k h_{\tilde{k}}}(h_k - \pi_k), \pi_k \leq h_k, \rho_k = \pi_k + h_{\tilde{k}} - h_k\}$$

So the tangent line to the parabola points into the cone exactly if $-2\sqrt{h_k h_{\tilde{k}}} < \frac{1}{2\omega_k \omega_{\tilde{k}}}(\omega_k^2 h_k + \omega_{\tilde{k}}^2 h_{\tilde{k}}) < 2\sqrt{h_k h_{\tilde{k}}}$, that is if $r < 0$. In this case, the critical point $(\pi_k, \rho_k, \sigma_k) = (h_k, h_{\tilde{k}}, 0)$ is clearly unstable, which agrees with our previous analysis. The tangent to the parabola does not point into the cone if $r > 0$. Figures 6 and 7 represent the two possibilities:

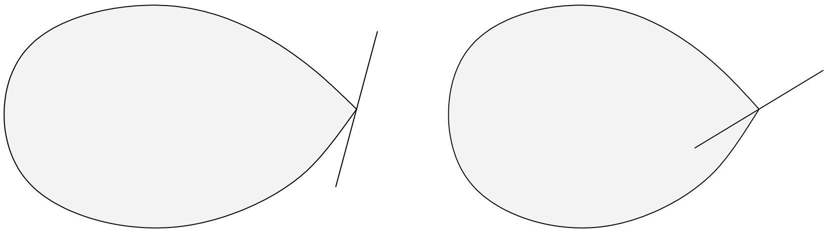

Figure 6: $r > 0$. **Figure 7:** $r < 0$.

This is a geometrical explanation for the motion of the eigenvalues. In the case that $r > 0$, we now see that $\mathcal{K}_k$, restricted to $(P_{h_k, h_{\tilde{k}}}/\mathbb{Z}_2) \cap \mathcal{I}_k^{-1}(h_k - h_{\tilde{k}})$, is extremal at $(h_k, h_{\tilde{k}}, 0)$. In other words, $(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ is a stable relative equilibrium inside the singular fiber $(S^2_{h_k} \times S^2_{h_{\tilde{k}}}) \cap \mathcal{I}_k^{-1}(h_k - h_{\tilde{k}})$. A theorem of Montaldi [**45**] then states that $(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ is stable in $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$.

We can study the Hamiltonian Hopf bifurcation in more detail by incorporating the nonlinear terms of the Hamiltonian into our analysis. So we must compute the second order approximation of the parabola $\alpha(\pi_k)$ and the cone $(P_{h_k, h_{\tilde{k}}}/\mathbb{Z}_2) \cap \mathcal{I}_k^{-1}(h_k - h_{\tilde{k}})$ at the singular point and at the critical value of the parameter $r = 0$. If the parabola is more curved than the cone, the bifurcation is completely different from the one where the cone is more curved than the parabola. The bifurcation is degenerate when the cone and the parabola are equally curved, that is when both second order derivatives are equal. We do not treat that case. After a short calculation in which we compare the curvatures of the cone and the parabola at the singularity, one finds that the character of the bifurcation depends on the parameter

$$s := 4\omega_k^2\omega_{\tilde{k}}^2 h_k^2 + 4\omega_k^2\omega_{\tilde{k}}^2 h_{\tilde{k}}^2 + (6\omega_k^2\omega_{\tilde{k}}^2 - \omega_k^4 - \omega_{\tilde{k}}^4)h_k h_{\tilde{k}}$$

It is not very difficult to arrive at the following conclusions:

1. If on one of the half lines defined by $r = 0$ one has that $s > 0$, then the Hamiltonian Hopf bifurcation on this half line is such that a stable relative equilibrium (=periodic solution) emerges from the critical point as the critical point becomes unstable. This relative equilibrium is indicated as a dot in Figure 8.
2. If on one of the half lines defined by $r = 0$ one has that $s < 0$, then the Hamiltonian Hopf bifurcation on this half line is such that an unstable relative equilibrium (=periodic orbit) is annihilated by the critical point as the critical point becomes unstable. The relative equilibrium is indicated with a dot in Figure 9.

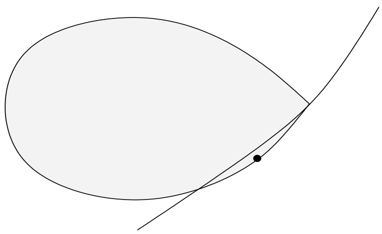

Figure 8: $-1 \ll r < 0$ and $s > 0$.

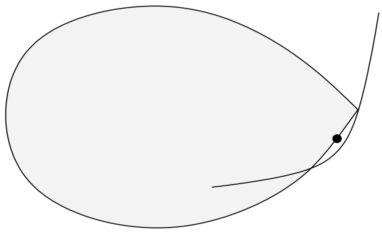

Figure 9: $0 < r \ll 1$ and $s < 0$.

We have considered an entirely geometric way to study the Hamiltonian Hopf bifurcation and the stability change of the relative equilibrium $(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$. The equilibrium $(-h_k, 0, 0, -h_{\tilde{k}}, 0, 0)$ can of course be handled in the same way.

3.7. Pinched tori and monodromy

We have studied how the level sets of $\mathcal{K}_k$ foliate the singular reduced phase space $(P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2) \cap \mathcal{I}_k^{-1}(h_k - h_{\tilde{k}})$ locally near the singularities and thus we could analyse the details of the Hamiltonian Hopf bifurcation at these singular points. In this section we will give some remarks on the *global* geometry of both the reduced phase space and the phase space of the original normal form.

We shall see that in the reduced system on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ there are homoclinic and heteroclinic connections between the relative equilibria $\pm(h_k, 0, 0, h_{\tilde{k}}, 0, 0)$ if $r < 0$. These connections are pinched tori. In the system on $T^*\mathbb{R}^{n-1}$ the pinched tori are reconstructed as whiskered tori with high dimensional coinciding stable and unstable manifolds. The presence of pinched tori results in nontrivial monodromy: the regular tori (Liouville tori) do not form a trivial torus bundle.

We reach these conclusions by simply drawing a picture of $(P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2)\cap\mathcal{I}_k^{-1}(h_k-h_{\tilde{k}})$ and its foliation into the level sets of $\mathcal{K}_k$. Recall that $(P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2)\cap\mathcal{I}_k^{-1}(h_k-h_{\tilde{k}})$ is a topological disk that contains one singular point if $h_k \neq h_{\tilde{k}}$ and two singular points if $h_k = h_{\tilde{k}}$. Each point inside the disk represents two three-dimensional tori in $\mathcal{A}_k$. The regular points on the boundary of the disk each represent one three dimensional torus. The singular points, which also lie on the boundary of the disk, represent a 'singular' two-dimensional torus. This singular torus has the interpretation of a superposition of travelling waves in the FPU lattice.

Let us first consider the case that $h_k = h_{\tilde{k}}$. In that case the reduced space is bounded by parabolas

$$(P_{h_k,h_{\tilde{k}}}/\mathbb{Z}_2)\cap\mathcal{I}_k^{-1}(0) = \{(\pi_k,\rho_k,\sigma_k)\in\mathbb{R}^3|\ |\sigma_k|\leq h_k^2-\pi_k^2\ ,\ \rho_k=\pi_k\}$$

It has two singular points which lie on the same level set of $\mathcal{K}_k$. This level set is also a parabola. Furthermore, note that in this situation $r = (\omega_k^4+\omega_{\tilde{k}}^4-14\omega_k^2\omega_{\tilde{k}}^2)h_k^2$, which by simple goniometric formulas is equal to $r = 16(1-\omega_k^2\omega_{\tilde{k}}^2)h_k^2$. Hence r is negative if and only if $\omega_k\omega_{\tilde{k}} > 1$ if and only if $n/12 < k < n/4$. But then the reduced space simply looks like in Figure 10:

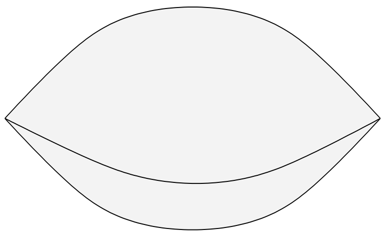

Figure 10: The heteroclinic connection in the reduced context.

We observe that there is a heteroclinic connection between the two singular points. In the reconstructed system on $S^2_{h_k}\times S^2_{h_{\tilde{k}}}$ this corresponds to a doubly pinched torus: two focus-focus singular points of which the stable and unstable manifolds coincide. In the original phase space $\mathcal{A}_k \cong T^*\mathbb{R}^4 \subset T^*\mathbb{R}^{n-1}$, this doubly pinched torus is again reconstructed as a heteroclinic connection between two-dimensional tori. They are connected by their 'whiskers' which have dimension four and are both diffeomorphic to $\mathbb{R}\times T^3$.

The heteroclinic connection has the following interpretation. For large negative values of time, the solutions on the heteroclinic connection look like a superposition of travelling waves in one direction. As time runs, these waves stop travelling and change direction. For large positive time values, the waves travel in the opposite direction.

If one starts close to the heteroclinic connection, that is with a motion that is nearly the superposition of two travelling waves with equal energy and in equal direction but not exactly on the heteroclinic connection, then after a certain time both travelling waves will come to a halt and turn around until the motion looks very much like the superposition of two travelling waves the directions and energies of which are again almost equal, although the direction is opposite to the direction in the beginning. This 'relaxation oscillation' continues and the superposed waves keep changing direction.

In the case that $\omega_k \omega_{\tilde{k}} < 1$, i.e. for $1 \leq k < n/12$, we have that $r > 0$ so the singular points are stable and there are no pinched tori. The case $k = n/12$ is degenerate: r is exactly zero and the parabola coincides with the boundary of the reduced space. We omit the analysis of this last case.

Let us now briefly also consider the situation where $h_k \neq h_{\tilde{k}}$ and $r < 0$. The singular level set then generically looks as in Figure 11:

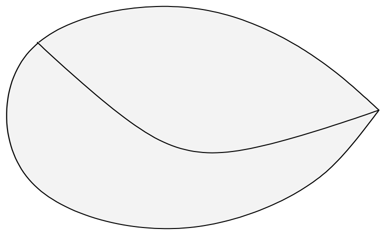

Figure 11: One of the homoclinic connections in the reduced context.

We see that there is a homoclinic connection that connects the singular point to itself. In the reconstructed system on $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ this corresponds to a singly pinched torus: the stable and unstable manifold of the focus-focus singular point coincide. In $\mathcal{A}_k \subset T^*\mathbb{R}^{n-1}$ the pinched torus is a homoclinic connection of a two-dimensional torus to itself. The two-dimensional torus again represents the superposition of travelling waves in the same direction with wave number k and $\tilde{k}$, which now do not have equal energy.

This completely describes the interaction between travelling waves with wave number k and travelling waves with wave number $n/2 - k$. The travelling waves do not interchange any energy. Still, their influence on one another is such that travelling waves can drastically change their momenta and thus their directions.

3.7.1. Monodromy. We observed that the foliation of the normal form has pinched tori. As was shown in [**43**] and [**66**], the presence of a pinched torus implies that the regular Liouville tori in $S^2_{h_k} \times S^2_{h_{\tilde{k}}}$ do not constitute a trivial torus bundle. Instead, they have monodromy and the monodromy map is known. When we reconstruct, we see that the regular tori in $T^*\mathbb{R}^{n-1}$ can not form a trivial bundle either. Nontrivial monodromy is an important obstruction to the existence of global action-angle variables as was shown in [**16**].

Recall that a pinched torus is present in the normal form if $n \geq 6$ is even. We conclude that if $n \geq 6$ is even, then the integrable normal form (3.5) does not admit global action-angle variables. This is remarkable as for every odd n it does.

We have now described how the level sets of the integrals of the Birkhoff normal form (3.5) globally foliate the phase space. In the next section we shall investigate what happens in the original FPU lattice with Hamiltonian (3.2).

3.8. Numerical comparison for 16 and 32 particles

We have analytically proven the existence of whiskered tori with coinciding stable and unstable manifolds in the Birkhoff normal form of the periodic FPU lattice. These objects have the interpretation of direction reversing travelling waves. It is natural to ask whether these homo- and heteroclinic connections can also be found in the original FPU lattice and the answer to this question is most likely no: the original FPU system is a nonintegrable perturbation of its normal form and hence the stable and unstable manifolds of the original system will generically have no intersection at all or transversal intersections. In the latter case the angle of intersection will be quite small, so this may lead to small-scale chaos. On the other hand, it was proven in [**65**] that near a pinched torus the Kolmogorov condition holds. The Kolmogorov condition is the nondegeneracy condition that has to be fulfilled for application of the KAM theorem. Hence one expects that many of the Liouville tori in the normal form lying close to the homo- or heteroclinic connection will survive as KAM tori in the original system. And therefore we expect to see many solutions of the original system which exhibit the relaxation oscillation between travelling waves in various directions that was described in the previous section. I tried to detect this relaxation oscillation in the original system by doing some basic numerical integrations of the solutions of the FPU system. All the numerical results in this section are obtained from the original Hamiltonian (3.2) and they are compared with the analytical predictions made from the normal form.

Let us first study the periodic FPU lattice with $n = 16$ particles, a number chosen by Fermi, Pasta and Ulam themselves. We shall investigate low energy solutions that start out as a superposition of two travelling waves with wave numbers $k = 3$ and $\tilde{k} = \frac{16}{2} - 3 = 5$. Note that $\frac{n}{12} = \frac{4}{3} < k = 3 < \frac{n}{4} = 4$, so if we give both waves equal energy and equal direction, then we start very close to the heteroclinic connection of the normal form and we expect the solution to reverse its direction once every while.

Let us choose the initial conditions $Q(0) = (0, 0, .237, 0, .194, 0,\ 0, 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, 0)$ and $P(0) = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, .322, 0, .264, 0, 0)$, such that $\mathcal{H}_3(0) = \mathcal{H}_5(0) = b_3(0) = b_5(0) = .0625$. The total energy is indeed quite low: $H = 0.1742$. The angular momenta $b_3(t)$ and $b_5(t)$ measure the direction of the waves. The normal form predicts that b_3 and b_5 remain equal as $\mathcal{I}_3 = b_3 - b_5$ is a constant of motion for the normal form. Moreover, we expect that both b_3 and b_5 exhibit a relaxation oscillation between the extremal values .0625 and $-.0625$ since this is exactly what happens on the Liouville tori of the normal form. The true values of b_3 and b_5 in the course of time are plotted in Figure 12. Note that both $b_3(t)$ and $b_5(t)$ have been plotted but that we see only one curve: it turns out that in the original system

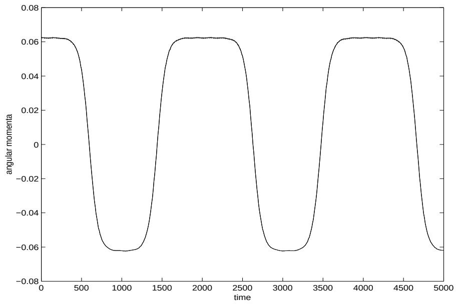

Figure 12: Superposed travelling waves with wave numbers 3 and 5 in the original FPU lattice with 16 particles interact as predicted by the normal form: the two angular momenta exhibit a relaxation oscillation between their maximal and minimal values.

the angular momenta b_3 and b_5 remain exactly equal all the time at this energy level, just as was predicted by the normal form. Furthermore, $b_3(t)$ and $b_5(t)$ vary between their maximal and minimal values at the given energy. The influence of the heteroclinic connection of the normal form is clearly visible here: the angular momenta seem to stick to their maximal and minimal value for quite some time, before moving off again.

For comparison, I also investigated how waves with wave numbers 2 and 5 interact in the system with 16 particles. Note that $\tilde{2} \neq 5$ so that in the normal form there is no interaction at all. Let us see numerically what happens in the original system. I chose $Q(0) = (0, .286, 0, 0, .194, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$ and $P(0) = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, .322, 0, 0, .264, 0)$, such that $\mathcal{H}_2(0) = \mathcal{H}_5(0) = b_2(0) = b_5(0) = .0625$. The total energy is $H = 0.1528$. The values of b_2 and b_5 are depicted on the same time-scale in Figure 13:

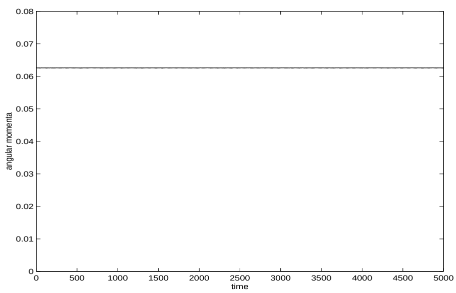

Figure 13: As predicted from the normal form, waves with wave numbers 2 and 5 do not interact in the original system.

Exactly as was analytically predicted by the normal form, b_2 and b_5 remain constant in the original system: the waves do not change their directions.

I moreover studied how the waves with wave numbers 3 and 5 interact at a higher energy level, where one does not expect that the solutions of the original system follow the predictions of the normal form. So we start with $Q(0) = (0, 0, .474, 0, .388, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$ and $P(0) = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, .645, 0, .527, 0, 0)$, such that $\mathcal{H}_2(0) = \mathcal{H}_5(0) = b_3(0) = b_5(0) = .25$ and the total energy is quite high: $H = 0.7048$. The angular momenta $b_3(t)$ and $b_5(t)$ are shown in Figure 14.

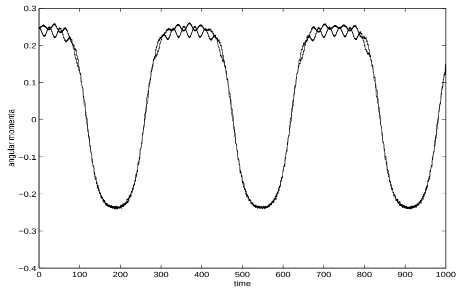

Figure 14: Also at a higher energy level, the normal form is a good approximation.

Note that the results are still reasonably well in agreement with the normal form predictions: the angular momenta b_3 and b_5 are almost equal all the time and exhibit a relaxation oscillation. Even at this high energy level the normal form still constitutes a very good approximation! This is a remarkable observation.

Finally, I numerically integrated the original FPU lattice with 32 particles for initial conditions $Q_k(0) = P_k(0) = 0$ for all k except $Q_7(0) = .222$, $Q_9(0) = .201$, $P_{23}(0) = .311$, $P_{25}(0) = .282$ such that $\mathcal{H}_7(0) = \mathcal{H}_9(0) = b_7(0) = b_9(0) = .0625$ and $H = 0.1762$. The normal form predicts that the travelling waves with wave number 7 and 9 change direction and we plot both angular momenta b_7 and b_9 in Figure 15.

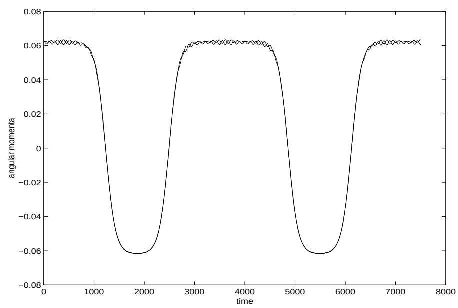

Figure 15: At low energy, the lattice with 32 particles behaves exactly as was predicted by the normal form.

The numerical results of the original system are again in agreement with the normal form. But at a higher energy the normal form is no longer a good approximation when $n = 32$. If one chooses the initial conditions $Q_k(0) = P_k(0) = 0$ for all k except $Q_7(0) = .444$, $Q_9(0) = .402$, $P_{23}(0) = .622$, $P_{25}(0) = .563$, then $\mathcal{H}_7(0) = \mathcal{H}_9(0) = b_7(0) = b_9(0) = .25$ and $H = 0.7091$. This time, the numerics show that b_7 and b_9 do not remain equal. Neither do they oscillate between the extremal values .25 and $-.25$. See the result in Figure 16.

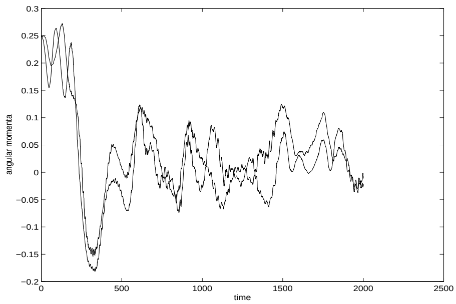

Figure 16: For $n = 32$ the solutions of the original system do not follow the normal form predictions at higher energy.

From this figure we see that the domain of validity of the normal form shrinks if n grows. This is to be expected, because when n is very large, near-resonances start spoiling the validity of the normal form. Still, it turns out that the normal form predicts the behaviour of the original FPU lattice (3.2) surprisingly well, sometimes even at energies where one would not expect this anymore.

3.9. Conclusions and discussion

We studied the Liouville integrable Birkhoff normal form of the periodic FPU β-lattice with an even number of particles. This normal form constitutes an approximation of the original FPU lattice in the low-energy domain of the phase space. The integrals of the normal form are quadratic and quartic functions of the phase space variables. Using the geometric methods of regular and singular reduction [**11**], we showed that the foliation of the phase space has singular elements, whiskered tori with coinciding stable and unstable manifolds, also called pinched tori.

It is well-known [**43**], [**66**] that pinched tori imply monodromy: the Liouville tori of the normal form do not form a trivial torus bundle over the set of regular values of the integrals. This is important information about how the Liouville tori are glued together globally, for instance on an energy level set. Among others, monodromy is an important topological obstruction to the existence of global action-angle variables. Because the Birkhoff normal form approximates the FPU system especially well in the low energy domain, we expect that the KAM tori on the low energy level sets are 'glued together' similarly. This will be proved in Chapter 4.

At the same time, our study reveals interesting dynamical information. We are able to determine how waves with different wave numbers interact in the normal form. It turns out that waves with wave number k can only interact with waves of which the wave number is $n/2 - k$. And even though these waves do not exchange any energy, their interaction is far from trivial. The pinched tori that were mentioned before are homoclinic and heteroclinic connections between solutions which are a superposition of travelling waves with these wave numbers. Thus it can happen that these superposed travelling waves change their direction.

The homoclinic and heteroclinic connections which exist in the normal form, are most probably not present in the original FPU system: under perturbations the stable and unstable manifolds will generically not intersect or at least intersect transversely. The angle of intersection will be quite small then, so this may lead to small-scale chaos. But in this chapter we focused on the regular dynamics.

From [**65**] one expects for instance that many of the Liouville tori in the normal form that lie close to the homo- or heteroclinic connection will survive as KAM tori in the original system. Therefore, many solutions of the original system should exhibit a relaxation oscillation between travelling waves in various directions. We indeed find this relaxation oscillation numerically in the original FPU lattices (3.2) with 16 and 32 particles. They form a class of interesting new solutions of the periodic FPU lattice. Surprisingly, the FPU system follows the normal form predictions even at rather high energy levels, where the Birkhoff normal form is a very questionable approximation. It would be interesting to study how robust the Liouville tori near a pinched torus are under Hamiltonian perturbations.

The reader should note the enormous qualitative differences in the behaviour of lattices with an odd and an even numbers of particles. Of course, these differences will gradually disappear when $n \to \infty$, as due to near-resonances, the domain of validity of the normal form approximation will shrink for growing n. For larger n, reversing waves will then only be observable at smaller and smaller energies. On the other hand, according to our simulations the cases $n = 16$ and $n = 32$ are in this sense still not very large.

Finally, the reader should be aware of other wave reversal phenomena that have been observed in the literature. I especially refer to [**7**] which studies the *'boomeron'*, a soliton that comes back.

CHAPTER 4

A Cantor set of tori with monodromy

We write down an asymptotic expression for action coordinates in an integrable Hamiltonian system with a focus-focus equilibrium. From the singularity in the actions we deduce that the Arnol'd determinant grows infinitely large near the pinched torus. Moreover, we prove that it is possible to globally parameterise the Liouville tori by their frequencies. If one perturbs this integrable system, then the KAM tori form a Whitney smooth family: they can be smoothly interpolated by a torus bundle that is diffeomorphic to the bundle of Liouville tori of the unperturbed integrable system. As is well-known, this bundle of Liouville tori is not trivial. Our result implies that the KAM tori have monodromy. In semi-classical quantum mechanics, quantisation rules select sequences of KAM tori that correspond to quantum levels. Hence a global labelling of quantum levels by two quantum numbers is not possible. This chapter is based on reference [**58**]

4.1. Introduction

In this chapter we study singular Lagrangean foliations of focus-focus type in two degree of freedom integrable Hamiltonian systems. Such foliations consist of a nontrivial bundle of two-dimensional regular Liouville tori and one singular surface, a pinched torus, see also [**11**], [**73**] or later in this chapter. This type of foliation has been found in various two degree of freedom Hamiltonian systems, for instance in the hydrogen atom in crossed fields [**14**], the Fermi-Pasta-Ulam lattice [**55**] and various molecular systems [**60**]. The most famous example is perhaps the spherical pendulum, see [**16**]. Note that nontrivial torus bundles can also occur in non-Hamiltonian dynamical systems [**13**].

Some authors have studied what happens in a perturbation of a Hamiltonian system with such a foliation. Horozov [**29**] was the first to show that for the spherical pendulum the so-called Arnol'd determinant is nonzero at every regular value of the energy-momentum map. This nondegeneracy condition is traditionally called the Kolmogorov condition and it makes the KAM theorem work. In [**65**] it was proved by Tien Zung that the Kolmogorov condition is satisfied in a full neighbourhood of any pinched torus of focus-focus type. In this chapter the results of [**65**] will be made more specific. Based on a computation of Vũ Ngọc [**73**], we shall explicitly describe the limiting behaviour of the frequency map and the Arnol'd determinant near a pinched torus. The latter grows infinitely large. The Kolmogorov condition requires that the Liouville tori of an integrable system can locally be parameterised by their frequencies. We will see that in the vicinity of a pinched torus, this can even be done globally, in a sense that we will describe later.

What happens to the singular foliation if one perturbs the integrable system? The pinched torus, being a high dimensional homoclinic connection, most likely breaks up into a homoclinic tangle with complicated geometry. A Cantor set of Liouville tori survives as KAM tori.

It is well-known, see [**11**], [**16**], [**43**], [**66**], that the Liouville tori near a pinched torus do not form a trivial torus bundle, but have monodromy. In [**14**] the question was posed whether this global geometry remains present in the KAM tori of the perturbed system. In this chapter we will show that this is the case. It turns out that the KAM tori in the perturbed system form a Whitney smooth family that is diffeomorphic to the bundle of Liouville tori in the integrable system. This means that the KAM tori have monodromy. The geometry of KAM tori in nearly integrable Hamiltonian systems is also discussed by Broer et al. in [**4**]. Their approach is completely different from the one in this chapter: the authors actually use a partition of unity for gluing together local Whitney smooth families of KAM tori.

The fact that KAM tori can have monodromy is particularly interesting for semi-classical quantum mechanics. Quantum monodromy in integrable systems has been analysed using the quantum energy-momentum map, see [**12**], [**14**], [**60**] and [**72**]. Semi-classical quantisation theory selects regular sequences of Liouville tori in the classical integrable system which correspond to quantum levels in the quantum system. In the semi-classical limit, with Planck's constant going to zero, these quantum levels form locally a regular lattice of which the points can be labelled by quantised actions. But if monodromy is present in the Liouville tori, then any global labelling of the quantum levels by two quantum numbers is impossible, since there is a defect in the lattice which results in a shift in the global lattice structure, see [**12**] and [**72**].

The only problem is that most two degree of freedom Hamiltonian systems are not integrable, even though it might be possible to approximate them by an integrable system. Our result explains that monodromy is also present in nonintegrable systems that are perturbations of an integrable system with a focus-focus singularity. Semi-classical quantisation theory states that the quantum levels are in this case described by sequences of KAM tori, see [**41**]. Monodromy in these KAM tori will again constitute an obvious obstruction to the global labelling of the quantum levels by two quantum numbers. The problems with the global labelling of quantum levels and the phenomenon of redistribution of quantum states have been studied extensively and have also been found experimentally, see for instance [**14**], [**20**] and [**60**].

In [**55**] and Chapter 3 of this thesis it was shown that focus-focus equilibria, pinched tori and monodromy can also occur in the Birkhoff normal form of the famous FPU lattice. Remarkably, their influence could also be observed in numerical integrations of the original lattice equations, even at rather high energy and in lattices of high dimension, where one would usually question the validity of a normal form approximation. One may therefore conjecture that the measure of the surviving KAM tori is exceptionally large in perturbations of integrable Hamiltonian systems with focus-focus singularities. A detailed study is necessary to prove such a conjecture and this chapter can be considered as a starting point for such an analysis.

4.2. Mathematical background

Let us recall the Hamiltonian monodromy theorem. Let M be a four dimensional real analytic symplectic manifold with symplectic form σ. Suppose that we have two real analytic Poisson commuting Hamiltonians $H_1, H_2 : M \to \mathbb{R}$, so $\{H_1, H_2\} = 0$. The map $H = (H_1, H_2) : M \to \mathbb{R}^2$ is called the energy-momentum map. We want study how the level sets $H^{-1}(h)$ of the energy-momentum map foliate the symplectic manifold M. At regular points, this foliation is Lagrangean, because H_1 and H_2 commute. A point $m \in M$ is called a focus-focus equilibrium if $X_{H_1}(m) = X_{H_2}(m) = 0$ and there are canonical coordinates (q, p) (that is $\sigma = \sum_{i=1}^{2} dq_i \wedge dp_i$) near m such that $(q, p)(m) = 0$ and

$$H_1 = a(q_1p_2 - q_2p_1) + b(q_1p_1 + q_2p_2) + \text{ higher order terms}$$

$$H_2 = c(q_1p_2 - q_2p_1) + d(q_1p_1 + q_2p_2) + \text{ higher order terms}$$

where $ad - bc \neq 0$. Let us moreover assume that H has the following properties:

1. There is an open neighbourhood $U \subseteq \mathbb{R}^2$ of 0 such that 0 is the only critical value of H in U.
2. For every $u \in U\backslash\{0\}$, the fiber $H^{-1}(u)$ is connected and compact.
3. The singular fiber $H^{-1}(0)$ is connected and compact and m is its only singular point.

The foliation of $H^{-1}(U)$ in level sets of H is a singular Lagrangean foliation with one singular point. The Arnol'd-Liouville theorem says that the regular fibers $H^{-1}(u)$ $(u \in U\backslash\{0\})$ form a smooth bundle of two-dimensional tori. The Hamiltonian monodromy theorem states that this bundle is not trivial. In fact, using a suitable basis for the fundamental group of the torus $H^{-1}(\bar{u})$ $(\bar{u} \in U\backslash\{0\})$ and identifying this torus with the lattice $\mathbb{R}^2/\mathbb{Z}^2$, the monodromy map of the bundle is given by the matrix $\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$. The Hamiltonian monodromy theorem was proved by Matveev [**43**] and Tien Zung [**66**]. The monodromy of the bundle is an obvious obstruction to the existence of global action angle coordinates on $H^{-1}(U\backslash\{0\})$, see [**16**].

The singular fiber $H^{-1}(0)$ is a pinched torus: an immersed sphere with one point of transversal self-intersection. Its set of nonsingular points, $H^{-1}(0)\backslash\{m\}$ is diffeomorphic to a cylinder.

Let us write

$$K_1 = q_1p_2 - q_2p_1 \quad , \quad K_2 = q_1p_1 + q_2p_2 \ \text{ and } K = (K_1, K_2)$$

Near m, the following linearisation result holds and is due to Eliasson [**19**]. There exist real analytic canonical coordinates $x = (q, p) : W \to T^*\mathbb{R}^2$ in a neighbourhood W of m such that $x(m) = 0$ and $H = \lambda \circ K \circ x$ for some real analytic local diffeomorphism λ of $\mathbb{R}^2$. This means that in W, $K \circ x$ and H define the same level sets. We also say that $K \circ x$ is a momentum map for the foliation given by the energy-momentum map H. But this implies that $K \circ x$ has a unique extension to a function on $H^{-1}(W)$ that is constant on the level sets of H. By the local submersion theorem, this extension is analytic too. We conclude that $K \circ x$ can be extended to a global real analytic momentum map for the Lagrangean foliation near the pinched torus. In other words, since we will only be interested in a neighbourhood of the pinched torus, we can and will assume that $H|_W = K \circ x$.

Let $F_0 : M \to \mathbb{R}$ be an arbitrary real analytic Hamiltonian function which Poisson commutes with H_1 and H_2, that is F_0 is a function of H_1 and H_2 only. We also write F_0 for $F_0 \circ H$. Clearly, the Hamiltonian vector field X_{F_0} is integrable: its flow leaves the level sets of H invariant. The motion in the Liouville tori is simply periodic or quasi-periodic. One may wonder whether this quasi-periodic behaviour persists when we perturb the Hamiltonian function F_0. In order to apply the KAM theorem, one must show that the Liouville tori of the integrable system defined by F_0 can locally be parameterised by their frequencies. We shall show that this is possible under the assumption that m is a linearly unstable equilibrium point of X_{F_0}.

Moreover, we want to study the geometry in the KAM tori by giving a smooth torus bundle that interpolates them. Theorems providing interpolation results for KAM tori usually only work for perturbations of integrable systems admitting global action-angle coordinates. This type of theorem will be used at an intermediate stage. This chapter then provides an example of a nontrivial Whitney smooth bundle of KAM tori.

4.3. Global action-angle coordinates

Vũ Ngọc in [**73**] derives an expression for action coordinates near a pinched torus from a local analysis near the focus-focus singularity in Eliasson's canonical coordinates (q, p). We recall this result here.

Let us first define the function $\arg : \mathbb{R}^2 \backslash \{0\} \to \mathbb{R}$ by $\arg : (r\cos\phi, r\sin\phi) \mapsto \phi$. Note that arg is of course a multivalued function, meaning that as a function from $\mathbb{R}^2\backslash\{0\} \to \mathbb{R}/_{2\pi\mathbb{Z}}$ it is well-defined. Over a positively oriented circle around the origin the value of arg increases 2π. But after choosing a fixed branch, arg becomes locally a uniquely defined analytic function. We have the following

Proposition 4.1. *There exists a real analytic function $s = s(H)$ defined on an open neighbourhood $\tilde{U} \subset \mathbb{R}^2$ of $\{H = 0\}$ such that*

$$a_1(H) = H_1 \ , \ a_2(H) = \frac{1}{2\pi}\left(H_2 \ln|H| + H_1 \arg H\right) + s(H) =: \psi(H)$$

define a set of local action coordinates near every point in $\tilde{U}\backslash\{0\}$.

The proof can be found in [**73**]. Obviously, $a_1(H) = H_1$ ($= K_1$ in Eliasson's coordinates) defines a Hamiltonian vector field in Eliasson's coordinates which has a 2π-periodic flow. Therefore it is an action. The other action is obtained as the Arnol'd integral

$$a_2(H) = \frac{1}{2\pi}\int_{\gamma_h} \alpha$$

where α is a one-form such that $d\alpha = \sigma$, see [**16**]. Such a one-form exists locally near every Liouville torus since the foliation in tori is Lagrangean. γ_h is a closed curve on the Liouville torus $H^{-1}(h)$ which is chosen so that an integral curve of $X_{a_1} = X_{H_1}$ and γ_h together form a basis of the fundamental group of the torus $H^{-1}(h)$. Obviously, this integral depends analytically on H, hence the function s is analytic. In [**73**] it was shown that the Taylor expansion of $s - s(0)$ classifies the singular Lagrangean foliation in an open neighbourhood of the pinched torus, up to a symplectomorphism.

Let us examine the coordinate transformation $H \mapsto a$ in more detail. We shall for convenience write

$$\Psi : (H_1, H_2) \mapsto (a_1, a_2) = (H_1, \psi(H_1, H_2))$$

If we choose a branch of arg, then Ψ is a single valued real analytic map on the domain $\mathbb{R}^2_* := \mathbb{R}^2 \backslash \mathbb{R}_{\geq 0}(1, 0)$ intersected with the open neighbourhood $\tilde{U}$. The Jacobi determinant of Ψ is

$$\det D\Psi(H) = \frac{\partial \psi(H)}{\partial H_2} = \frac{1}{2\pi}\left(\ln|H| + 1\right) + \frac{\partial s(H)}{\partial H_2}$$

which is obviously negative and hence nonzero in a small enough open neighbourhood of $\{H = 0\}$. Let us choose a little annulus $V := \{\rho_1 < |H| < \rho_2\}$ in the intersection of this neighbourhood with $\tilde{U}$. It is easy to verify that $\Psi : V_* := V \backslash \mathbb{R}_{\geq 0}(1, 0) \to \mathbb{R}^2$ is injective, because the map $H_2 \mapsto \psi(a_1, H_2)$ has strictly negative derivative and makes a negative jump at $H_2 = 0$ if $a_1 > 0$. Therefore, Ψ is a real analytic diffeomorphism between V_* and $A := \Psi(V_*)$. Ψ 'opens' V_*, that is at different branches of arg, the bounding half line $\mathbb{R}_{\geq 0}(1, 0)$ is mapped by Ψ to different half lines, see Figure 1.

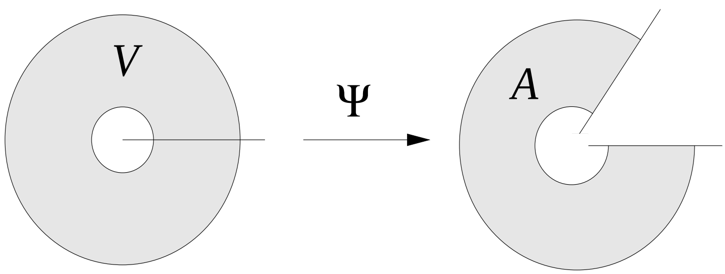

Figure 1: The map $\Psi : V_* \to A$.

Let us write $M_V := H^{-1}(V) \subset M$ for the nontrivial bundle of Liouville tori over V.

Proposition 4.2. *There exist global action-angle coordinates on the subbundle* $H^{-1}(V_*) \subset M_V$. *This means that there exist an open set* $A \subset \mathbb{R}^2$ *and a* C^∞ *diffeomorphism* $\Phi_0 : H^{-1}(V_*) \to A \times T^2$ *with the properties that* $\Phi_0^*(da \wedge d\phi) = \sigma$ *and* $p \circ \Phi_0 = \Psi \circ H$. *Here* $p : A \times T^2 \to A$ *denotes the projection on the first coordinate.*

Proof. Note that V_* is contractible to a point. Therefore the bundle $H^{-1}(V_*)$ over V_* is topologically trivial, see [**63**] pp. 53. This implies that there is a homotopy between the identity map i on $H^{-1}(V_*)$ and a map ϕ that sends $H^{-1}(V_*)$ to a single Lagrangean fiber. The difference of the pullbacks $i^*\sigma - \phi^*\sigma = \sigma - 0 = \sigma$ is hence exact on $H^{-1}(V_*)$. Finally, $\Psi : V_* \to A$ is a diffeomorphism. According to Theorem 2.2 in [**16**] these facts are sufficient for the existence of C^∞ global action-angle coordinates on $H^{-1}(V_*)$. □

4.4. Frequencies

Under the assumption that the focus-focus equilibrium point m is linearly unstable for the vector field X_{F_0}, we will show that the frequency map $\omega := \frac{\partial F_0}{\partial a} : A \to \Omega := \omega(A)$ is a real analytic diffeomorphism. Knowing that $\Psi : V_* \to A$ is a diffeomorphism, we only need to show that $\omega \circ \Psi : V_* \to \Omega$ is a diffeomorphism. We explicitly calculate $\omega \circ \Psi$ as follows. First of all, note that $\omega(a) = \frac{\partial F_0(a)}{\partial a} = \left.\frac{\partial F_0(H)}{\partial H}\right|_{H=H(a)} \circ \frac{\partial H(a)}{\partial a}$ where

$$\frac{\partial H(a)}{\partial a} = \left(\left.\frac{\partial \Psi(H)}{\partial H}\right|_{H=H(a)} \right)^{-1} = \begin{pmatrix} 1 & 0 \\ \partial\psi(H(a))/\partial H_1 & \partial\psi(H(a))/\partial H_2 \end{pmatrix}^{-1}$$

Using the fact that

$$\frac{\partial \psi(H)}{\partial H_1} = \frac{1}{2\pi} \arg H + \frac{\partial s(H)}{\partial H_1} \quad \text{and} \quad \frac{\partial \psi(H)}{\partial H_2} = \frac{1}{2\pi} (\ln|H| + 1) + \frac{\partial s(H)}{\partial H_2}$$

we arrive at the following expression for $\omega \circ \Psi : H \mapsto \omega(H)$:

$$\begin{aligned} \omega_1(H) =& \frac{\partial F_0(H)}{\partial H_1} - \frac{\partial F_0(H)}{\partial H_2} \frac{\frac{1}{2\pi}\arg H + \frac{\partial s(H)}{\partial H_1}}{\frac{1}{2\pi}(\ln|H|+1) + \frac{\partial s(H)}{\partial H_2}} \\ \omega_2(H) =& \frac{\partial F_0(H)}{\partial H_2} \frac{1}{\frac{1}{2\pi}(\ln|H|+1) + \frac{\partial s(H)}{\partial H_2}} \end{aligned} \tag{4.1}$$

Note that $\lim_{H\to 0} \omega(H) = (\partial F_0(0)/\partial H_1, 0)$. Recall that this limit is taken over $H \in \mathbb{R}^2_*$ and that we have chosen a fixed branch of arg. The following proposition describes the limiting behaviour of the derivative matrix $\frac{\partial \omega(H)}{\partial H}$ near $H = 0$.

Proposition 4.3.

$$\lim_{H\to 0} \begin{pmatrix} \ln|H| & 0 \\ 0 & \frac{\ln^2|H|}{2\pi} \end{pmatrix} \frac{\partial \omega(H)}{\partial H} \begin{pmatrix} H_2 & -H_1 \\ -H_1 & -H_2 \end{pmatrix} = \frac{\partial F_0(0)}{\partial H_2} \,\mathrm{Id} \tag{4.2}$$

This follows from a straightforward analysis based on (4.1). We are now in position to show that $\omega \circ \Psi : V_* \to \Omega$ is a diffeomorphism if the annulus V is chosen close enough to the origin $H = 0$.

Corollary 4.4. *$DX_{F_0}(m)$ has an eigenvalue off the imaginary axis if and only if $\frac{\partial F_0(0)}{\partial H_2} \neq 0$. In this case the Arnol'd determinant* $\det\left(\frac{\partial \omega(H)}{\partial H}\right)$ *goes to infinity as $|H|$ goes to zero. If the annulus V is chosen small enough, then the map $\omega \circ \Psi : V_* \to \Omega$ is a real analytic diffeomorphism. Hence, $\omega : A \to \Omega$ is a real analytic diffeomorphism.*

Proof The first statement is trivial since

$$DX_{F_0}(m) = \frac{\partial F_0(0)}{\partial H_1} DX_{H_1}(m) + \frac{\partial F_0(0)}{\partial H_2} DX_{H_2}(m)$$

and $DX_{H_1}(m)$ and $DX_{H_2}(m)$ commute and respectively have purely imaginary and purely real eigenvalues. The second statement follows by taking the the determinant of (4.2) which yields that

$$\frac{1}{2\pi}|H|^2 \ln^3 |H| \det(\frac{\partial \omega(H)}{\partial H}) \to -(\frac{\partial F_0(0)}{H_2})^2 \neq 0$$

and hence $\det(\frac{\partial \omega(H)}{\partial H}) \to \infty$ as $H \to 0$. According to Proposition 4.2 we can now choose the annulus V in such a way that for every $H \in V_*$

$$\begin{pmatrix} \ln|H| & 0 \\ 0 & \frac{\ln^2|H|}{2\pi} \end{pmatrix} \frac{\partial \omega(H)}{\partial H} \begin{pmatrix} H_2 & -H_1 \\ -H_1 & -H_2 \end{pmatrix} = \frac{\partial F_0(0)}{\partial H_2} \; (\; \mathrm{Id} + M(H)\;)$$

for some matrix $M(H)$ of which the elements each have norm less than $\frac{1}{10}$. This clearly implies that $\det(\frac{\partial \omega(H)}{\partial H}) \neq 0$ for $H \in V_*$. It is easy to show that this implies that $\omega \circ \Psi : V_* \to \Omega$ is injective. Pick $H^{(1)}$ and $H^{(2)}$ in V_*. We connect $H^{(1)}$ and $H^{(2)}$ by a curve γ consisting of a circle segment from $H^{(1)}$ to $\frac{|H^{(1)}|}{|H^{(2)}|}H^{(2)}$ and a line segment from $\frac{|H^{(1)}|}{|H^{(2)}|}H^{(2)}$ to $H^{(2)}$. A straightforward but rather long computation shows that $\omega(H^{(2)}) - \omega(H^{(1)}) = \int_\gamma \frac{\partial \omega}{\partial H} \cdot ds \neq 0$, expressing that $\omega \circ \Psi$ is injective. This proves that $\omega \circ \Psi$ and ω are real analytic diffeomorphisms. □

We conclude that if $DX_{F_0}(m)$ has an eigenvalue with nonzero real part, then it is possible to choose the annulus V close enough to the origin $H = 0$ such that both the action map $\Psi : V_* \to A$ and the frequency map $\omega : A \to \Omega$ are diffeomorphisms.

V_*, A and Ω are open, contractible, bounded sets with a piecewise smooth boundary, see Figures 1 and 2.

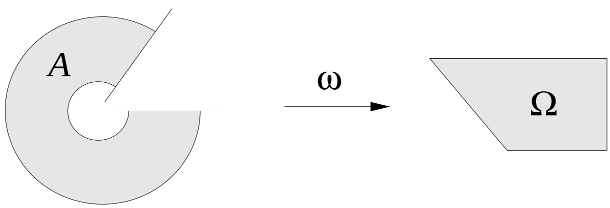

Figure 2: The map $\omega : A \to \Omega$.

4.5. Monodromy in the KAM tori

We shall argue that if one perturbs the completely integrable Hamiltonian F_0 on M a bit, the monodromy of the Liouville tori in M_V is still present in the surviving KAM tori. It turns out that the KAM tori form a Whitney smooth torus bundle. They can be interpolated by a smooth torus bundle that is diffeomorphic to M_V. This type of interpolation theorem is well-known for perturbations of an integrable Hamiltonian system for which

1. global action-angle coordinates exist.
2. the frequency map is a global diffeomorphism.

See [**5**] or [**52**]. Obviously, M_V does not meet these requirements, since it is not a trivial bundle. According to the previous paragraphs, the bundle $H^{-1}(V_*) \subset M_V$ does satisfy 1. and 2. We now apply the standard KAM theorem on this subbundle and see that this suffices to get an interpolation result for all the KAM tori in M_V.

A well-known KAM interpolation theorem is for instance given in [**52**] by Pöschel. The setting of Pöschel's theorem is the following:

Let $A \subset \mathbb{R}^2$ be an open subset. Consider the symplectic manifold $A \times T^2$ with symplectic form $d\phi \wedge da$ and real analytic Hamiltonian function $\tilde{F}_0(a)$. Assume that $\omega = \frac{\partial \tilde{F}_0}{\partial a} : A \to \mathbb{R}^2$ is a global diffeomorphism on its image, which is the set of frequencies Ω. Obviously, under the diffeomorphism $\Phi_1 = \omega^{-1} \times \mathrm{Id} : \Omega \times T^2 \to A \times T^2$, the Hamiltonian vector field $X_{\tilde{F}_0} = \frac{\partial \tilde{F}_0}{\partial a_1}\frac{\partial}{\partial \phi_1} + \frac{\partial \tilde{F}_0}{\partial a_2}\frac{\partial}{\partial \phi_2}$ on $A \times T^2$ pulls back to the vector field

$$\Phi_1^* X_{\tilde{F}_0} = \omega_1 \frac{\partial}{\partial \phi_1} + \omega_2 \frac{\partial}{\partial \phi_2}$$

on $\Omega \times T^2$. Pöschel's theorem says the following for perturbations of X_{F_0}:

Theorem 4.5 (KAM)**.** *Let $\tau > 1$ be a fixed given number. Then there exists a positive constant δ such that for every small enough γ and every C^∞ Hamiltonian function $\tilde{F}(a, \phi)$ with*

$$||\tilde{F} - \tilde{F}_0|| < \delta\gamma^2$$

the following holds: there exists a C^∞ near identity diffeomorphism $\Phi_2 : \Omega \times T^2 \to \Omega \times T^2$ which on $\Omega_\gamma \times T^2$ conjugates the vector field $\Phi_1^* X_{\tilde{F}}$ to the vector field $\Phi_1^* X_{\tilde{F}_0}$, that is

$$\Phi_2^* \Phi_1^* X_{\tilde{F}} \big|_{\Omega_\gamma \times T^2} = (\Phi_1 \circ \Phi_2)^* X_{\tilde{F}} \big|_{\Omega_\gamma \times T^2} = \Phi_1^* X_{\tilde{F}_0}$$

Here Ω_γ is defined as the set of frequencies $\omega \in \Omega$ that have distance at least γ to the boundary of Ω and satisfy the Diophantine inequalities

$$|(\omega, k)| \geq \gamma |k|^{-\tau} \quad \forall\ k \in \mathbb{Z}^2$$

By construction, $\Phi_2(\omega, \phi) = (\omega, \phi)$ if ω has distance less than $\gamma/2$ to $\partial\Omega$.

Remark 4.6. *The norm $|| \cdot ||$ is a combination of a C^∞ supremum norm and a C^∞ Hölder norm for smooth functions on $A \times T^2$, see* [**52**] *pp. 662-663 and 690.*

Remark 4.7. *Pöschel also assumes that $\tilde{F}_0$ has a complex analytic extension to a neighbourhood of A in $\mathbb{C}^2$. We avoid this by switching to a smaller, compact A*

if necessary, which in our case can be arranged by choosing the annulus V appropriately.

Remark 4.8. *Pöschel uses the freedom in the Whitney extension theorem to construct Φ_2 such that $\Phi_2(\omega, \phi) = (\omega, \phi)$ if ω has distance less than $\gamma/2$ to $\partial\Omega$, see* [**52**] *pp. 681-682. This has the effect that Φ_2 becomes a C^∞ diffeomorphism from $\Omega \times T^2$ to $\Omega \times T^2$. We will see that this has even more advantages.*

Remark 4.9. *The domain Ω in Section 4.4 of this chapter is bounded and has a piecewise smooth boundary. Therefore one quickly derives from the definition of Ω_γ that the Lebesgue measure of $\Omega \backslash \Omega_\gamma$ is of order γ. This means that there are positive constants L and γ_0 such that the Lebesgue measure of $\Omega \backslash \Omega_\gamma$ is smaller then $L\gamma$ if $\gamma < \gamma_0$.*

Theorem 4.5 says that the tori with frequencies ω in the Cantor set $\Omega_\gamma \subset \Omega$ survive a small enough Hamiltonian perturbation. The surviving KAM tori form a Whitney smooth family of tori, that is they can be interpolated by a smooth bundle of tori that lie close to the original tori.

We can now simply apply Pöschel's theorem for perturbations of a Hamiltonian system on $A \times T^2$, where $A = \Psi(V_*)$. Then it is only a small step to our main theorem:

Theorem 4.10. *Let V be an annulus around $\{H = 0\}$ such that Ψ and ω are real analytic diffeomorphisms on V_* and $A = \Psi(V_*)$. According to the results of Sections 4.3 and 4.4, such a V exists if $DX_{F_0}(m)$ has an eigenvalue that is not purely imaginary. Then there exists a positive constant δ such that for every small enough γ and every C^∞ Hamiltonian function $F : M_V \to \mathbb{R}$ with*

$$||(F - F_0) \circ \Phi_0^{-1}|| < \delta\gamma^2$$

the following holds: there exists a C^∞ near identity diffeomorphism $\Phi : M_V \to M_V$ and a Cantor set $V_\gamma \subset V$ such that

$$\Phi^* X_F \big|_{H^{-1}(V_\gamma)} = X_{F_0}$$

The Lebesgue measure of $V \backslash V_\gamma$ is of order γ.

Proof. For the given Hamiltonians $F_0, F : M_V \to \mathbb{R}$, define $\tilde{F}_0 = F_0 \circ \Phi_0^{-1} = F_0 \circ \Psi^{-1}$ and $\tilde{F} = F \circ \Phi_0^{-1}$ on $A \times T^2$. Recall that $\Psi : V_* \to A$ is the transformation to actions whereas $\Phi_0 : H^{-1}(V_*) \to A \times T^2$ is the transformation to actions and angles. Note that $\tilde{F}_0$ is analytic if F_0 is analytic, since Ψ is analytic. According to Pöschel's theorem, there is a positive constant δ such that if $||\tilde{F} - \tilde{F}_0|| < \delta\gamma^2$, then there exists a near identity transformation $\Phi_2 : \Omega \times T^2 \to \Omega \times T^2$ such that

$$\Phi_2^* \Phi_1^* X_{\tilde{F}} \big|_{\Omega_\gamma \times T^2} = \Phi_1^* X_{\tilde{F}_0}$$

But because Φ_0 is symplectic, $X_{F_0} = \Phi_0^* X_{\tilde{F}_0}$ and $X_F = \Phi_0^* X_{\tilde{F}}$. It follows that

$$\Phi_2^* \Phi_1^* (\Phi_0^{-1})^* X_F \big|_{\Omega_\gamma \times T^2} = \Phi_1^* (\Phi_0^{-1})^* X_{F_0}$$

and hence

$$(\Phi_0^{-1} \circ \Phi_1 \circ \Phi_2 \circ \Phi_1^{-1} \circ \Phi_0)^* X_F \big|_{H^{-1}(V_\gamma)} = \Phi_0^* (\Phi_1^{-1})^* \Phi_2^* \Phi_1^* (\Phi_0^{-1})^* X_F \big|_{H^{-1}(V_\gamma)} = X_{F_0}$$

where V_γ is defined as $V_\gamma := (\omega \circ \Psi)^{-1}(\Omega_\gamma)$. Thus, $H^{-1}(V_\gamma) = (\Phi_1^{-1} \circ \Phi_0)^{-1}(\Omega_\gamma \times T^2)$. The Lebesgue measure of $\Omega \backslash \Omega_\gamma$ is of order γ. Because the Jacobi determinant of $(\omega \circ \Psi)^{-1}$ is bounded on Ω, the Lebesgue measure of $V \backslash V_\gamma$ is of order γ too.

Let us now define the map $\Phi : M_V \to M_V$ as follows:

$$\Phi(m) = \begin{cases} (\Phi_0^{-1} \circ \Phi_1 \circ \Phi_2 \circ \Phi_1^{-1} \circ \Phi_0)(m) \ , \text{ if } m \in H^{-1}(V_*) \\ m \ , \text{ if } m \in H^{-1}(\mathbb{R}_{\geq 0}(1,0)) \end{cases}$$

Because $\Phi_2(\omega, \phi) = (\omega, \phi)$ in an open neighbourhood of $\partial\Omega$, Φ has the property that in a full neighbourhood of the set $H^{-1}(V \cap \mathbb{R}_{\geq 0}(1,0))$ it is the identity map. Furthermore, $\Phi|_{H^{-1}(V_*)} : H^{-1}(V_*) \to H^{-1}(V_*)$ is a diffeomorphism. Hence, Φ is a diffeomorphism. As we already argued, it has the required conjugation property on $H^{-1}(V_\gamma)$. $\square$

The diffeomorphism $\Phi : M_V \to M_V$ in Theorem 4.10 maps the Liouville torus $H^{-1}(v)$, $(v \in V_\gamma)$ of the unperturbed integrable system defined by F_0 to a KAM torus of the perturbed system defined by F. This means that the KAM tori can be interpolated by a family of tori that is diffeomorphic to M_V: the KAM-tori have monodromy.

4.6. Discussion

The results obtained in this chapter generalise [**65**] in which it is proved that the Kolmogorov condition is satisfied near a focus-focus singular value. We obtain explicit quantitative estimates on the behaviour of the Arnol'd determinant near a pinched torus and show that it grows to infinity. But there is more. By cutting away a measure zero set of Liouville tori, we have obtained a trivial torus bundle on which global action-angle coordinates exist. The tori in this bundle can globally be parameterised by their frequencies. This enables us to use the standard KAM theorem, which says that in a perturbed system certain tori survive and that these tori are part of a smooth structure. By a simple gluing argument, we show that the KAM tori near a pinched torus form a nontrivial Whitney smooth bundle that is diffeomorphic to the original bundle of Liouville tori. This justifies the statement that the KAM tori in a perturbed singular foliation of focus-focus type have monodromy.

CHAPTER 5

A forced spring-pendulum

In this chapter we study a parametrically forced spring-pendulum that was introduced by Tondl and Verhulst [**67**]. This forced spring-pendulum is an example of a time-periodic Hamiltonian system, in which the forcing models the influence of a complicated external deterministic system. We develop a Birkhoff normal form theory for such systems, that can be applied near periodic orbits. First of all, we show that the Birkhoff normalisation can be performed at the level of Hamiltonian functions. This nicely simplifies computations. Moreover, as usual the normal form allows a dimension-reduction. We focus our attention on two and a half degree of freedom systems: two degree of freedom time-periodic Hamiltonian systems such as our forced spring-pendulum. We distinguish between full and nongenuine resonances. The nongenuinely resonant normal form is integrable. In an example of a fully resonant normal form, we detect interesting single- and multi-pulse solutions.

5.1. Introduction

Springs, pendula and spring-pendula have always been popular toys for mathematicians and physicists. The well-known mathematical pendulum is a Hamiltonian system with one degree of freedom. The integrable spherical pendulum [**11**], [**16**] has two degrees of freedom. So does the spring-pendulum, see [**68**], which is nonintegrable but allows an integrable approximation. There has also been an increasing interest lately in the three degree of freedom swing-spring, see [**18**], which has a circle symmetry and therefore a second integral.

But in this chapter we shall be interested in a less classical example that was introduced by Tondl and Verhulst [**67**]: a two degree of freedom spring-pendulum with parametric excitation as in Figure 1. The excitation can account for various external forces and influences. To be more precise, we study the forced spring-pendulum as a first step to understanding a system of coupled spring-pendula, such as a chain or lattice of spring-pendula. The forcing is thus a very simple model for the influence of the other spring-pendula on the spring-pendulum under consideration.

Our forced spring-pendulum can be described as follows. We denote the position of the pendulum mass by its Cartesian coordinates $q = (q_1, q_2) \in \mathbb{R}^2$, the origin of $\mathbb{R}^2$ being located at the suspension point of the spring. If we assume that the spring-pendulum is excited by a force with period 2π, then the phase space of this mechanical system is $T^*\mathbb{R}^2 \times S^1 = T^*\mathbb{R}^2 \times \mathbb{R}/2\pi\mathbb{Z}$ with coordinates $x = (q_1, q_2, p_1, p_2, t)$. The Hamiltonian function $H : T^*\mathbb{R}^2 \times S^1 \to \mathbb{R}$ determines the nonautonomous

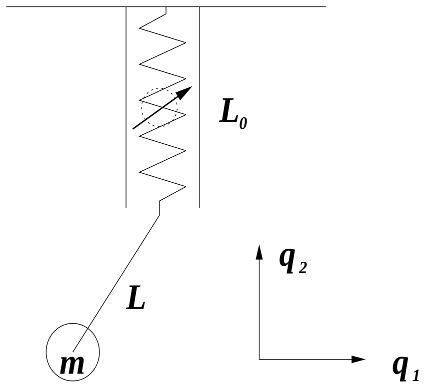

Figure 1: The parametrically forced spring-pendulum.

time-periodic Hamiltonian vector field on $T^*\mathbb{R}^2 \times S^1$ by

$$X_H + \frac{\partial}{\partial t} := \sum_{j=1}^{n} \frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j} + \frac{\partial}{\partial t}$$

In other words, we have the system of ordinary differential equations

$$\dot{q}_j = \frac{\partial H}{\partial p_j}\ ,\ \dot{p}_j = -\frac{\partial H}{\partial q_j}\ ,\ \dot{t} = 1$$

The Hamiltonian function H of our forced spring-pendulum is the sum of a kinetic and a potential energy. The potential energy has a gravitational component and a component depending on the elongation of the spring.

Denoting the rest-length of the spring by L_0, and the length of the pendulum by L, the elongation of the spring is verified to be $q_2 + L_0 + \sqrt{L^2 - q_1^2}$. The Hamiltonian function will therefore read

$$H = \frac{1}{2}(p_1^2 + p_2^2) + gq_2 + \frac{k}{2}(1 + \varepsilon\cos(t))\left(q_2 + L_0 + \sqrt{L^2 - q_1^2}\right)^2 \qquad (5.1)$$

Note that we assume that the spring mass is $m = 1$, which can be arranged by rescaling the phase space variables if necessary. The gravitational constant is denoted by $g > 0$ and the spring constant by $k > 0$. ε is a small parameter, $|\varepsilon| \ll 1$.

The stress-strain relation of the spring varies slightly and periodically in time. This assumption of variable stiffness is realistic in many cases, when the spring-pendulum is subject to external forces. But it can also be a simple model for the complicated forces that act when the spring-pendulum is coupled to another deterministic system. One can for instance imagine it being part of a kind of Fermi-Pasta-Ulam lattice of spring-pendula: a chain of spring-pendula with nearest neighbour interaction. The influence of the nearest neighbours is then modelled by a very simple forcing term.

It is important to remark that Hamiltonian (5.1) has a symmetry: the reflection $(q_1, q_2, p_1, p_2, t) \mapsto (-q_1, q_2, -p_1, p_2, t)$. This implies that the hyperplane $\{(q, p, t) \in T^*\mathbb{R}^2 \times S^1 \mid q_1 = p_1 = 0\}$ is invariant. This hyperplane describes the purely vertical motions of the spring-pendulum.

When $\varepsilon = 0$, the Hamiltonian system is autonomous. The autonomous system has been studied a lot and is well-understood, see for instance [**68**]. It will have a periodic solution: the downward position given by $\{q_1 = p_1 = p_2 = 0, q_2 = -L_0 - L - g/k, t \in S^1\}$. For $\varepsilon \neq 0$ the system is nonautonomous and it is therefore much more complicated. We shall study it with the method of Birkhoff normalisation. This basically means that we introduce an extra symmetry in the equations of motion by choosing appropriate coordinates and approximating the equations of motion. This usually simplifies the analysis.

We assume that the reader is familiar with the well-known Birkhoff normal form method for autonomous Hamiltonian systems near elliptic equilibria as described in for instance [**10**], [**54**] or Chapter 2 of this thesis. The Birkhoff normalisation of time-periodic Hamiltonian vector fields near periodic orbits is an extension of this theory. An important result in this chapter will be that, just as in the classical Hamiltonian setting, the procedure of Birkhoff normalisation can be performed at the level of Hamiltonian functions. This is a not so trivial theoretical result, leading to a considerable simplification of practical computations.

As always, an extra symmetry is present in the Birkhoff normal form. For autonomous Hamiltonian systems this extra symmetry by Noether's theorem can be associated with an extra integral, other than the Hamiltonian function itself. The normal form of an autonomous two degree of freedom Hamiltonian system is therefore Liouville integrable: by the theorem of Liouville-Arnol'd, its solutions move quasi-periodically and lie on invariant tori. This has implications for the original Hamiltonian system: using the KAM theorem one can usually prove that many of these invariant tori persist. Moreover, the size of chaos in the original two degree of freedom system will be exponentially small. On the other hand, in autonomous three or more degree of freedom Hamiltonian systems, near-integrable behaviour will generally be much less prevalent. It is known that already the normal form, in spite of its two integrals, can display large scale chaos, see [**17**] and [**22**].

Time-periodic Hamiltonian systems in general have no integrals at all. Neither will the induced symmetry of the normal form directly result in an extra integral, although it turns out that the normal form can be reduced to a classical Hamiltonian system. We will focus our attention on the so-called 'two and a half degree of freedom' systems. These are the two degree of freedom systems with time-periodic Hamiltonians. Dimensionally they are in between the two and three degree of freedom autonomous Hamiltonian systems.

The forced spring-pendulum of Tondl and Verhulst is an example of a two and a half degree of freedom Hamiltonian system and its normal form can be reduced to an autonomous two degree of freedom Hamiltonian system. We will study it for several combinations of resonances. It turns out that the nongenuinely resonant Birkhoff normal form is completely integrable. In the case of full resonance, we find some interesting multi-pulse solutions in the normal form of the forced spring-pendulum.

5.2. Time-periodic Birkhoff normalisation

In this section, we shall describe the method of Birkhoff normalisation for time-periodic Hamiltonian vector fields. The phase space of these vector fields is $T^*\mathbb{R}^n \times S^1 = T^*\mathbb{R}^n \times \mathbb{R}/_{2\pi\mathbb{Z}}$ with coordinates $x = (q, p, t) = (q_1, \ldots, q_n, p_1, \ldots, p_n, t)$. This space is endowed with the canonical two-form $dq \wedge dp := \sum_j dq_j \wedge dp_j$. With this two-form, each of the fibers $T^*\mathbb{R}^n \times \{t\}$ is a symplectic manifold. For a function $H : T^*\mathbb{R}^n \times S^1 \to \mathbb{R}$, let us define the vector field X_H as follows:

$$X_H = \sum_{j=1}^{n} \frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j}$$

Note that X_H is tangent to the fibers $T^*\mathbb{R}^n \times \{t\}$ and can therefore be interpreted as a family of autonomous Hamiltonian systems on the fibers $T^*\mathbb{R}^n \times \{t\} \cong T^*\mathbb{R}^n$, parameterised by $t \in S^1$ and with Hamiltonian functions $H(\cdot, t) : (q, p) \mapsto H(q, p, t)$. This means that H is a constant of motion for X_H as

$$\mathcal{L}_{X_H} H := dH \cdot X_H = \sum_{j=1}^{n} \frac{\partial H}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial H}{\partial p_j}\frac{\partial H}{\partial q_j} + \frac{\partial H}{\partial t} \cdot 0 = 0$$

Of more practical relevance are vector fields of the form $X_H + \frac{\partial}{\partial t}$. These vector fields are nonautonomous, i.e. time runs with speed one. H will generally not be a constant of motion now as

$$\mathcal{L}_{X_H + \frac{\partial}{\partial t}} H := dH \cdot (X_H + \frac{\partial}{\partial t}) = dH \cdot \frac{\partial}{\partial t} = \frac{\partial H}{\partial t}$$

Now we shall describe how the Birkhoff normal form can be constructed. Normal forms are usually computed by making appropriate coordinate changes, following a stepwise procedure. These coordinate changes are themselves the time one maps of flows of vector fields. Therefore, we first make the following definitions that help in computing how one vector field transforms under the flow of another:

Definition 5.1. *Let $\mathcal{V}$ denote the set of smooth vector fields on $T^*\mathbb{R}^n \times S^1$. For $X \in \mathcal{V}$, denote the flow of X by $(t, x) \mapsto e^{tX}(x)$. For $X, Y \in \mathcal{V}$ we then define the Lie bracket $[X, Y] \in \mathcal{V}$ as follows:*

$$[X, Y] := \left.\frac{d}{dt}\right|_{t=0} (e^{tX})^* Y = \left.\frac{d}{dt}\right|_{t=0} Te^{-tX} Y \circ e^{tX}$$

In coordinates, writing $X = \sum_j X_j \frac{\partial}{\partial x_j}, Y = \sum_j Y_j \frac{\partial}{\partial x_j}$, we find that

$$[X, Y] = \sum_{i,j} (\frac{\partial Y_i}{\partial x_j} X_j - \frac{\partial X_i}{\partial x_j} Y_j) \frac{\partial}{\partial x_i}$$

Let $\mathcal{F}$ be the set of smooth functions on $T^*\mathbb{R}^n \times S^1$. For $F, G \in \mathcal{F}$, we then define the Poisson bracket $\{F, G\} \in \mathcal{F}$ as follows:

$$\{F, G\} := (dq \wedge dp)(X_F, X_G) = dF \cdot X_G = -dG \cdot X_F$$

In coordinates,

$$\{F, G\} = \sum_{j=1}^{n} \frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j}$$

$\mathcal{V}$ is a Lie algebra under the Lie bracket and so is $\mathcal{F}$ under the Poisson bracket. With the help of the formulas for the Lie and Poisson brackets in local coordinates, it is not difficult to express the Lie bracket of time-periodic Hamiltonian vector fields in terms of Poisson brackets. This leads to the following simplifications:

Proposition 5.2. *Let $F, G \in \mathcal{F}$. Then*

$$[X_F, X_G] = X_{-\{F,G\}} \text{ and } [X_F, \frac{\partial}{\partial t}] = X_{-\frac{\partial F}{\partial t}} \tag{5.2}$$

The first identity says that $F \mapsto X_F, \mathcal{F} \to \mathcal{V}$ is a Lie-algebra anti-homomorphism. The second identity tells us that the Lie-bracket of two time-periodic Hamiltonian vector fields is always fiber-preserving. Proposition 5.2 makes the computation of the Lie bracket a lot easier: we can compute it at the level of Hamiltonian functions.

As the Lie bracket $[X, Y]$ is bilinear in X and Y, the operator ad_X defined by $\mathrm{ad}_X(Y) := [X, Y]$ is a linear map from $\mathcal{V}$ to $\mathcal{V}$. As $\mathcal{V}$ is a vector space, ad_X can also be interpreted as a vector field on $\mathcal{V}$ sending $Y \in \mathcal{V}$ to $\mathrm{ad}_X(Y) \in \mathcal{V} = T_Y\mathcal{V}$. The family $t \mapsto (e^{tX})^*Y$ satisfies the linear differential equation $\frac{d}{dt}(e^{tX})^*Y = \mathrm{ad}_X((e^{tX})^*Y)$ with initial condition $(e^{0X})^*Y = Y$. Assuming that $\mathrm{ad}_X : \mathcal{V} \to \mathcal{V}$ is a continuous operator with respect to some norm, this differential equation can easily be solved and has solution

$$(e^{tX})^*Y = e^{t\mathrm{ad}_X}(Y) = \sum_{n=0}^{\infty}(t\mathrm{ad}_X)^n(Y) \tag{5.3}$$

This formula is of course only correct in a subset of $T^*\mathbb{R}^n \times S^1$ where the time-t flow of X is defined and ad_X is a bounded operator. Let us assume that this is the case.

With the help of Proposition 5.2, for time-periodic Hamiltonian vector fields formula (5.3) can be rewritten as

Theorem 5.3.

$$(e^{-X_F})^*(X_G + \frac{\partial}{\partial t}) = X_{H'} + \frac{\partial}{\partial t}$$

in which

$$H' = e^{\mathrm{ad}_F}G + \left(\int_0^1 e^{\tau \mathrm{ad}_F} d\tau\right)\left(\frac{\partial F}{\partial t}\right) \tag{5.4}$$

and $\mathrm{ad}_F : \mathcal{F} \to \mathcal{F}$ *is defined by* $\mathrm{ad}_F(G) = \{F, G\}$.

Proof: From formula (5.3) we know that

$$(e^{-X_F})^*(X_G + \frac{\partial}{\partial t}) = e^{\mathrm{ad}_{-X_F + 0\frac{\partial}{\partial t}}}(X_G + \frac{\partial}{\partial t}) = e^{\mathrm{ad}_{-X_F}}X_G + e^{\mathrm{ad}_{-X_F}}\frac{\partial}{\partial t}$$

By Proposition 5.2, the result now follows from the facts that $\mathrm{ad}_{-X_F}X_G = X_{\mathrm{ad}_F G}$, $(\mathrm{ad}_{-X_F})^0\frac{\partial}{\partial t} = \frac{\partial}{\partial t}$, and that for $n \geq 1$ we have $(\mathrm{ad}_{-X_F})^n\frac{\partial}{\partial t} = X_{(\mathrm{ad}_F)^{n-1}\frac{\partial F}{\partial t}}$. □

This theorem says that when we pull back a time-periodic Hamiltonian vector field $X_G + \frac{\partial}{\partial t}$ under the time-1 flow of a fiber-preserving Hamiltonian vector field X_{-F}, then we obtain a new time-periodic Hamiltonian vector field $X_{H'} + \frac{\partial}{\partial t}$ which has Hamiltonian

$$H' = e^{\mathrm{ad}_F} G + \int_0^1 e^{\tau \mathrm{ad}_F} d\tau \frac{\partial F}{\partial t} = \sum_{n=0}^{\infty} \left(\frac{1}{n!} (\mathrm{ad}_F)^n G + \frac{1}{(n+1)!} (\mathrm{ad}_F)^n \frac{\partial F}{\partial t} \right)$$

Let us now assume that the Lie algebra of Hamiltonian functions $\mathcal{F}$ is graded:

$$\mathcal{F} = \bigoplus_{k=0}^{\infty} \mathcal{F}_k$$

meaning that every Hamiltonian can at least formally be written as an infinite sum of Hamiltonians. This grading usually has the interpretation of an ordering of the Hamiltonian functions with respect to asymptotic smallness. We require that

$$\{\mathcal{F}_k, \mathcal{F}_l\} \subset \mathcal{F}_{k+l} \text{ and } \frac{\partial \mathcal{F}_k}{\partial t} \subset \mathcal{F}_k$$

Example 5.4. *Let $\mathcal{F}_k$ be the set of homogeneous polynomials of degree $k+2$ in the phase space variables (q, p) with smooth t-dependent coefficients. This is an example of a grading.*

Example 5.5. *Let $\varepsilon \in \mathbb{R}$ be an extra parameter on which the Hamiltonian functions depend. Let $\mathcal{F}_k$ be the set of functions on $T^*\mathbb{R}^n \times S^1$ of the form $\varepsilon^k F$ where F is some function on $T^*\mathbb{R}^n \times S^1$ independent of ε. This is an example of a grading.*

Suppose we are given a Hamiltonian $H = H_0 + H_1 + H_2 + \ldots \in \mathcal{F}$ with $H_k \in \mathcal{F}_k$. We would like to normalise it by a sequence of transformations. Given a Hamiltonian $F_1 \in \mathcal{F}_1$, we can transform

$$(e^{-X_{F_1}})^* (X_H + \frac{\partial}{\partial t}) = X_{H_0 + H_1' + \ldots} + \frac{\partial}{\partial t} = X_{\underbrace{H_0}_{\in \mathcal{F}_0} + \underbrace{H_1 + \{F_1, H_0\} + \frac{\partial F_1}{\partial t}}_{\in \mathcal{F}_1} + \ldots\ldots} + \frac{\partial}{\partial t}$$

The dots stand for terms in $\mathcal{F}_k$ with $k \geq 2$.

We want to simplify the Hamiltonian $H_1 + \{F_1, H_0\} + \frac{\partial F_1}{\partial t} = H_1 - (\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(F_1)$ by choosing the correct F_1. In other words, we want F_1 to solve the homological equation

$$(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(F_1) = H_1$$

which would make that $H_1' = 0$, a nice simplification. Unfortunately, the homological equation often can not be solved. Therefore, let us make an important assumption now. We assume that the linear operator $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t} : \mathcal{F} \to \mathcal{F}$ is semi-simple, which means that

$$\mathcal{F} = \ker(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}) \oplus \mathrm{im}(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$$

As $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$ leaves every $\mathcal{F}_k$ invariant, $\mathcal{F}_k = (\mathrm{kerad}_{H_0} - \frac{\partial}{\partial t}) \oplus \mathrm{im}(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$ automatically. In particular H_1 is uniquely decomposed as $H_1 = H_1^k + H_1^i$, with $H_1^k \in \ker(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$, $H_1^i \in \mathrm{im}(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$. Now choose an $F_1 \in \mathcal{F}_1$ such that $(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(F_1) = H_1^i$. Then we see that $H_1' = H_1^k \in \ker(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$. But now we can again write $H_2' = H_2'^k + H_2'^i$ and normalise H_2'. Etcetera. It is clear that by suitable choices one can for any finite $r \geq 1$ find a sequence of transformations $e^{-X_{F_1}}, \ldots, e^{-X_{F_r}}$ that 'normalise' $H = H_0 + H_1 + H_2 + \ldots$ up to order r.

We summarise this result as follows:

Theorem 5.6 (Time-periodic Birkhoff normal form theorem)**.** *Let a Hamiltonian $H = H_0 + H_1 + \ldots \in \mathcal{F}$ be given on $T^*\mathbb{R}^n \times S^1$ such that $H_k \in \mathcal{F}_k$ for all k and $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t} : \mathcal{F} \to \mathcal{F}$ is semi-simple. Then for every $r \geq 1$ there is an open neighbourhood U of $\{0\} \times S^1$ and a symplectic diffeomorphism $\Phi : U \to T^*\mathbb{R}^n \times S^1$ with the properties that Φ leaves the fibers $T^*\mathbb{R}^n \times \{t\}$ invariant, $\Phi^*(dq \wedge dp) = dq \wedge dp$ and*

$$\Phi^*(X_H + \frac{\partial}{\partial t}) = X_{H_0 + \overline{H_1} + \ldots + \overline{H_r} + \ldots} + \frac{\partial}{\partial t}$$

such that

$$(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(\overline{H}_k) = 0$$

for all $1 \leq k \leq r$. The truncated Hamiltonian $\overline{H} = H_0 + \overline{H}_1 + \ldots + \overline{H}_r$ is called a Birkhoff normal form of H of order r.

Clearly, the original time-periodic Hamiltonian vector field $X_H + \frac{\partial}{\partial t}$ is conjugate to the Birkhoff normal form vector field $X_{\overline{H}} + \frac{\partial}{\partial t}$, modulo a very small perturbation term. Studying $X_{\overline{H}} + \frac{\partial}{\partial t}$, we can therefore obtain interesting information about the flow of $X_H + \frac{\partial}{\partial t}$.

5.3. Reduction to the Poincaré section

Suppose we are given a Hamiltonian in normal form, that is a time-periodic Hamiltonian function

$$\overline{H} = H_0 + \overline{H}_1 + \ldots + \overline{H}_r \tag{5.5}$$

defined on $T^*\mathbb{R}^n \times S^1$, which is such that

$$(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(\overline{H}_k) = 0 \tag{5.6}$$

for every $1 \leq k \leq r$. This first of all means that

$$\mathcal{L}_{X_{H_0} + \frac{\partial}{\partial t}} \overline{H}_k = -(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(\overline{H}_k) = 0$$

So each $\overline{H}_k$ is a constant of motion for the flow of $X_{H_0} + \frac{\partial}{\partial t}$. The $\overline{H}_k$ are hence called *invariants*.

But Proposition 5.2 implies also that

$$[X_{H_0} + \frac{\partial}{\partial t}, X_{\overline{H}_k}] = 0$$

i.e. these vector fields Lie-commute. This means that the flows of the vector fields $X_{H_0} + \frac{\partial}{\partial t}$ and $X_{\overline{H}_1+\ldots+\overline{H}_r}$ commute. Hence, the flow of the total system $X_{H_0+\overline{H}_1+\ldots+\overline{H}_r} + \frac{\partial}{\partial t}$ is simply the composition of the flow of $X_{H_0} + \frac{\partial}{\partial t}$ and the flow of $X_{\overline{H}_1+\ldots+\overline{H}_r}$. Assuming that the flow of $X_{H_0} + \frac{\partial}{\partial t}$ is rather trivial to compute, it remains to investigate the flow of $X_{\overline{H}_1+\ldots+\overline{H}_r}$. But the latter leaves all the fibers $T^*\mathbb{R}^n \times \{t\}$ invariant. Moreover, note that $X_{\overline{H}_1+\ldots+\overline{H}_r}|T^*\mathbb{R}^n \times \{t\}$ and $X_{\overline{H}_1+\ldots+\overline{H}_r}|T^*\mathbb{R}^n \times \{s\}$ are conjugate via the time-$(t-s)$-map of $X_{H_0} + \frac{\partial}{\partial t}$. Hence it suffices to study the system in only one of the fibers: we may fix an arbitrary time $t \in S^1$ and consider the system $X_{\overline{H}_1(\cdot,t)+\ldots+\overline{H}_r(\cdot,t)}$ on the *Poincaré section* $T^*\mathbb{R}^n \times \{t\} \cong T^*\mathbb{R}^n$. This is a classical Hamiltonian system with n degrees of freedom which describes the motion from one orbit of the $(X_{H_0} + \frac{\partial}{\partial t})$-flow to another. Note that this system has an integral: the Hamiltonian $\overline{H}_1(\cdot,t) + \ldots + \overline{H}_r(\cdot,t)$.

As usual for normal forms, we can thus perform an important dimension reduction. Moreover, the Hamiltonian $\overline{H}_1(\cdot,t) + \ldots + \overline{H}_r(\cdot,t)$ on $T^*\mathbb{R}^n \times \{t\}$ obviously has a symmetry, namely the time-2π-map (Poincaré map) of $X_{H_0} + \frac{\partial}{\partial t}$.

5.4. Polynomial Hamiltonians with periodic coefficients

In the following, we shall assume that the Hamiltonian H has the following form:

$$H = H_0(q,p) + \sum_{k=1}^{m} \varepsilon^k H_k(q,p,t) + \mathcal{O}(\varepsilon^{m+1}) \tag{5.7}$$

in which $0 \leq |\varepsilon| \ll 1$ is a small parameter and H_0 is a quadratic harmonic oscillator Hamiltonian of the form

$$H_0(q,p) = \sum_{j=1}^{n} \frac{\omega_j}{2}(q_j^2 + p_j^2) \tag{5.8}$$

We allow the $\varepsilon^k H_k$ to be members of the class

$$\mathcal{F}_k := \{ \ \varepsilon^k \sum_{|\alpha|+|\beta|<\infty} c_{\alpha,\beta}(t) q^\alpha p^\beta \text{ for certain } c_{\alpha,\beta} \in C^1(S^1) \ \} \tag{5.9}$$

So the H_k are polynomials in (q,p) of finite degree and with continuously differentiable time-periodic coefficients. Clearly, $\mathcal{F} := \bigoplus_{k\geq 0} \mathcal{F}_k$ is a graded Lie-algebra. We will show that in this context it is possible to bring the Hamiltonian in normal form near $\{0\} \times S^1$.

For the actual computation of the normal form it is convenient to introduce complex coordinates by making the symplectic transformation:

$$\begin{pmatrix} x_j \\ y_j \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \begin{pmatrix} q_j \\ p_j \end{pmatrix}$$

In these canonical coordinates,

$$H_0 = \sum_{j=1}^{n} i\omega_j x_j y_j$$

and the H_k are linear combinations of terms of the form $f(t)x^\alpha y^\beta$. The action of $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$ on these terms is as follows:

$$\mathrm{ad}_{H_0} - \frac{\partial}{\partial t} : f(t)x^\alpha y^\beta \mapsto \left(i\langle \omega, \beta - \alpha \rangle f(t) - \frac{df(t)}{dt} \right) x^\alpha y^\beta$$

Theorem 5.7. *With H_0 given as in (5.8), $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$ is semi-simple on the $\mathcal{F}_k$ given in (5.9). Therefore, in an open neighbourhood of $\{0\} \times S^1$ we can bring the Hamiltonian (5.7) into Birkhoff normal form of arbitrary finite order.*

Proof: Every element of $\mathcal{F}_k$ can after the transformation $(q,p) \mapsto (x,y)$ be written as a sum of terms $\varepsilon^k f(t)x^\alpha y^\beta$. Such a term is in the image of $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$ if and only if there exists a 2π-periodic solution g to the ordinary differential equation

$$i\langle \omega, \beta - \alpha \rangle g(t) - \frac{dg(t)}{dt} = \varepsilon^k f$$

The solution to this equation can be found by variation of constants:

$$g(t) = g_0 e^{i\langle \omega, \beta - \alpha \rangle t} - \int_0^t e^{i\langle \omega, \beta - \alpha \rangle (t-\xi)} \varepsilon^k f(\xi) d\xi \tag{5.10}$$

The constant g_0 has to be chosen such that $g(0) = g(2\pi)$, which makes g a smooth function on S^1. This is obviously possible if $\langle \omega, \beta - \alpha \rangle \notin \mathbb{Z}$. Hence, if $\langle \omega, \beta - \alpha \rangle \notin \mathbb{Z}$, then $\varepsilon^k f(t)x^\alpha y^\beta$ is in the image of $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$. It remains to consider the case that $\langle \omega, \beta - \alpha \rangle \in \mathbb{Z}$. In that case let us write $f(t) = (f(t) - F(t)) + F(t)$ where

$$F(t) = \frac{1}{2\pi} e^{i\langle \omega, \beta - \alpha \rangle t} \int_0^{2\pi} e^{-i\langle \omega, \beta - \alpha \rangle \xi} f(\xi) d\xi$$

Clearly, $i\langle \omega, \beta - \alpha \rangle F(t) - \frac{dF(t)}{dt} = 0$, so $\varepsilon^k F(t)x^\alpha y^\beta$ is in the kernel of $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$. Moreover, one can solve the equation $i\langle \omega, \beta - \alpha \rangle g(t) - \frac{dg(t)}{dt} = \varepsilon^k (f(t) - F(t))$ as $\int_0^{2\pi} e^{-i\langle \omega, \beta - \alpha \rangle \xi} (f(\xi) - F(\xi)) d\xi = 0$. Thus $\varepsilon^k (f(t) - F(t))x^\alpha y^\beta$ is in the image of $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$. We conclude that every term of the form $\varepsilon^k f(t)x^\alpha y^\beta$ is the sum of a term in im $(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$ and a term in ker $(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})$.

This proves that $\mathrm{ad}_{H_0} - \frac{\partial}{\partial t}$ is semi-simple. By the theory of the previous sections, Hamiltonian (5.7) can thus be brought in normal form. □

5.5. Invariants

From the proof of Theorem 5.7, we know that the Birkhoff normal form of a Hamiltonian of the described class is a linear combination of terms

$$e^{i\langle \omega, \beta - \alpha \rangle t} x^\alpha y^\beta \text{ for which } \langle \omega, \beta - \alpha \rangle \in \mathbb{Z}$$

Note also that after the reduction to a Poincaré section, i.e. after fixing a $t \in S^1$, it will be a linear combination of terms of the form $x^\alpha y^\beta$ for which $\langle \omega, \beta - \alpha \rangle \in \mathbb{Z}$. Either of these terms are called *polynomial invariants* as they are constants of motion for the flow of $X_{H_0} + \frac{\partial}{\partial t}$. Let us investigate these polynomial invariants in more detail now.

Note first of all that the normal mode energies

$$C_j := ix_jy_j = \frac{1}{2}(p_j^2 + q_j^2)$$

are invariants for any choice of ω as $\omega_j - \omega_j = 0$. We denote the vector invariant $C := (C_1, \ldots, C_n) = (ix_1y_1, \ldots, ix_ny_n)$. Any other invariant can be multiplied by C^α to obtain again another invariant, hence we will from now on only look for invariants $e^{i\langle\omega,\beta-\alpha\rangle t}x^\alpha y^\beta$ for which $\alpha_j\beta_j = 0$ for all j. So given a $\gamma \in \mathbb{Z}^n\backslash\{0\}$ for which $\langle\omega,\gamma\rangle \in \mathbb{Z}$ we have a unique invariant: define $\alpha_j = (|\gamma_j| - \gamma_j)/2$ and $\beta_j = (|\gamma_j| + \gamma_j)/2$, then $e^{i\langle\omega,\beta-\alpha\rangle t}x^\alpha y^\beta$ is a complex invariant. We may assume that $\gcd(\gamma_j) = 1$ and that $\gamma_{\min\{i|\gamma_i\neq 0\}} > 0$. Then we define the real invariants

$$A_{\alpha,\beta} := \mathrm{Re}\ e^{i\langle\omega,\beta-\alpha\rangle t}x^\alpha y^\beta$$

$$B_{\alpha,\beta} := \mathrm{Im}\ e^{i\langle\omega,\beta-\alpha\rangle t}x^\alpha y^\beta$$

These quantities satisfy

$$A^2_{\alpha,\beta} + B^2_{\alpha,\beta} = C^{\alpha+\beta}$$

and the Poisson structure identities

$$\{A_{\alpha,\beta}, B_{\alpha,\beta}\} = \frac{1}{2}C^{\alpha+\beta}\sum_j \frac{\beta_j^2 - \alpha_j^2}{C_j}$$

$$\{A_{\alpha,\beta}, C\} = (\beta-\alpha)B_{\alpha,\beta}\ ,\ \{B_{\alpha,\beta}, C\} = (\alpha-\beta)A_{\alpha,\beta}\ ,\ \{C_j, C_k\} = 0$$

Note that the $\overline{H}_k$ are polynomial functions of these invariants.

5.6. Two and a half degrees of freedom

In this section we consider the two and a half degree of freedom case, that is we assume that our phase space is $T^*\mathbb{R}^2 \times S^1$ and our Hamiltonian function is

$$H = H_0(q,p) + \sum_{k=1}^{r} \varepsilon^k H_k(q,p,t) + \mathcal{O}(\varepsilon^{r+1})$$

where

$$H_0 = \frac{\omega_1}{2}(q_1^2 + p_1^2) + \frac{\omega_2}{2}(q_2^2 + p_2^2)$$

and $\varepsilon^k H_k \in \mathcal{F}_k$, that is the H_k are polynomials in (q,p) with differentiable time-periodic coefficients.

In the coming subsections we will investigate what the normal form will look like for various choices of $\omega = (\omega_1, \omega_2)$, in other words which invariants we may encounter in the case of two and a half degrees of freedom.

5.6.1. Nonresonant flow. Let us assume that the linear frequencies ω_1, ω_2 and 1 are completely nonresonant, meaning that $\langle \omega, \gamma \rangle \notin \mathbb{Z}$ for all $\gamma \in \mathbb{Z}^2 \backslash \{0\}$. Then the invariants are C_1 and C_2 and products of these. They Poisson commute: $\{C_1, C_2\} = 0$. This implies that the normal form $\overline{H}_1 + \ldots + \overline{H}_r$ on $T^*\mathbb{R}^2$ is a polynomial function of C_1 and C_2. Moreover, C_1 and C_2 are constants of motion for the normal form flow. Hence, the normal form equations are completely integrable and solutions move on invariant tori.

5.6.2. Nongenuine resonance. Assume that $\omega_1 \notin \mathbb{Q}$ (the case that $\omega_2 \notin \mathbb{Q}$ is equivalent), but that a relation exists of the form $\gamma_1\omega_1 + \gamma_2\omega_2 = m \in \mathbb{Z}$, for certain $\gamma_1, \gamma_2 \in \mathbb{Z}$ with $\gamma_2 > 0$ and $\gcd(\gamma_1, \gamma_2, m) = 1$. We speak of 'nongenuine resonance' in this case. Examples are $(\omega_1, \omega_2) = (\sqrt{2}, 3)$ or $(\omega_1, \omega_2) = (\sqrt{2}, 2\sqrt{2})$. In this situation, $\delta_1\omega_1 + \delta_2\omega_2 = \omega_1(\delta_1 - \delta_2\gamma_1/\gamma_2) + \delta_2 m/\gamma_2$ which is not in $\mathbb{Z}$ unless $\delta_1\gamma_2 = \delta_2\gamma_1$. This means that any relation of the form $\delta_1\omega_1 + \delta_2\omega_2 \in \mathbb{Z}$ is a multiple of the relation $\gamma_1\omega_1 + \gamma_2\omega_2 = m$ and each invariant is a product of the invariants C_1, C_2 and the imaginary and real parts of $A + iB = e^{imt}y_1^{\gamma_1}y_2^{\gamma_2}$ (if $\gamma_1 > 0$) or $A + iB = e^{imt}x_1^{-\gamma_1}y_2^{\gamma_2}$ (if $\gamma_1 < 0$). From the Poisson relations

$$\{A, C\} = \gamma B \ , \ \{B, C\} = -\gamma A$$

we infer that $E := \gamma_2 C_1 - \gamma_1 C_2$ is a Casimir: it Poisson commutes with A, B and C. This implies that the normal form Hamiltonian $\overline{H}_1(\cdot, t) + \ldots + \overline{H}_r(\cdot, t)$ on $T^*\mathbb{R}^2$, being a polynomial function of A, B and C, is integrable, the integrals being $\overline{H}_1(\cdot, t) + \ldots + \overline{H}_r(\cdot, t)$ and E. Its solutions generically move on invariant tori.

The equations of motion of the integrable normal form on $T^*\mathbb{R}^2$ can be studied as follows. The invariants $(A, B, C_1, C_2) \in \mathbb{R}^4$ satisfy

$$A^2 + B^2 = C_1^{|\gamma_1|} C_2^{|\gamma_2|} \ , \ C_1, C_2 \geq 0 \tag{5.11}$$

Fixing the value of the Casimir, $E = \gamma_2 C_1 - \gamma_1 C_2 = e$, allows for a reduction to a two dimensional reduced phase space which can be embedded in three dimensional Euclidean space:

$$\Sigma := \{ \ (A, B, C_2) \in \mathbb{R}^3 \mid A^2 + B^2 = (\frac{e + \gamma_1 C_2}{\gamma_2})^{|\gamma_1|} C_2^{|\gamma_2|} \ , \ C_2 \geq 0 \ , \ e + \gamma_1 C_2 \geq 0 \ \}$$

This is a two-dimensional orbifold in three-space, which is foliated in the level sets of the Hamiltonian $\overline{H} = \overline{H}_1 + \ldots + \overline{H}_r$. This means that we can make drawings of the reduced phase space and the level sets of $\overline{H}$. A bifurcation analysis can thus easily be performed. Σ is an unbounded surface if $\gamma_1 > 0$ and a bounded surface if $\gamma_1 < 0$. Moreover, it can have singularities, the analysis of which is not very difficult.

We conclude that for two and a half degrees of freedom, the analysis of the normal form in the case of nongenuine resonance, resembles very much the analysis of a resonant two degree of freedom normal form. The major difference is that the reduced phase space can be noncompact.

5.6.3. Full resonance. The only truly nontrivial case is that of full resonance. This occurs when $\omega_1 = \frac{r_1}{s_1} \in \mathbb{Q}, \omega_2 = \frac{r_2}{s_2} \in \mathbb{Q}$, where $\gcd(r_j, s_j) = 1$. Then there are minimal integers k, l, m, n such that

$$k\omega_1 + l\omega_2 = 0$$

$$m\omega_1 + n\omega_2 = 1$$

and every other relation is of the form

$$K(k\omega_1 + l\omega_2) + L(m\omega_1 + n\omega_2) = (Kk + Lm)\omega_1 + (Kl + Ln)\omega_2 = L$$

that is a linear combination of the two minimal relations. Apart from the reduction to the Poincaré section $T^*\mathbb{R}^2$, we can generally not decrease the dimension any further. We can only observe that the reduced system on $T^*\mathbb{R}^2$ will have a discrete symmetry: the time-2π flow (Poincaré map) of $X_{H_0} + \frac{\partial}{\partial t}$ from $T^*\mathbb{R}^2 \to T^*\mathbb{R}^2$ given in coordinates by

$$\Phi : \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} \mapsto \begin{pmatrix} q_1 \cos 2\pi\omega_1 + p_1 \sin 2\pi\omega_1 \\ q_2 \cos 2\pi\omega_2 + p_2 \sin 2\pi\omega_2 \\ p_1 \cos 2\pi\omega_1 - q_1 \sin 2\pi\omega_1 \\ p_2 \cos 2\pi\omega_2 - q_2 \sin 2\pi\omega_2 \end{pmatrix}$$

The map Φ has finite order: if K is the smallest common multiple of s_1 and s_2, then $\Phi^K = \mathrm{Id}$.

5.7. Example: the forced spring-pendulum

Recall the forced spring-pendulum of Section 5.1. We saw that when $\varepsilon = 0$, it has a periodic solution given by $p_1 = p_2 = q_1 = 0, q_2 = -L_0 - L - g/k$. We define

$$\omega_1 = \sqrt{g/L}\ ,\ \omega_2 = \sqrt{k}$$

and we introduce new canonical coordinates

$$(Q_1, Q_2, P_1, P_2) = (\sqrt{\omega_1}q_1, \sqrt{\omega_2}(q_2 + L_0 + L + g/k), p_1/\sqrt{\omega_1}, p_2/\sqrt{\omega_2})$$

and Taylor-expand the Hamiltonian H around $Q = P = 0$. Using that $\sqrt{L^2 - Q_1^2/\omega_1} = L - \frac{1}{2L\omega_1}Q_1^2 - \frac{1}{8L^3\omega_1^2}Q_1^4 + \ldots$, we arrive at the following:

$$\begin{aligned} H = {} & \frac{\omega_1}{2}(P_1^2 + Q_1^2) + \frac{\omega_2}{2}(P_2^2 + Q_2^2) + \mu Q_1^2 Q_2 + \lambda_1 Q_1^4 + \ldots \\ & + \varepsilon \cos(t) \left(\lambda_2 Q_2 + \frac{\omega_1}{2}Q_1^2 + \frac{\omega_2}{2}Q_2^2 + \mu Q_1^2 Q_2 + \lambda_1 Q_1^4 + \ldots\right) \end{aligned} \tag{5.12}$$

We thus find that ω_1 and ω_2 are the eigenfrequencies of the spring-pendulum. The dots indicate terms of order $\mathcal{O}(||Q||^5)$. Together with $\omega_1 > 0$ and $\omega_2 > 0$, the parameter

$$\mu = -k^{\frac{3}{4}}/2\sqrt{gL} < 0$$

can be freely be chosen by tuning the parameters in the system, whereas

$$\lambda_1 = \frac{\mu^2}{2}\left(\frac{1}{\omega_2} + \frac{\omega_1^2}{\omega_2^3}\right) > 0 \text{ and } \lambda_2 = -\frac{\omega_1\omega_2}{2\mu} > 0$$

are dependent variables. To bring the Hamiltonian (5.12) into a form that is appropriate for Birkhoff normalisation, we rescale variables $(Q,P)=\varepsilon(q,p)$ and obtain

$$H=\frac{\omega_1}{2}(p_1^2+q_1^2)+\frac{\omega_2}{2}(p_2^2+q_2^2)+\lambda_2\cos(t)q_2+$$
$$+\,\varepsilon\left(\mu q_1^2q_2+\frac{\omega_1}{2}\cos(t)q_1^2+\frac{\omega_2}{2}\cos(t)q_2^2\right)+\varepsilon^2\left(\lambda_1q_1^4+\mu\cos(t)q_1^2q_2\right)+\mathcal{O}(\varepsilon^3)$$

Due to the inhomogeneous term at order $\mathcal{O}(\varepsilon^0)$, this Hamiltonian is not in the standard form for time-periodic normalisation, as described in Section 5.4. But such a standard form can easily be obtained as follows. When $\omega_2\neq 1$, then the $\mathcal{O}(\varepsilon^0)$ part of $X_H+\frac{\partial}{\partial t}$ has at least one solution of frequency 1, which we subtract to obtain new variables:

$$Q_1=q_1,P_1=p_1,Q_2=q_2+\frac{\lambda_2\omega_2}{\omega_2^2-1}\cos(t),P_2=p_2-\frac{\lambda_2}{\omega_2^2-1}\sin(t)$$

This transformation is the time-1 map of the flow of $X_F+0\frac{\partial}{\partial t}$ for $F=\frac{\lambda_2}{\omega_2^2-1}(\omega_2p_2\cos(t)$ $+q_2\sin(t))$. With the help of formula (5.4) and using that $\{F,\frac{\partial F}{\partial t}\}=-\omega_2(\frac{\lambda_2}{\omega_2^2-1})^2$ is constant, we therefore obtain the new Hamiltonian

$$\begin{aligned}H=&\frac{\omega_1}{2}(P_1^2+Q_1^2)+\frac{\omega_2}{2}(P_2^2+Q_2^2)+\\&+\ \varepsilon\left(\mu Q_1^2Q_2+\lambda_3Q_2+\lambda_4Q_1^2\cos(t)+\frac{\omega_2}{2}Q_2^2\cos(t)+\lambda_3Q_2\cos(2t)\right)+\\&+\ \varepsilon^2\left(\lambda_1Q_1^4+\lambda_5Q_1^2+\mu Q_1^2Q_2\cos(t)+\lambda_5Q_1^2\cos(2t)\right)+\mathcal{O}(\varepsilon^3)\end{aligned}\tag{5.13}$$

in which

$$\lambda_3=\frac{-\omega_1\omega_2^3}{4\mu(1-\omega_2^2)},\lambda_4=\frac{\omega_1}{2}\left(1-\frac{\omega_2^2}{1-\omega_2^2}\right)\text{ and }\lambda_5=\frac{-\omega_1\omega_2^2}{4(1-\omega_2^2)}$$

are again dependent variables.

We have shown that except when $\omega_2=1$, the time-dependent Hamiltonian of the forced spring-pendulum can be brought in the standard form (5.13). The latter defines a system consisting of two independent oscillators, perturbed by a time-dependent periodic Hamiltonian. It has a reflection symmetry and hence an invariant hyperplane $\{Q_1=P_1=0\}$. Up to order $\mathcal{O}(\varepsilon^0)$, the circle $\{Q=P=0\}\times S^1$ is invariant. The system is ready for normalisation near this circle.

5.8. Normal form of the spring-pendulum

The eventual formula for the normal form of (5.13) depends of course heavily on the resonance relations that exist between the eigenvalues ω_1 and ω_2. We will treat a few interesting cases here, in which nontrivial resonant terms already occur at order $\mathcal{O}(\varepsilon)$.

5.8.1. Nongenuine resonance 1. Consider the example $\omega_1=\frac{1}{2},\omega_2\notin\mathbb{Q},\omega_2\neq\frac{1}{2}\sqrt{2}$. Then the only resonance relation reads $2\omega_1=1$ and according to Section 5.5 the invariants are

$$C_1 = \frac{1}{2}(P_1^2 + Q_1^2),\ C_2 = \frac{1}{2}(P_2^2 + Q_2^2)$$
$$A = \text{Re } y_1^2 e^{it} = \frac{1}{2}(P_1^2 \cos(t) + 2P_1Q_1 \sin(t) - Q_1^2 \cos(t))$$
$$B = \text{Im } y_1^2 e^{it} = \frac{1}{2}(P_1^2 \sin(t) - 2P_1Q_1 \cos(t) - Q_1^2 \sin(t))$$

A short computation tells us that the normal form Hamiltonian is up to order $\mathcal{O}(\varepsilon)$ given by

$$\overline{H} = \frac{1}{2}C_1 + \omega_2 C_2 - \frac{\varepsilon\lambda_4}{2}A$$

where $\lambda_4 \neq 0$. Fixing the value of the Casimir $E = -2C_2 = e \leq 0$, we can analyse the reduced phase space

$$\Sigma = \{(A, B, C_1) \in \mathbb{R}^3 | A^2 + B^2 = C_1^2, C_1 \geq 0\}$$

Σ is an unbounded cone, foliated by the level sets of the reduced Hamiltonian $\varepsilon\overline{H}_1 = -\frac{\varepsilon\lambda_4}{2}A$, see Figure 2.

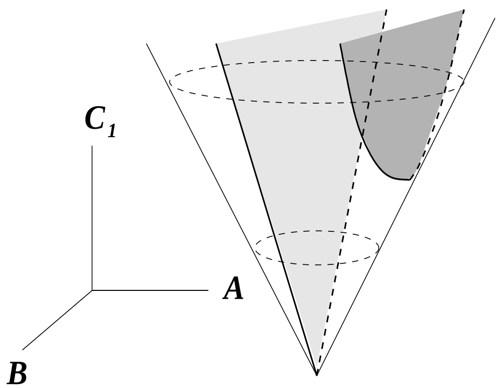

Figure 2: The foliation of the reduced phase space.

It is clear from the figure that the origin $A = B = C_1 = 0$, that represents the second normal mode solution $(C_1 = 0, C_2 = -e/2)$, is unstable. The amplitude of the first normal mode will grow unboundedly. A similar thing happens if we choose $\omega_1 \notin \mathbb{Q}, \omega_2 = \frac{1}{2}$.

5.8.2. Nongenuine resonance 2. Another important example of nongenuine resonance occurs when $2\omega_1 = \omega_2 \notin \mathbb{Q}$. In this case, no time-dependent resonant terms can exist. The analysis is therefore the same as for the autonomous spring-pendulum and it is well-known. The $\omega_1 : \omega_2 = 1 : 2$-resonance leads in autonomous Hamiltonian systems to various nontrivial phenomena, see [**10**], [**11**] or [**68**], even in the integrable Birkhoff normal form. It is generally considered the most important resonance in two degrees of freedom. Let us briefly recall the normal form analysis up to order $\mathcal{O}(\varepsilon)$ here.

The Birkhoff normal form Hamiltonian is autonomous and computed to be

$$\overline{H} = \frac{\omega_1}{2}(P_1^2 + Q_1^2) + \frac{\omega_2}{2}(P_2^2 + Q_2^2) + \frac{\mu\varepsilon}{4}(Q_1^2 Q_2 + 2Q_1P_1P_2 - Q_2P_1^2)$$

The Hamiltonian system $X_{\overline{H}} + \frac{\partial}{\partial t}$ on $T^*\mathbb{R}^2 \times S^1$ of course reduces to a classical Hamiltonian system on $T^*\mathbb{R}^2$, which is integrable with as integrals $\overline{H}_1$ and the 'linear energy' Casimir

$$E = \frac{1}{2}(P_1^2 + Q_1^2) + (P_2^2 + Q_2^2)$$

Let us also compute invariants. The only nontrivial resonance relation is $-2\omega_1 + \omega_2 = 0$ and the invariants thus are

$$C_1 = \frac{1}{2}(Q_1^2 + P_1^2)\ ,\ C_2 = \frac{1}{2}(Q_2^2 + P_2^2)$$

$$A = \mathrm{Re}\ x_1^2 y_2 = \frac{1}{2\sqrt{2}}(Q_1^2P_2 - P_1^2P_2 - 2Q_1P_1Q_2)$$

$$B = \mathrm{Im}\ x_1^2 y_2 = \frac{1}{2\sqrt{2}}(P_1^2Q_2 - Q_1^2Q_2 - 2Q_1P_1P_2)$$

satisfying the relations

$$A^2 + B^2 = C_1^2 C_2\ ,\ C_1 \geq 0\ ,\ C_2 \geq 0$$

Fixing the value of the Casimir $E = C_1 + 2C_2 = e \geq 0$, we can then embed our reduced phase space in $\mathbb{R}^3$ as

$$\Sigma = \{(A, B, C_1) | A^2 + B^2 = C_1^2(e - C_1)/2, 0 \leq C_1 \leq e\}$$

Σ is a topological sphere with one cone-like singularity at $(A, B, C_1) = (0, 0, 0)$. In terms of the invariants, the normal form Hamiltonian is $\overline{H} = \omega_1 C_1 + \omega_2 C_2 - \frac{\mu\varepsilon}{\sqrt{2}}B$. Σ is hence foliated by the level sets of the reduced Hamiltonian $\varepsilon\overline{H_1} = -\frac{\mu\varepsilon}{\sqrt{2}}B$, see Figure 3.

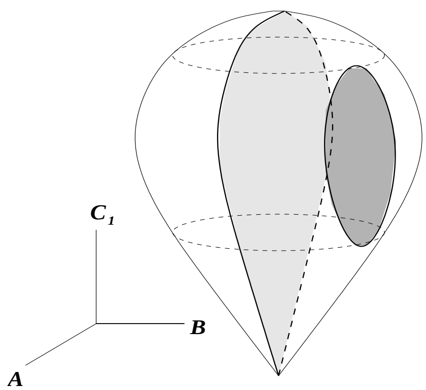

Figure 3: The foliation of the reduced phase space for the 1:2-resonance.

The level sets of $\varepsilon\overline{H}_1$ are the intersections of planes of constant B with the depicted balloon-shaped surface. Almost every such level set is a circle, which corresponds to an invariant Liouville torus in the integrable system on $T^*\mathbb{R}^2$. Two of the level sets are elliptic relative equilibria, each corresponding to a periodic 'jumping' orbit in $T^*\mathbb{R}^2$, see also [**15**]. There is one hyperbolic singular relative equilibrium (the tip of the cone). It corresponds to vertical spring-pendulum motion: the second normal mode given by $C_1 = 0, C_2 = e/2$. This normal mode is unstable. The singular point is connected to itself by its coinciding stable and unstable manifolds, lying in the level set $\overline{H}_1 = -\mu B/\sqrt{2} = 0$. Reconstructed in $T^*\mathbb{R}^2$ this is a 'Möbius figure-8' that connects the second normal mode solution to itself, see Figure 4.

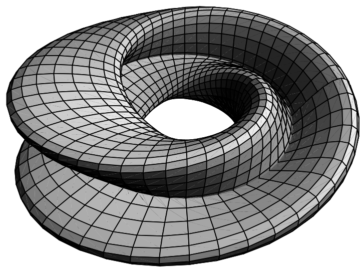

Figure 4: The homoclinic connection defined by $E = e, \overline{H}_1 = 0$.

The Möbius figure-8 is filled with homoclinic orbits. See [**15**] for more details.

5.8.3. Full resonance. Our forced spring-pendulum will of course be much more intriguing when its eigenvalues display full resonance. As we can not study every possible resonance, we shall assume again that $2\omega_1 = \omega_2$, but this time such that $\omega_j \in \mathbb{Q}$. Of course we still need the assumption that $\omega_2 \neq 1$, but we shall moreover assume that $\omega_2 \neq \frac{1}{2}, 2$. This implies that again no time-dependent resonant terms occur at order $\mathcal{O}(\varepsilon)$, so that up to this order the Birkhoff normal form analysis is exactly as in Section 5.8.2. But time-dependent resonant terms can indeed show up now at order $\mathcal{O}(\varepsilon^2)$ and we shall tune our parameters such that this is the case. Our Birkhoff normal form will then have the form

$$\overline{H} = H_0(Q,P) + \varepsilon\overline{H}_1(Q,P) + \varepsilon^2\overline{H}_2(Q,P,t) =$$
$$\frac{\omega_1}{2}(P_1^2+Q_1^2)+\frac{\omega_2}{2}(P_2^2+Q_2^2)+\frac{\mu\varepsilon}{4}(Q_1^2Q_2+2Q_1P_1P_2-Q_2P_1^2)+\varepsilon^2\overline{H}_2(Q,P,t)$$

such that

$$(\mathrm{ad}_{H_0} - \frac{\partial}{\partial t})(\overline{H}_2) = 0$$

As an example, we compute the $\mathcal{O}(\varepsilon^2)$ normal form for a particular resonance. We choose $\omega_1 = \frac{3}{2}, \omega_2 = 3$, so that $1 : \omega_1 : \omega_2 = 2 : 3 : 6$. After a rather long second order normal form computation, we then find that

$$\overline{H}_2 = -\frac{\mu^2}{2^3\cdot 3}(Q_1^2+P_1^2)(Q_2^2+P_2^2) + \frac{\mu^2}{2^6}(Q_1^2+P_1^2)^2$$
$$-\frac{3^3\cdot 17^2}{2^{15}}(Q_1^2+P_1^2) - \frac{3^3}{2^3\cdot 5\cdot 7}(Q_2^2+P_2^2) - \frac{3^6}{5\cdot 2^8\mu}(Q_2\cos(3t) - P_2\sin(3t))$$

According to Section 5.3, we can now reduce to a classical Hamiltonian system on $T^*\mathbb{R}^2$ with Hamiltonian function $\varepsilon\overline{H}_1 + \varepsilon^2\overline{H}_2(\cdot,t)$ where t is fixed and arbitrary, say $t=0$. The Hamiltonian then is a polynomial in (Q,P). For simplicity, we rescale time by a factor $1/\varepsilon$ to obtain the Hamiltonian $\overline{H}_1+\varepsilon\overline{H}_2$. The lowest order part of this Hamiltonian, $\overline{H}_1$, is integrable with as integrals $\overline{H}_1$ itself and the linear energy Casimir $E = H_0/\omega_1$. The quadratic vector field $X_{\overline{H}_1}$ leaves the level sets $E^{-1}(e)\subset T^*\mathbb{R}^2$ invariant. For each $e>0$, this level set is a compact ellipsoid that contains two periodic 'jumping' orbits, a lot of Liouville tori and a Möbius figure-8 that connects the circle $\{Q_1 = P_1 = 0, Q_2^2+P_2^2 = e\}$ to itself. Taking the union over all $e\geq 0$, we get an unbounded homoclinic connection $\{\overline{H}_1 = 0\}$ that connects the invariant hyperplane $\{Q_1 = P_1 = 0\}$ to itself. This hyperplane consists exactly of the stationary points of $\overline{H}_1$. Outside the hyperplane, the homoclinic connection $\{\overline{H}_1 = 0\}$ is a smooth 3-dimensional manifold. It is filled with homoclinic solutions

$$\begin{pmatrix} Q_1(\tau)\\ P_1(\tau)\\ Q_2(\tau)\\ P_2(\tau)\end{pmatrix}_{e,\alpha} = \begin{pmatrix} \sqrt{2e}\cosh^{-1}(\mu\sqrt{e}\,\tau/2)\sin\alpha\\ \sqrt{2e}\cosh^{-1}(\mu\sqrt{e}\,\tau/2)\cos\alpha\\ \sqrt{e}\tanh(\mu\sqrt{e}\,\tau/2)\sin 2\alpha\\ \sqrt{e}\tanh(\mu\sqrt{e}\,\tau/2)\cos 2\alpha\end{pmatrix} \tag{5.14}$$

One readily checks that the orbit $(Q_{e,\alpha}(\tau), P_{e,\alpha}(\tau))$ lies inside $E^{-1}(e)\cap\overline{H}_1^{-1}(0)$. The Casimir value $e\geq 0$, the angle $\alpha\in S^1$ and the time $\tau\in\mathbb{R}$ parameterise the homoclinic connection $\{\overline{H}_1 = 0\}\backslash\{Q_1 = P_1 = 0\}$. We once again see that the homoclinic orbits in (5.14) connect the plane $\{Q_1 = P_1 = 0\}$ to itself.

The full system $X_{\overline{H}_1+\varepsilon\overline{H}_2}$ on $T^*\mathbb{R}^2$ is a small Hamiltonian perturbation of the quadratic, integrable, ellipsoid-preserving system $X_{\overline{H}_1}$. The invariant symplectic hyperplane $\{Q_1 = P_1 = 0\}$ is now not filled with equilibria, but fibered by the level sets of

$$\overline{H}_2\big|_{Q_1=P_1=0} = -\frac{3^3}{2^3\cdot 5\cdot 7}(Q_2^2+P_2^2) - \frac{3^6}{5\cdot 2^8\mu}Q_2$$

These level sets are circles centered at $(Q_2,P_2) = (-\frac{3^3\cdot 7}{2^4\mu}, 0)$, see Figure 5.

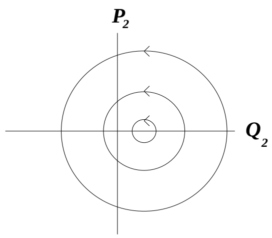

Figure 5: The motion in slow manifold $\{Q_1 = P_1 = 0\}$ in the case $\varepsilon > 0$.

Clearly, the motion in this slow manifold is periodic.

Perturbations of ellipsoid-preserving quadratic vector fields were recently studied by J.M. Tuwankotta [**69**]. Using bifurcational and numerical techniques, this author studies dissipative perturbations of such vector fields, which commonly arise from certain atmosphere models. Our problem can be considered as a Hamiltonian variant.

Hamiltonian perturbations of integrable systems have moreover been studied a lot by using the KAM theorem. This theorem says that under a certain nondegeneracy condition, many of the invariant tori of an integrable system will persist under nonintegrable perturbations. We expect to see many of these KAM-tori in the system induced by $\overline{H}_1 + \varepsilon\overline{H}_2$. But in our further analysis, we will mostly be interested in the remnants of the homoclinic connection defined by $\overline{H}_1 = 0$. In the coming subsection, we will therefore study the $2:3:6$-normal form of the spring-pendulum by a Melnikov analysis.

5.8.4. Melnikov analysis. It is an interesting question whether some of the homoclinic orbits of the vector field $X_{\overline{H}_1}$ will survive in the flow of $X_{\overline{H}_1+\varepsilon\overline{H}_2}$ when ε is small but nonzero. A theorem of Fénichel [**34**] ensures that the stable and unstable manifolds of every compact part $\{Q^2 + P_2^2 \leq R^2, Q_1 = P_1 = 0\}$ of the slow manifold will persist for $\varepsilon \neq 0$ but small enough. With the help of a Melnikov integral we can approximate the distance between these stable and unstable manifolds. A nondegenerate zero of the Melnikov integral will then correspond to a homoclinic single-pulse solution, see [**38**] or [**26**]. Melnikov integrals are commonly studied, but not if the homoclinic connection has a rather complicated geometry as is the case here. The Melnikov integral, which up to first order in ε measures the $\overline{H}_1$-distance between the first branches of the stable and unstable manifold, is computed by integrating the infinitesimal increment $d\overline{H}_1 \cdot X_{\overline{H}_2}$ of H_1 along the homoclinic orbits of $X_{\overline{H}_1}$, that is:

$$M(e,\alpha) = \int_{-\infty}^{\infty} \{\overline{H}_1, \overline{H}_2\}(Q_{e,\alpha}(\tau), P_{e,\alpha}(\tau))d\tau$$

in which $(Q_{e,\alpha}(\tau), P_{e,\alpha}(\tau))$ is as given in (5.14). The evaluation of the Melnikov integral is surprisingly simple. Note first of all that when $\gamma_2 + \delta_2$ is even, then $\int_{-\infty}^{\infty} \{\overline{H}_1, Q_{e,\alpha}^{\gamma} P_{e,\alpha}^{\delta}\}(\tau)d\tau = 0$, as $\tau \mapsto \{\overline{H}_1, Q_{e,\alpha}^{\gamma} P_{e,\alpha}^{\delta}\}(\tau)$ is an odd function. For the spring-pendulum in $2:3:6$-resonance, we hence quickly compute that

$$M(e,\alpha) = -\frac{3^6}{5 \cdot 2^8 \mu} \int_{-\infty}^{\infty} \{\overline{H}_1, Q_2\}\big|_{(Q,P)=(Q_{e,\alpha}(\tau),P_{e,\alpha}(\tau))} \, d\tau = -\frac{3^6}{5 \cdot 2^7 \mu} \sqrt{e} \sin(2\alpha)$$

Clearly, at every $e > 0, \alpha = 0 \mod \pi/2$, this M has a transversal zero: $M = 0, \operatorname{grad} M \neq 0$. According to the implicit function theorem, the stable and unstable manifolds must therefore have a two-dimensional intersection at $\mathcal{O}(\varepsilon)$-distance of these zeros, corresponding to a one-parameter family of homoclinic one-pulse orbits.

5.9. Multi-pulse solutions

In this section we conjecture that apart from the one-pulse solutions that were found in the previous section, multi-pulse solutions can exist in the normal form of the 2 : 3 : 6 resonant spring-pendulum. We give a heuristic argument here, using geometric perturbation theory as in [**27**]. A full proof would unfortunately have a large number of nontrivial estimates, which is far beyond the scope of this chapter.

We first of all note that at the point $(Q_1, P_1, Q_2, P_2) = (0, \sqrt{2e}, 0, 0)$, the homoclinic connection $\{\overline{H}_1 = 0\}$ intersects transversely with the hyperplane $\{P_2 = 0\}$. So do the stable manifold W^s and the unstable manifold W^u of the perturbed vector field $X_{\overline{H}_1+\varepsilon\overline{H}_2}$, lying at $\mathcal{O}(\varepsilon)$-distance of the original homoclinic connection $\{\overline{H}_1 = 0\}$. The intersections are two-dimensional. According to the previous section, W^s and W^u moreover intersect transversely themselves, which results in a transversal intersection of $W^s \cap \{P_2 = 0\}$ with $W^u \cap \{P_2 = 0\}$ inside $\{P_2 = 0\}$ at $\mathcal{O}(\varepsilon)$-distance of the line segment $\{(0, s, 0, 0) | 0 < \sqrt{2e} - \mathcal{O}(1) < s < \sqrt{2e} + \mathcal{O}(1)\} \subset \{P_2 = 0\}$ on which the Melnikov function has its transversal zero. See Figure 6.

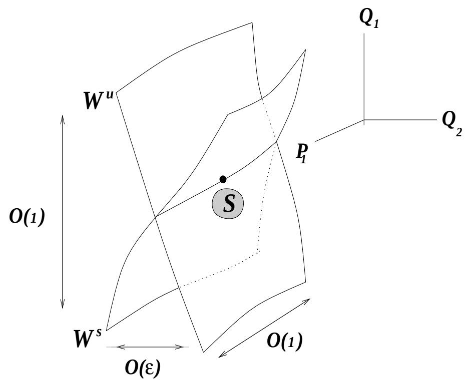

Figure 6: Transversal intersection of the stable and unstable manifolds inside the plane $\{P_2 = 0\}$ near the point $(Q_1, P_1, Q_2) = (0, \sqrt{2e}, 0)$.

Let us now take a small collection S of points in $W^u \cap \{P_2 = 0\}$, at $\mathcal{O}(e^{-1/\varepsilon})$-distance of the stable manifold W^s, and at $\mathcal{O}(\varepsilon)$-distance of $(Q_1, P_1, Q_2, P_2) = (0, \sqrt{2e}, 0, 0)$, see Figure 6. We are interested in the image $\mathcal{P}(S)$ of S under the Poincaré map $\mathcal{P}$ that maps some points of $\{P_2 = 0\}$ back to $\{P_2 = 0\}$. The points in S lie on orbits of $X_{\overline{H}_1+\varepsilon\overline{H}_2}$ that, starting in S and closely following one of the unperturbed homoclinic orbits, reach within $\mathcal{O}(1)$-time the neighbourhood

$$\Delta = \{(Q, P) \in T^*\mathbb{R}^2 | \ |Q_1|, |P_1| < \delta, Q_2^2 + P_2^2 < R^2\}$$

of the slow manifold, near the point $(Q_1, P_1, Q_2, P_2) = (0, 0, 0, \sqrt{e})$. We assume that δ is small enough such that Fénichel coordinates can be found in Δ, see [**27**] or [**34**].

Our orbit will enter Δ at $\mathcal{O}(e^{-1/\varepsilon})$-distance of W^s and stay in Δ for a time of at least $\mathcal{O}(1/\varepsilon)$. In Δ, the orbit will follow Fénichel's equations and stay close to the circle $\{Q_1 = P_1 = 0, (Q_2 + \frac{3^3.7}{2^4\mu})^2 + P_2^2 = e\}$. It will move along this circle over a distance of $\mathcal{O}(1)$ until it leaves Δ, at $\mathcal{O}(e^{-1/\varepsilon})$-distance of W^u. Note that we can make our orbit stay arbitrarily long in Δ, by choosing its initial point in S sufficiently close to W^s. Hence the orbits can make arbitrarily many rotations in Δ. Some of these orbits leave Δ again near the point $(Q_1, P_1, Q_2, P_2) = (0, 0, 0, -\sqrt{e})$. Staying close to one of the unperturbed homoclinic orbits, they will return to $\{P_2 = 0\}$ again, at a distance of $\mathcal{O}(e^{-1/\varepsilon})$ from W^u and of $\mathcal{O}(\varepsilon)$ from $(0, \sqrt{2e}, 0, 0)$.

Depending on exact estimates, that we have omitted, the image $\mathcal{P}(S)$ of S will consist of at least a finite number of surfaces, two of which are drawn in Figure 7.

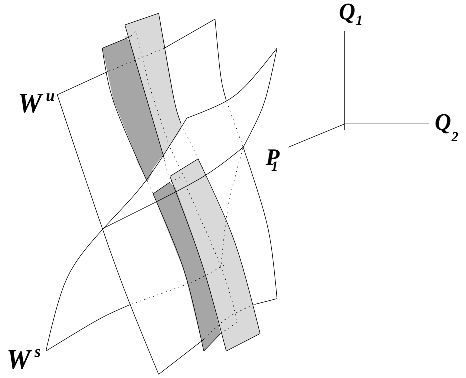

Figure 7: Two parts of $\mathcal{P}(S)$.

Clearly, $\mathcal{P}(S)$ intersects W^s in at least a finite number of curves. Each point of intersection corresponds to a 2-pulse solution: it lies in W^s and is taken by $\mathcal{P}^{-1}$ to W^u. Hence, there is a finite number of one-parameter families of two-pulse solutions.

But we can continue and take a small set $S' \subset \mathcal{P}(S)$, at $\mathcal{O}(e^{-1/\varepsilon})$-distance of W^u and at $\mathcal{O}(\varepsilon)$-distance of $(0, \sqrt{2e}, 0, 0)$. $\mathcal{P}(S')$ will again intersect W^s in finitely many curves. Each point on such a curve represents a three-pulse solution. Etc. In this way it follows that:

Theorem 5.8 (Conjecture)**.** *For small enough ε and for $n \in \mathbb{N}_{\geq 2}$, $n = \mathcal{O}(1)$, the flow of $X_{\overline{H}_1 + \varepsilon \overline{H}_2}$ on $T^*\mathbb{R}^2$ contains an $\mathcal{O}(1)$ number of one-parameter families of homoclinic n-pulse solutions at $\mathcal{O}(\varepsilon)$-distance of the original three-dimensional homoclinic connection $\{\overline{H}_1 = 0\}$.*

5.10. Discussion

To gain more understanding in the behaviour of a forced spring-pendulum, this chapter started by describing a Birkhoff normal form theory for time-periodic Hamiltonian systems. It turned out that the normal form of a time-periodic Hamiltonian system can be computed at the level of Hamiltonian functions. This simplifies computations a lot. Moreover we have described the dimension reduction that can be performed for the normal form equations.

The Birkhoff normal form of the forced spring-pendulum has been computed for various examples of resonances. When the eigenvalues of the Hamiltonian admit a nongenuine resonance, then the equations of motion are integrable. On the other hand, the solutions of the normal form can easily become unbounded.

Some very interesting phenomena can occur when the eigenvalues display full resonance. We computed the normal form of the $2:3:6$-resonant forced spring-pendulum. Up to first order, the reduced normal form Hamiltonian on $T^*\mathbb{R}^2$ is integrable and it contains an invariant plane, connected to itself by a three dimensional homoclinic connection. In the second order normal form, many of the Liouville tori of the integrable system will survive as KAM tori, but the homoclinic connection breaks up: the time-periodic forcing destroys it. By a Melnikov analysis, we showed however that one-parameter families of one-pulse homoclinic solutions survive. We argue moreover that finitely many one-parameter families of homoclinic multi-pulse solutions must exist. As an entirely solid proof of the latter statement is beyond the scope of this chapter, we have formulated it as a conjecture. With a more detailed analysis, it may even be possible to prove stronger results. For instance, one may wonder if the perturbed flow contains a horseshoe map. This could show the existence of chaos and the nonintegrability of the fully resonant normal form. A more thorough investigation is necessary to prove this.

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Samenvatting

Natuurkundige, biologische, economische en andere door wetenschappers bestudeerde systemen, worden dikwijls beschreven met een wiskundig model. Zo'n model wordt geformuleerd op basis van observaties, kennis en logisch redeneren.

Een beroemd voorbeeld is de zwaartekrachtwet van Galilei, die de beweging van een vallend voorwerp beschrijft. Al argumenterend en experimenterend formuleerde de sterrenkundige Galilei deze 'wet' in 1638. De zwaartekrachtwet zegt: 'de snelheid van een vallend voorwerp neemt iedere seconde met dezelfde hoeveelheid toe.'

Deze regel is eenvoudig in het gebruik, blijkt vaak perfect te kloppen en is daarom erg waardevol. We kunnen er bijvoorbeeld mee uitrekenen hoe hard een appel de grond raakt als deze vanaf zekere hoogte uit een boom valt. Maar soms klopt er niets van Galilei's wet: door de grote luchtweerstand is de valsnelheid van een parachutist maar beperkt en het is ook al eeuwen bekend dat hemellichamen zich heel anders gedragen dan vallende appels. In deze gevallen is een ingewikkelder model nodig om zinnige uitspraken over de werkelijkheid te kunnen doen.

Het opstellen van een wiskundig model is een kunst op zich, maar in dit proefschrift vragen we ons niet zozeer af hoe een model tot stand komt of in welke mate het toepasbaar is. Dit proefschrift is juist een studie naar de wiskundige eigenschappen van bestaande modellen. Onder de aanname dat die modellen tot op zekere hoogte kloppen, zijn de conclusies uit de wiskundige analyse waardevol en kunnen ze worden geïnterpreteerd als eigenschappen van de werkelijkheid die we trachten te modelleren.

De modellen in dit proefschrift zijn modellen uit de *klassieke mechanica*. De wetten van de klassieke mechanica zijn wiskundige regels die de beweging van natuurkundige objecten bepalen, door de krachten op en tussen deze objecten te beschrijven. Voorbeelden zijn Galilei's zwaartekrachtwet en de beroemde wetten van Kepler die de beweging van de planeten vastleggen. In het moderne wiskundige taalgebruik worden al deze wetten geformuleerd als een *differentiaalvergelijking*. Wanneer de aanvankelijke staat van een klassiek mechanisch systeem bekend is, dan bepaalt deze differentiaalvergelijking hoe het systeem zich in de toekomst zal gedragen. De bewegingen van het systeem zijn impliciet, doch ondubbelzinnig vastgelegd door de differentiaalvergelijking. Dit betekent echter niet dat we ook weten hoe die beweging daadwerkelijk zal zijn.

Een wiskundige stelt zich tot taak om door berekeningen en redeneringen expliciete uitspraken te doen over de oplossingen van het wiskundige model. Dus om vragen te beantwoorden als: met welke snelheid zal een voorwerp dat luistert naar de wet van Galilei, de grond raken als het op tien meter hoogte wordt losgelaten? Of: zal de aarde, ervan uitgaande dat haar beweging correct beschreven wordt door de wetten van Kepler, nog lang in haar huidige cirkelbaan om de zon blijven ronddraaien? Deze puur wiskundige vragen houden de wetenschap al eeuwen bezig. Helaas is het vaak ontstellend moeilijk ze te beantwoorden.

Het klassiek mechanische systeem dat centraal staat in dit proefschrift heet de *Fermi-Pasta-Ulam keten.* Dit is een soort ketting, bestaande uit een groot aantal kralen die krachten op elkaar uitoefenen. De Fermi-Pasta-Ulam keten staat model voor een eenvoudige eendimensionale atoomstructuur. Kennis van het model is daarom van fundamenteel belang voor het begrijpen van natuurkundige systemen als eenvoudige kristallen, lange moleculen, draden of snaren. Het model werd in de jaren vijftig van de twintigste eeuw gezamenlijk geformuleerd door de beroemde natuurkundige en nobelprijswinnaar Fermi, computerexpert Pasta en wiskundige Ulam. De wetten van de klassieke mechanica schrijven zoals gewoonlijk precies voor hoe de kralen in de ketting elkaar beïnvloeden. Desondanks vergt het een behoorlijke dosis wiskunde om erachter te komen hoe de keten zich zal gaan gedragen.

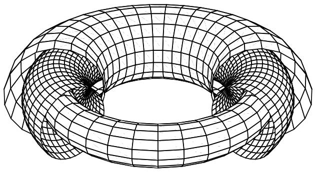
Al vroeg in de geschiedenis van het Fermi-Pasta-Ulam model werden enkele aspecten van dit gedrag ontdekt in computerexperimenten. Computerexperimenten stellen ons in staat om het gedrag van een model in beperkte mate te onderzoeken, ook als we niet veel van dit model begrijpen. De uitkomsten van de experimenten waren verrassend: ze druisten volledig in tegen de natuurkundige intuïtie van de vijftiger jaren en waren bovendien geenszins theoretisch wiskundig te verklaren. Eigenlijk bleek de keten zich veel gestructureerder en ordelijker te gedragen dan Fermi, Pasta en Ulam hadden verwacht. En uit latere computerexperimenten bleek keer op keer dat dit keurige gedrag structureel was. Al met al heeft men zich hier lange tijd over verwonderd. In de jaren die volgden, raakte onze kennis over niet-lineaire differentiaalvergelijkingen in een stroomversnelling. Er werden dan ook verscheidene wiskundige theorieën geponeerd die als verklaring voor het 'Fermi-Pasta-Ulam probleem' moesten dienen. Maar deze waren altijd mager onderbouwd.

In de jaren zeventig en tachtig was het stil rond de Fermi-Pasta-Ulam keten, maar sinds een jaar of tien staat het model weer veel in de belangstelling van natuurkundigen, aangezien we nu beter dan ooit in staat zijn het model wiskundig te begrijpen. Ook dit proefschrift beoogt een bijdrage te leveren aan ons theoretisch wiskundig begrip van de Fermi-Pasta-Ulam keten. Een deel van de observaties van Fermi, Pasta en Ulam wordt in dit proefschrift wiskundig verklaard. Maar ook worden door een wiskundige analyse enkele nieuwe, voorheen onbekende verschijnselen ontdekt.

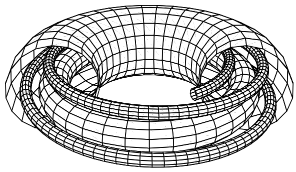
De exacte resultaten uit dit proefschrift zijn op deze plek moeilijk te verwoorden. Niet in de laatste plaats omdat de wiskunde van de Fermi-Pasta-Ulam keten zich afspeelt in een hoogdimensionale ruimte die men zich moeilijk voor kan stellen. Het is de ruimte van de posities en snelheden van alle deeltjes in de keten en deze ruimte heeft veel meer dimensies dan de ons omringende drie-dimensionale ruimte.

In dit proefschrift wordt allereerst een aantal voorheen onbekende oplossingen van het Fermi-Pasta-Ulam model berekend. Over de oplossingen die we niet kunnen berekenen, doen we een aantal kwalitatieve uitspraken. Een belangrijke conclusie is dat we wiskundig kunnen *bewijzen* dat de meeste laag-energetische oplossingen van de Fermi-Pasta-Ulam keten zich 'keurig' gedragen. Het blijkt dat in de hoogdimensionale ruimte waarin het model gedefinieerd is, zekere eenvoudige meetkundige objecten voorkomen waarover de oplossingen van de differentiaalvergelijking zich bewegen. Deze meetkundige objecten zijn *torussen.* In eenvoudige gevallen kan men bij een torus denken aan het oppervlak van de binnenband van een fiets. Het feit dat de beweging op torussen plaatsvindt, verklaart in grote mate dat deze beweging gestructureerd en eenvoudig is. Dit resultaat is dan ook van belang voor ons begrip van het Fermi-Pasta-Ulam probleem.

Een ander interessant resultaat is dat de gevonden torussen op allerlei verschillende manieren gesitueerd kunnen zijn ten opzichte van elkaar. Zo kunnen ze in elkaar gelegen zijn zoals in Figuur 1, of juist om elkaar heen geknoopt zoals in Figuur 2.



Figuur 1: Torussen in elkaar.



Figuur 2: Torussen in en om elkaar.

De soms ingewikkelde meetkundige ligging van torussen ten opzichte van elkaar heeft een interessante natuurkundige interpretatie: er kunnen golfbewegingen voorkomen in de Fermi-Pasta-Ulam keten die plotseling en drastisch van aard veranderen. Deze golven waren nog niet eerder waargenomen, maar nu we ze kunnen voorspellen, blijkt het gemakkelijk ze in computerexperimenten terug te vinden.

Het wiskundige gereedschap dat nodig is om de hierboven beschreven analyse uit te voeren, wordt in dit proefschrift verzameld en verder ontwikkeld. De wiskundige sleutelwoorden zijn *integreerbaarheid, quasi-periodieke beweging, normaalvormen, symmetrie en monodromie.* Vervolgens wordt uitgelegd hoe dit gereedschap moet worden gebruikt om wiskundige conclusies te kunnen trekken over de Fermi-Pasta-Ulam keten en andere mechanische systemen en worden deze conclusies natuurkundig geïnterpreteerd.

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Curriculum Vitae

Op 5 februari 1977 ben ik in Utrecht geboren. Sindsdien woonde ik in Culemborg, waar ik in 1995 mijn gymnasiumdiploma behaalde aan het Koningin Wilhelmina College. Daarna ging ik Wiskunde en Natuurkunde studeren aan de Universiteit Utrecht. In 1999 studeerde ik af in de Toegepaste Wiskunde en startte mijn aanstelling als aio aan de faculteit Wiskunde en Informatica van diezelfde universiteit. Dit betekent dat ik de afgelopen jaren onderwijs heb gegeven, lid was van het onderzoeksbestuur van de vakgroep Wiskunde en op reis ging naar Peyresq, Cala Gonone, Snowbird, Enschede, Bandung, Rome en Hasselt. Maar natuurlijk heb ik vooral veel tijd besteed aan het promotieonderzoek dat leidde tot dit proefschrift.

Born in Utrecht on February the 5th, 1977, I graduated from high school in 1995. In 1999 I obtained my Masters degree in Applied Mathematics at the University of Utrecht and I started my PhD research. During the last years I gave lectures, was a member of the research board of the faculty, refereed articles, attended conferences, visited foreign institutes and wrote this thesis.