An integrable approximation for the Fermi-Pasta-Ulam lattice

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Abstract

This contribution presents a review of results obtained from computations of approximate equations of motion for the Fermi-Pasta-Ulam lattice. These approximate equations are obtained as a finite-dimensional Birkhoff normal form. It turns out that in many cases, the Birkhoff normal form is suitable for application of the KAM theorem. In particular this proves Nishida's 1971 conjecture stating that almost all low-energetic motions of the anharmonic Fermi-Pasta-Ulam lattice with fixed endpoints are quasi-periodic. The proof is based on the formal Birkhoff normal form computations of Nishida, the KAM theorem and discrete symmetry considerations.

1 Introduction

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 [9]. It consists of a number of equal point masses that nonlinearly interact with their nearest neighbors. Assuming the lattice consists of a finite number of particles N and satisfies periodic boundary conditions, the physical variables of the FPU lattice are the positions q_j $(j \in \mathbb{Z}/N\mathbb{Z})$ of the particles, see Figure 1, and their conjugate momenta p_j $(j \in \mathbb{Z}/N\mathbb{Z})$.

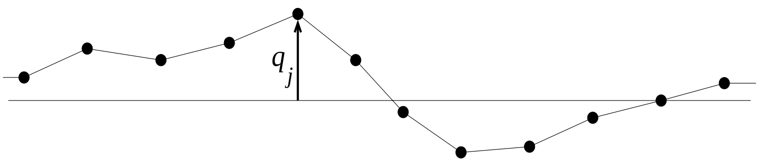

Figure 1: Schematic picture of the FPU lattice.

Positions and momenta are elements of the $2N$-dimensional space of q_j's and p_j's, the cotangent bundle $T^*\mathbb{R}^N$. Equipped with the canonical symplectic form $dq \wedge dp := \sum_{j=1}^{N} dq_j \wedge dp_j$ this is a symplectic manifold and a Hamiltonian function

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$H : T^*\mathbb{R}^N \to \mathbb{R}$ generates the Hamiltonian vector field X_H implicitly defined by the relation $dq \wedge dp(X_H, \cdot) = dH$. That is the integral curves of X_H are the solutions of the system of ordinary differential equations

$$\dot{q}_j = \frac{\partial H}{\partial p_j} \ , \ \dot{p}_j = -\frac{\partial H}{\partial q_j} \ , \ j \in \mathbb{Z}/N\mathbb{Z} \ .$$

For the 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.

Fermi, Pasta and Ulam were interested in the statistical properties of the nonlinear FPU lattice. In fact, they expected that it would attain a thermal equilibrium, as is expected in statistical mechanics. This means that the initial energy of the lattice should be redistributed and, averaged over time, equipartitioned among all the Fourier modes of the lattice, see [18]. They performed a numerical experiment to investigate how and at what time-scale this would occur. The astonishing result of their integrations was that there was no sign of energy equipartition at all, see [9] and [18]: energy that was initially put in one Fourier mode, was shared by only a few other modes. Moreover, within a rather short time nearly all the energy in the system returned to the initial mode. This recurrent behaviour has been observed in experiments on the FPU lattice with quite small as well as very large numbers of particles, on short and long time-scales, and we are led to believe that at low energy the FPU lattice behaves more or less quasi-periodically. This observation was a big surprise. On the other hand, when the initial energy of the lattice is larger then a certain threshold, equipartition indeed occurs.

For a theoretical understanding of the Fermi-Pasta-Ulam experiment, one has often tried to link the FPU lattice to a completely integrable system. These are dynamical systems possessing a complete set of integrals of motion and therefore they display the regular type of behavior that was observed in the FPU experiment. More precisely, it is well-known [2] that periodic and quasi-periodic motion is typical in completely integrable finite-dimensional Hamiltonian systems due to the theorem of Liouville-Arnol'd. The FPU lattice is not completely integrable, but one can nevertheless remark the following.

Firstly, it turns out that the special FPU lattice for which

$$W(x) = \frac{1}{a^2}e^{ax} - \frac{1}{a^2}(1 + ax) = \frac{1}{2!}x^2 + \frac{a}{3!}x^3 + \frac{a^2}{4!}x^4 + \frac{a^3}{5!}x^5 + \ldots$$

is in fact completely integrable. This lattice is called the Toda lattice and it possesses a Lax pair representation, as was shown by Flaschka in [10]. For the general FPU lattice such a thing is definitely not true.

On the other hand, it is not difficult to derive integrable partial differential equations for the asymptotic evolution of long low-amplitude waves in FPU chains with a large number of particles. The first theoretical understanding of the Fermi-Pasta-Ulam experiment therefore came when Zabusky and Kruskal [30] formally derived that the evolution of long *unidirectional* waves of low amplitude is at lowest order governed by a Korteweg-de Vries (KdV) equation. For instance, one may set $\varepsilon := \frac{1}{N} \ll 1$ and assume the existence of a smooth function $u^L = u^L(\tau, \xi)$ such that $q_j(t) = \varepsilon u^L(\varepsilon^3 t, \varepsilon(t + j))$. By a simple Taylor-expansion, one now quickly derives that this two time-scale traveling wave Ansatz leads to the identity $u^L_{\tau\xi} = \frac{\alpha}{4} u^L_\xi u^L_{\xi\xi} + \frac{1}{24} u^L_{\xi\xi\xi\xi} + \mathcal{O}(\varepsilon^2)$. On setting $v^L = u^L_\xi$, this reduces to $v^L_\tau = \frac{\alpha}{4} v^L v^L_\xi + \frac{1}{24} v^L_{\xi\xi\xi} + \mathcal{O}(\varepsilon^2)$. This is the easiest way I know to formally obtain a KdV equation for the evolution of unidirectional waves -in this case traveling to the left.

By studying the KdV equation numerically, Kruskal and Zabusky discovered the stability of the interaction of its solitons. It was later proved by Gardner et al. [13] that the KdV equation has infinitely many integrals. In fact, Peter Lax realised that KdV is a member of a hierarchy of integrable equations that have a Lax-pair, and therefore a complete set of integrals. See [21] for a good overview of these results. We now know that the solutions of the KdV equation (and all other equations in the KdV hierarchy) are almost-periodic, with a dense set of quasi-periodic solutions, see [19]. This could explain, to some extent, the observation of quasi-periodicity in the FPU experiment, although the exact connection between FPU and KdV is not very clear from the above formal derivation.

In order to derive the KdV equation rigorously, one may proceed as follows. First one writes an exact evolution equation for an interpolation function u: setting again $\varepsilon := \frac{1}{N} \ll 1$, and assuming that $q_j(t) = \varepsilon u(t, \varepsilon j)$ for a smooth function $u = u(t, x), \mathbb{R} \times \mathbb{R}/\mathbb{Z} \to \mathbb{R}$, it is clear that $q_j(t)$ satisfies the FPU equations of motion if u satisfies the evolution equation

$$u_{tt}(t, x) = \frac{1}{\varepsilon} W' \left(\varepsilon u(t, x + \varepsilon) - \varepsilon u(t, x) \right) - \frac{1}{\varepsilon} W' \left(\varepsilon u(t, x) - \varepsilon u(t, x - \varepsilon) \right)$$

One should think of this equation as a second order ordinary differential equation on a space of smooth functions of x of period 1. One now proceeds by defining the discrete Riemann-invariants

$$\begin{aligned} U^L(t, x) &:= \frac{1}{\varepsilon} \left(u_t(t, x) + u(t, x + \varepsilon/2) - u(t, x - \varepsilon/2) \right) \\ U^R(t, x) &:= \frac{1}{\varepsilon} \left(u_t(t, x) - u(t, x + \varepsilon/2) + u(t, x - \varepsilon/2) \right) \end{aligned}$$

and observing, by Taylor expanding $u(t, x \pm \varepsilon/2)$ and $u(t, x \pm \varepsilon)$ with respect to ε, that the corresponding evolution equations for U^L and U^R can be expressed as

$$\begin{aligned} U^L_t &= \varepsilon U^L_x + \varepsilon^3 \left(\frac{\alpha}{4} (U^L - U^R)(U^L_x - U^R_x) + \frac{1}{24} U^L_{xxx} \right) + \mathcal{O}(\varepsilon^5) \\ U^R_t &= -\varepsilon U^R_x + \varepsilon^3 \left(\frac{\alpha}{4} (U^L - U^R)(U^L_x - U^R_x) - \frac{1}{24} U^R_{xxx} \right) + \mathcal{O}(\varepsilon^5) \end{aligned}$$

Quite remarkably, it turns out that it is possible to make a small transformation $(U^L, U^R) \mapsto (\tilde{U}^L, \tilde{U}^R) = (U^L, U^R) + \mathcal{O}(\varepsilon)$ in a suitable space of smooth periodic functions of x that removes all coupling terms from the above evolution equations.

In other words, the evolution equations for $\tilde{U}^L$ and $\tilde{U}^R$ can be expressed as

$$\begin{aligned}\tilde{U}_t^L =& \varepsilon\tilde{U}_x^L + \varepsilon^3\left(\frac{\alpha}{4}\tilde{U}^L\tilde{U}_x^L + \frac{1}{24}\tilde{U}_{xxx}^L\right) + \mathcal{O}(\varepsilon^5)\\ \tilde{U}_t^R =& -\varepsilon\tilde{U}_x^R + \varepsilon^3\left(\frac{\alpha}{4}\tilde{U}^R\tilde{U}_x^R - \frac{1}{24}\tilde{U}_{xxx}^R\right) + \mathcal{O}(\varepsilon^5)\end{aligned}$$

This means that $\tilde{u}^L(t,x) := \tilde{U}^L(t, x-\varepsilon t)$ and $\tilde{u}^R(t,x) := \tilde{U}^R(t, x+\varepsilon t)$ satisfy approximate KdV equations, arising after a coordinate transformation as a "resonant normal form". It is not very hard to prove the long (but finite) time validity of these KdV equations. A result of this kind was proved by Bambusi and Ponno in [3], where the above transformation is obtained by the so-called method of averaging and the above estimates are made precise. A similar result was obtained by Wayne and Schneider in [28], although these authors use a multiple scales method. I am at the moment not aware of any results stronger than the long time validity of the KdV equations. It seems to be completely unknown, for example, whether any of the quasi-periodic solutions of the KdV equations persist (as KAM tori) in the FPU lattice.

Persistence results for quasi-periodic tori are easier to obtain in the finite dimensional setting. In the remainder of this paper, we shall therefore view the FPU lattice as a finite dimensional dynamical system. As is well-known [2], periodic and quasi-periodic motion is typical in completely integrable finite dimensional Hamiltonian systems. Unfortunately, apart from the Toda lattice, the FPU lattice is not completely integrable. One possible explanation of the recurrent behaviour of the lattice is therefore based on the famous Kolmogorov-Arnol'd-Moser (KAM) theorem [2], [4]. This theorem explains that large measure Cantor sets of quasi-periodic motions can also exist in classes of nonintegrable Hamiltonian systems, namely those that can be viewed as small perturbations of certain integrable Hamiltonian systems. The restrictive requirement is that the integrable system that we are perturbing satisfies a nondegeneracy condition, which requires that each quasi-periodic motion of the integrable system has a different frequency. Even though various -again heuristic- arguments advocate this approach, and I mention in particular [17], the big problem is that it is not at all a priori clear whether the finite dimensional FPU lattice can really be viewed as a perturbation of such a *nondegenerate* integrable Hamiltonian system. The only obvious integrable approximation to the FPU lattice is its linearisation, which is highly degenerate as its frequency map is constant. Exactly this problem was pointed out for instance in the review paper by Ford [11] and the book by Weissert [29],

An interesting attempt to prove the applicability of the KAM theorem arises in a paper by T. Nishida [20], who in 1971 considered the FPU lattice with a finite number of particles, fixed endpoints and symmetric potential energy density function (the so-called β-lattice). Analogous to the normal form construction for the derivation of the two KdV equations, Nishida computes the so-called Birkhoff normal form for the finite dimensional FPU lattice. *Assuming* a rather strong nonresonance condition on the frequencies of this lattice, he shows that this normal form constitutes a nondegenerate integrable approximation to the original lattice Hamiltonian. In this way, he proves the applicability of the KAM theorem and the existence of a positive measure set of quasi-periodic motions in the nonlinear FPU lattice. But note that all of this is under the assumption of a nonresonance condition, which unfortunately is only satisfied in exceptional cases. The actual value of Nishida's computation therefore remains unclear.

This contribution is based on reference [25], which is devoted to a full proof of what Nishida intended to show. Let me summarize the main result of [25] as follows:

The Fermi-Pasta-Ulam lattice with fixed endpoints and an arbitrary finite number of moving particles possesses a completely integrable finite order Birkhoff normal form, which constitutes an integrable appoximation to the original Hamiltonian function. The integrals are the linear energies of the Fourier modes. When the potential energy density function of the lattice is an even function (β-lattice), this integrable approximation is nondegenerate in the sense of the KAM-theorem. This proves the existence of a large-measure set of quasi-periodic motions in the low-energy domain of the β-lattice.

The key to proving this result lies in the fact that Nishida's nonresonance condition, which a priori seems highly necessary for computing the Birkhoff normal form, is actually obsolete. As in [23], [24], which treat the FPU lattice with periodic boundary conditions, discrete symmetries are the key to proving Nishida's 'conjecture'. The results in [25] can be considered as an extension of [23] to the lattice with fixed endpoints.

I want to remark here that the results of this paper do not provide any explicit bounds on the domain of validity of the normal form approximation. In particular we have at this moment no estimates on the behaviour of this domain when n grows to infinity. The principal interest of the result lies in the fact that, at least to my knowledge, it is the first complete proof of the very existence of a positive measure set of quasi-periodic motions in the FPU lattice with fixed endpoints.

2 Discrete symmetry

The Hamiltonian function (1.1) of the periodic FPU lattice has discrete symmetries of which we shall discuss some dynamical consequences. Two important symmetries of the periodic FPU lattice are the linear mappings $R, S : T^*\mathbb{R}^N \to T^*\mathbb{R}^N$ defined by

$$\begin{aligned} R :&(q_1, q_2, \ldots, q_{N-1}, q_N; p_1, p_2, \ldots, p_{N-1}, p_N) \mapsto \\ &(q_2, q_3, \ldots, q_N, q_1; p_2, p_3, \ldots, p_N, p_1) \ , \\ S :&(q_1, q_2, \ldots, q_{N-1}, q_N; p_1, p_2, \ldots, p_{N-1}, p_N) \mapsto \\ &-(q_{N-1}, q_{N-2}, \ldots, q_1, q_N; p_{N-1}, p_{N-2}, \ldots, p_1, p_N) \ . \end{aligned}$$

It is easily checked that R and S are canonical transformations that leave the periodic FPU Hamiltonian (1.1) invariant, i.e. $R^*(dq \wedge dp) = S^*(dq \wedge dp) = dq \wedge dp$ and $R^*H(= H \circ R) = S^*H(= H \circ S) = H$. We call such transformations symmetries, as they conjugate the Hamiltonian vector field X_H to itself and hence commute with the time-t flows e^{tX_H} of X_H. Since the symmetries R and S satisfy the multiplication relations $R^N = S^2 = \mathrm{Id}$, $SR = R^{-1}S$, they constitute a representation in $T^*\mathbb{R}^N$ of the N-th dihedral group, the symmetry group of the N-gon, by symplectic mappings.

For every group G of symmetries, we can define the fixed point set

$$\mathrm{Fix}\, G = \{(q, p) \in T^*\mathbb{R}^N | P(q, p) = (q, p) \ \forall P \in G\} \ . \tag{2.1}$$

If G is a group of symmetries of a Hamiltonian function H, then Fix G is an invariant manifold for the flow of X_H. Classification of the fixed point sets of the different subgroups of D_N therefore leads to a collection of invariant manifolds, listed for instance in [24]. Other authors, cf. [5], have baptized these invariant manifolds *bushes of normal modes*. The restriction of a Hamiltonian vector field to a fixed point set of a group is often easy to compute:

Proposition 2.1 *When G is compact and consists of linear symplectic isomorphisms of $T^*\mathbb{R}^n$, then* $\mathrm{Fix}\, G$ *is a symplectic manifold with the restriction to* $\mathrm{Fix}\, G$ *of $dq \wedge dp$ as symplectic form. This implies that whenever X_H is tangent to* $\mathrm{Fix}\, G$, *in particular when H is G-symmetric,*

$$(X_H)|_{\mathrm{Fix}\; G} = X_{(H|_{\mathrm{Fix}\; G})}$$

A proof of this result can be obtained by averaging over the compact group G and is given in [25].

One particular fixed point set is of interest for this paper: let N be even, say $N = 2n + 2$, then the group $\langle S \rangle = \{\mathrm{Id}, S\}$ is given by:

$$\mathrm{Fix}\,\langle S \rangle = \{(q, p) \in T^*\mathbb{R}^N | q_j = -q_{2n+2-j}, p_j = -p_{2n+2-j}\ \forall j\}$$

Clearly, in Fix $\langle S \rangle$, $q_0 = q_{n+1} = p_0 = p_{n+1} = 0$. Thus we see that Fix $\langle S \rangle$ is filled with solutions $(q_1(t), \ldots, q_N(t); p_1(t), \ldots, p_N(t))$ for which the $(q_1(t), \ldots, q_n(t); p_1(t), \ldots, p_n(t))$ constitute the general solution curves of the FPU lattice with fixed endpoints and n moving particles. Hence we conclude that the FPU lattice with fixed endpoints and n particles is embedded in the periodic lattice with $N = 2n + 2$ particles.

3 Quasi-particles

The representation of D_N on $T^*\mathbb{R}^N$ is the sum of irreducible representations and it is natural to choose coordinates on $T^*\mathbb{R}^N$ that are adapted to these irreducible representations. This is commonly done by making a Fourier transformation $q \mapsto Q$ and lifting it to a symplectic "point transformation" on the cotangent bundle:

$$(q, p) \mapsto (Q, P)\ ,\ T^*\mathbb{R}^N \to T^*\mathbb{R}^N\ .$$

Such a transformation is explicitly given in [25]. The new coordinates (Q, P) are usually called *quasi-particles* or *phonons*. As the transformation $(q, p) \mapsto (Q, P)$ is symplectic, it is useful to express the Hamiltonian in terms of Q and P. If we write for (1.1)

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

where H_2 is a quadratic polynomial in (Q, P) and H_3 and H_4 cubic and quartic polynomials in Q, then we find that (see [18], [22] or [26])

$$H_2 = \sum_{k=1}^{N} \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2)\ . \tag{3.1}$$

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

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

This means that written down in quasi-particles, the equations of motion of the harmonic lattice ($\alpha = \beta = 0$) are simply the equations for $N-1$ uncoupled harmonic oscillators and, as $\omega_N = 0$, one free particle. In fact, the Hamiltonian system is Liouville integrable in this situation. Integrals are for instance the linear energies

$$E_k := \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2) \ . \tag{3.2}$$

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. The normal modes then interact in a complicated manner that is governed by the Hamiltonians $H_r = H_r(Q)$ ($r = 3, 4$). These Hamiltonians describe the interactions between the various Fourier modes.

It turns out that H is independent of $Q_N = \frac{1}{\sqrt{N}} \sum_j q_j$. Hence the total momentum $P_N = \frac{1}{\sqrt{N}} \sum_j p_j$ is a constant of motion and the equations for the remaining variables are completely independent of (Q_N, P_N). It is common to set the latter coordinates equal to zero, thus remaining with a system on $T^*\mathbb{R}^{N-1}$ with coordinates $(Q_1, \ldots, Q_{N-1}, P_1, \ldots, P_{N-1})$. As $\omega_1, \ldots, \omega_{N-1} > 0$, we can conclude that the origin $(Q, P) = 0$ is a dynamically stable equilibrium of this reduced system.

Assuming again that $N = 2n+2$, it follows from the definition of the quasi-particles given in [25] and the definition of S that

$$\mathrm{Fix}\langle S\rangle = \{(Q, P) \in T^*\mathbb{R}^{N-1} \mid Q_k = P_k = 0 \ \forall \ n+1 \le k \le N-1 \ \} \cong T^*\mathbb{R}^n \ .$$

The Hamiltonian of the fixed endpoint lattice is therefore

$$H|_{\mathrm{Fix}\langle S\rangle} = \sum_{k=1}^{n} \frac{1}{2}(P_k^2 + \Omega_k^2 Q_k^2) + H_3(Q_1, \ldots, Q_n, 0, \ldots, 0) + H_4(Q_1, \ldots, Q_n, 0, \ldots, 0)$$

To distinguish we have here used the notation $\Omega_k := \omega_k = 2\sin(\frac{k\pi}{2n+2})$ ($1 \le k \le n$) for the linear frequencies of the fixed endpoint lattice. We will continue to use the notation $E_k = \frac{1}{2}(P_k^2 + \Omega_k^2 Q_k^2)$ ($1 \le k \le n$) for the integrals of the linearisation of the fixed endpoint lattice.

4 The Birkhoff normal form

Nishida's idea was to study the Hamiltonian of the fixed endpoint lattice using Birkhoff normalisation, which 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. For $r \ge 2$, let $\mathcal{F}_r$ be the finite-dimensional space of homogeneous r-th degree polynomials in (Q, P) on $T^*\mathbb{R}^{N-1}$ and let $\mathcal{F} := \bigoplus_{r \ge 2} \mathcal{F}_r$. With the Poisson bracket $\{\cdot, \cdot\} : \mathcal{F} \times \mathcal{F} \to \mathcal{F}$ defined by

$$\{F, G\} := \sum_{k=1}^{N-1} \frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k} - \frac{\partial F}{\partial p_k}\frac{\partial G}{\partial q_k}$$

$\mathcal{F}$ is a so-called graded Lie-algebra, which means that $\{\mathcal{F}_r, \mathcal{F}_s\} \subset \mathcal{F}_{r+s-2}$. With this definition, we have for each $F \in \mathcal{F}$, the 'adjoint' linear operator

$$\mathrm{ad}_F : \mathcal{F} \to \mathcal{F} \ , \ G \mapsto \{F, G\}$$

We recall the following result, a complete proof of which can be found for instance in [6], [7] and [12]. It proceeds by constructing a sequence of symplectic "normal form transformations".

Theorem 4.1 (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 $H_r \in \mathcal{F}_r$ for each r and*

$$\mathrm{ad}_{H_2} : G \mapsto \{H_2, G\} \ , \ \mathcal{F}_r \to \mathcal{F}_r$$

is semi-simple (i.e. complex-diagonalizable) for every r. Then for every finite $s \geq 3$ 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

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

where

$$\mathrm{ad}_{H_2}(\overline{H}_r) = 0$$

for every $3 \leq r \leq s$. The transformed and truncated Hamiltonian $\overline{H} := H_2 + \overline{H}_3 + \ldots + \overline{H}_s$ is called a Birkhoff normal form of H of order s.

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 $t \mapsto e^{tX_{H_2}}$ is a continuous symmetry of $\overline{H}$.

Also, H and $\overline{H}$ are symplectically equivalent modulo a small perturbation of order $\mathcal{O}(||(Q, P)||^{s+1})$. 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 $||(Q, P)||$. With Gronwall's lemma, precise error estimates can be made.

Finally, I would like to mention the ill-known bijective correspondence between the relative equilibria of the Birkhoff normal form and the bifurcation equations for periodic solutions obtained by Lyapunov-Schmidt reduction, as is explained in [8].

For Hamiltonian systems with symmetry, the following elegant and well-known result is often useful, see [6] and [12]:

Theorem 4.2 *Let $H = H_2 + H_3 + \ldots \in \mathcal{F}$ and G be a group of linear symplectic symmetries of H. Then a normal form $\overline{H} = H_2 + \overline{H}_3 + \ldots + \overline{H}_s$ for H can be constructed such that also $\overline{H}$ is G-symmetric.*

This result follows as the normal form transformation of Theorem 4.1 can be chosen G-symmetric.

We shall also rely on the following result on normal forms of symmetric subsystems, which trivially follows from Proposition 2.1 and the proof of Theorem 4.2, as symmetric normal form transformations leave fixed point subsets invariant.

Corollary 4.3 *Let H be a Hamiltonian function with compact symmetry group G consisting of linear symplectic mappings. 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.*

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

This corollary tells us that it is sufficient to compute the normal form of the full system to know the normal forms of its symmetric subsystems. In particular, to find the normal form of an FPU lattice with fixed endpoints, it suffices to know the normal form of the appropriate periodic lattice. Normal forms of periodic lattices have been studied elaborately in [23].

5 Nishida's conjecture

In his 1971 paper, Nishida proved the following result:

Theorem 5.1 (Proven by Nishida in [20]) *Consider the FPU lattice with fixed endpoints, $\alpha = 0$, $\beta \neq 0$ and n arbitrary. Assume moreover the fourth order nonresonance condition on the $\Omega_k = 2\sin(\frac{k\pi}{2n+2})$ $(1 \leq k \leq n)$ requiring that*

$$\sum_{k=1}^{n}(l_k - m_k)\Omega_k \neq 0 \; \forall \, l, m \in \{0, 1, 2, \ldots\}^n \text{ with } \sum_{k=1}^{n} |l_k| + |m_k| = 4 \text{ and } \sum_{k=1}^{n} |l_k - m_k| \neq 0$$

Then the quartic Birkhoff normal form $\overline{H} = H_2 + \overline{H}_4$ of the lattice is a function of the action variables $a_k := E_k/\Omega_k$ $(1 \leq k \leq n)$ only and is therefore integrable. Moreover it satisfies the Kolmogorov nondegeneracy condition

$$\det \frac{\partial^2 \overline{H}}{\partial a_k \partial a_{k'}} \neq 0$$

This implies that almost all low-energy solutions of the β-lattice with fixed endpoints are quasi-periodic and move on invariant tori. More precisely, the relative Lebesgue measure of all these tori lying inside the small ball $\{0 \leq H \leq \varepsilon\}$, goes to 1 as ε goes to 0.

It turns out that the numbers

$$\sum_{k=1}^{n}(l_k - m_k)\Omega_k \ , \ \text{for} \ \sum_{k=1}^{n} |l_k| + |m_k| = 4$$

are simply the eigenvalues of ad_{H_2} on $\mathcal{F}_4$. Nishida's requirement that they be nonzero except in the trivial case that $l_k = m_k$ for all k thus just means that the subspace $\ker \mathrm{ad}_{H_2} \in \mathcal{F}_4$ in which $\overline{H}_4$ must lie is very low-dimensional. It must therefore be remarked here that the integrability of the normal form follows almost trivially from Nishida's nonresonance assumption. Nishida's article consists mainly of the explicit computation of the normal form $\overline{H}$ of H under the nonresonance assumption in order to check its nondegeneracy.

But unfortunately, resonances do occur, implying that Nishida's nonresonance condition is often violated. We have for instance the relations

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

$$\sin(\pi/6) + \sin(13\pi/30) - \sin(7\pi/30) - \sin(3\pi/10) = 0$$

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

which lead to a violation of Nishida's nonresonance condition if $n+1$ is a multiple of 21 or 15.

Nishida refers to an unpublished result of Izumi proving a much stronger nonresonance condition on the Ω_k in special cases. The result states that no $\mathbb{Z}$-linear relations between the Ω_k exist if $n+1$ is a prime number or a power of 2. I was not able to trace back Izumi's proof of this statement, but note that a more general result had already been obtained in 1959 by Hemmer [14], who actually derived an expression for the total number of independent $\mathbb{Z}$-linear relations between the Ω_k $(1 \leq k \leq n)$ in terms of Euler's phi-function. It turns out that no $\mathbb{Z}$-linear relations exist if and only if $n+1$ is a prime number or a power of 2.

Moreover, as the above examples illustrate, resonance relations between 4 eigenvalues exist for several n and Nishida's condition is therefore sometimes violated. In this paper we will nevertheless sketch a proof of 'Nishida's conjecture' that his theorem holds without having to impose any nonresonance condition.

6 Near-integrability

Let us start with a review of some observation in [23] for the periodic FPU lattice. First of all we note that, as the symmetry R is symplectic,

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

where we have used that H_2 is R-symmetric. From this result we read off that R^* and ad_{H_2} commute as linear operators $\mathcal{F}_r \to \mathcal{F}_r$, which means that they can be diagonalized simultaneously. In [23] this diagonalisation is accomplished with respect to the basis of monomials for $\mathcal{F}_r$. This is made explicit by introducing new canonical coordinates by a linear map $(Q,P) \mapsto (z,\zeta), T^*\mathbb{C}^N \to T^*\mathbb{C}^N$. The coordinates (z,ζ) could be call "superphonons". Their explicit definition is given in [25].

One can show that indeed ad_{H_2} and R^* act on monomials as follows: if $\Theta, \theta \in \{0,1,2,\ldots\}^{N-1}$ are multi-indices, then

$$\begin{aligned} \mathrm{ad}_{H_2} : z^\Theta \zeta^\theta &\mapsto \nu(\Theta,\theta) z^\Theta \zeta^\theta \\ R^* : z^\Theta \zeta^\theta &\mapsto e^{\frac{2\pi i \mu(\Theta,\theta)}{N}} z^\Theta \zeta^\theta \end{aligned}$$

in which ν and μ are defined as

$$\nu(\Theta,\theta) := \sum_{1 \leq k < \frac{N}{2}} i\omega_k(\theta_k - \theta_{N-k} - \Theta_k + \Theta_{N-k}) \; + i\omega_{\frac{N}{2}}(\theta_{\frac{N}{2}} - \Theta_{\frac{N}{2}}) \tag{6.1}$$

$$\mu(\Theta,\theta) := \sum_{1 \leq k < \frac{N}{2}} j(\Theta_k + \Theta_{N-k} - \theta_k - \theta_{N-k}) + \frac{N}{2}(\Theta_{\frac{N}{2}} - \theta_{\frac{N}{2}}) \mod N \tag{6.2}$$

First of all, this shows that ad_{H_2} and R^* are diagonal with respect to the basis of $\mathcal{F}_r$ consisting of the monomials $z^\Theta \zeta^\theta$ for which $|\Theta|+|\theta| := \sum_{j=1}^{N-1} |\Theta_j|+|\theta_j| = r$ and the corresponding eigenvalues are the $\nu(\Theta,\theta)$ and $e^{\frac{2\pi i\mu(\Theta,\theta)}{N}}$ respectively. In particular we observe that ad_{H_2} is semi-simple on every $\mathcal{F}_r$, so that Theorem 4.1 indeed applies. A $\mathbb{Z}$-linear relation in the frequencies ω_k is called a *resonance*. For this reason, the monomials $z^\Theta\zeta^\theta$ for which $\nu(\Theta,\theta)=0$ are called resonant monomials. They are important because they are exactly the ones that are not in im ad_{H_2} and thus, as is clear from Theorem 4.1, the ones that cannot be transformed away by Birkhoff normalisation. As $\Omega_k=\omega_k (1\le k\le n)$, Nishida's nonresonance condition would be a consequence of its analogon for periodic lattices, that can be formulated as follows:

'*When* $|\Theta|+|\theta|=4$ *and* $\nu(\Theta,\theta)=0$ *then* $\theta_{\frac{N}{2}}-\Theta_{\frac{N}{2}}=0$ *and* $\theta_k-\theta_{N-k}-\Theta_k+\Theta_{N-k}=0$ *for each* $1\le k<\frac{N}{2}$*.*'

Of course, this condition is not valid either.

By Theorem 4.2 we now know that the normal form of the periodic FPU Hamiltonian must be a linear combination of monomials $z^\Theta\zeta^\theta$ that are both resonant and symmetric, i.e. for which $\nu(\Theta,\theta)=0$ and $\mu(\Theta,\theta)=0 \mod N$. The following theorem was proven in [23].

Theorem 6.1

i) The set of multi-indices $(\Theta,\theta)\in\mathbb{Z}^{N-1}_{\ge 0}$ *for which* $|\Theta|+|\theta|=3,\ \mu(\Theta,\theta)=0$ *mod* N *and* $\nu(\Theta,\theta)=0$ *is empty.*

ii) The set of multi-indices $(\Theta,\theta)\in\mathbb{Z}^{N-1}_{\ge 0}$ *for which* $|\Theta|+|\theta|=4,\ \mu(\Theta,\theta)=0$ *mod* N *and* $\nu(\Theta,\theta)=0$ *is contained in the set defined by the relations* $\theta_k-\theta_{N-k}-\Theta_k+\Theta_{N-k}=\theta_{\frac{N}{2}}-\Theta_{\frac{N}{2}}=0$*.*

The proof of this result relies heavily on the number theoretic properties of the eigenvalues $\omega_k=2\sin(k\pi/N)$. In fact, the proof involves a full classification of third and fourth order resonance relations in the FPU eigenvalues, that is given in the Appendix to [23].

We have seen that resonance relations lead to several nontrivial resonant monomials. But according to Theorem 6.1 we now know that these nontrivial resonant monomials are not R-symmetric and hence cannot occur in the normal form of the periodic FPU lattice.

As a result, we see that there are no nonzero elements of $\mathcal{F}_3$ that are both resonant and R-symmetric. Hence $\overline{H}_3=0$ automatically. Also, the space ker $\mathrm{ad}_{H_2}\cap\mathcal{F}_4$ in which $\overline{H}_4$ has to lie, is quite low-dimensional.

7 Integrability of the normal form

In the previous section we saw, without computing $\overline{H}_3$ explicitly, that it must be zero for the Hamiltonian of the periodic FPU lattice, irrespective of α,β and n. By Corollary 4.3, we can therefore conclude that $\overline{H}_3=0$ for every FPU lattice with fixed endpoints, despite the resonances in the eigenvalues of the fixed endpoint chain.

Similarly, one can hope to understand the structure of $\overline{H}_4$ for the FPU lattice with fixed endpoints by studying the $\overline{H}_4$ of the corresponding periodic FPU lattice.

Theorem 6.1 above told us that the latter satisfies serious restrictions. Indeed it turns out that, despite fourth order resonances, the $\overline{H}_4$ of the fixed endpoint lattice is very simple.

Theorem 7.1 (Conjectured by Nishida in [20]) *Independent of n, α and β, the quartic Birkhoff normal form $\overline{H} = H_2 + \overline{H}_4$ of the FPU lattice with fixed endpoints (3.3) is integrable with integrals E_k $(1 \leq k \leq n)$, defined in (3.2).*

The details of the proof of this corollary are given in [25]. The idea of the proof is very simple: Theorem 6.1 tells us which monomials of order 4 are invariant under R^* and lie in $\ker \mathrm{ad}_{H_2}$. The restriction of each of these monomials to $\mathrm{Fix}\langle S\rangle$ turns out to be a function of the variables E_k $(1 \leq k \leq n)$. We will not repeat the proof here.

Note that the integrability of the normal form of the fixed endpoint lattice is caused by a *hidden* symmetry, i.e. by the symmetry of the periodic lattice in which it is embedded. It must also be remarked here that it is very exceptional for a high-dimensional resonant Hamiltonian system to have an integrable normal form.

The dynamics of the truncated normal form $H_2 + \overline{H}_4$ is very simple. In fact, the regular level sets of the integral map $E : T^*\mathbb{R}^n \to \mathbb{R}^n$ that sends $(Q, P) \mapsto (E_1, \ldots, E_n)$ are smooth n-dimensional tori on which the flow of the normal form can be computed by a transformation to action-angle coordinates $(Q, P) \mapsto (a, \varphi)$. More explicitly, 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

$$\varphi_k = \arg(P_k, \Omega_k Q_k) \ , \ a_k = E_k/\Omega_k = \frac{1}{2\Omega_k}(P_k^2 + \Omega_k^2 Q_k^2) \ , \ 1 \leq k \leq n$$

Then (φ, a) are canonical coordinates: $dQ \wedge dP = d\varphi \wedge da$. So in these coordinates the equations of motion read

$$\dot{a}_k = 0 \ , \ \dot{\varphi}_k = \Omega_k + \frac{\partial \overline{H}_4(a)}{\partial a_k}$$

This simply defines periodic or quasi-periodic motion. Remark: (ϕ, a) are sometimes called 'symplectic polar coordinates'.

8 Nondegeneracy

To verify that the normal form $\overline{H}$ is nondegenerate in the sense of the KAM theorem, we examine the frequency map Ω which assigns to each invariant torus the frequencies of the flow on it:

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

The nondegeneracy condition requires that Ω be a local diffeomorphism, which is the case 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, one needs to compute the Birkhoff normal form explicitly, where until now we had been able to avoid this. In the next theorem we shall present the normal form of the FPU Hamiltonian in the case that $H_3 = 0$, i.e. $\alpha = 0$. This lattice, that has no cubic terms, is usually referred to as the β-lattice.

Theorem 8.1 (Conjectured by Nishida in [20]) *If $\alpha = 0$, then a quartic Birkhoff normal form of FPU lattice with fixed endpoints is given by $\overline{H} = H_2 + \overline{H}_4$, where*

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

This simply follows from a long computation such as presented in [23], [26], [27], [15] and [16] of the normal form of the β-lattice with periodic boundary conditions and restricting it to $\mathrm{Fix}\langle S\rangle$. The result was also obtained directly for the fixed endpoint lattice by Nishida in [20] under his nonresonance assumption.

It is easy to prove the invertibility of the matrix $\frac{\partial^2 \overline{H}_4}{\partial a_k \partial a_{k'}}$. Its nondegeneracy was also checked by Nishida himself by applying elementary row and column operations to compute the determinant that turns out to be nonzero. Thus we conclude:

Corollary 8.2 (Conjectured by Nishida in [20]) *If $\alpha = 0$ and $\beta \neq 0$, then the integrable quartic Birkhoff normal form $\overline{H} = H_2 + \overline{H}_4$ of the FPU lattice with fixed endpoints (3.3) 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 $\{0 \le H \le \varepsilon\}$, goes to 1 as ε goes to 0.*

Nishida, and we, chose to compute normal form $H_2 + \overline{H}_4$ only for the β-lattice. This computation is already quite long, but it becomes even harder when $\alpha \neq 0$. It should nevertheless also be possible to write down an expression for the fixed endpoints normal form if $\alpha \neq 0$. For checking Kolmogorov's condition this will actually be necessary. We know a priori that the resulting normal form will be integrable and depends quadratically on the E_k. Preliminary results by Henrici and Kappeler, partially referred to in [15] and [16] seem to prove exactly what one expects, namely that Kolmogorov's nondegeneracy condition is satisfied for 'generic' α and β.

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