A SYMMETRIC NORMAL FORM FOR THE FERMI PASTA ULAM CHAIN

BOB RINK
Mathematics Institute, Utrecht University, PO Box 80.010, 3508 TA Utrecht, The Netherlands
E-mail: rink@@math.uu.nl

The Fermi Pasta Ulam chain with periodic boundary conditions admits discrete and continuous symmetries. These symmetries allow one to formulate important restrictions on the Birkhoff normal form of this Hamiltonian system. We derive integrability properties and KAM statements. Hence the combination of symmetry and resonance in the periodic Fermi Pasta Ulam chain explains its quasiperiodic behaviour. This article contains a summary of the results obtained in references [11] and [12]

1 Introduction

The Fermi Pasta Ulam chain with periodic boundary conditions is a model for point masses moving on a circle with nonlinear forces acting between the nearest neighbours. Let us set $q_j \in \mathbb{R}$ to be the position of the j-th particle ($j = 1, \ldots, n$) with respect to a certain reference position on the circle. The space of positions $q = (q_1, \ldots, q_n)$ of the particles in the chain is $\mathbb{R}^n$. The space of positions and conjugate momenta is the cotangent bundle $T^*\mathbb{R}^n$ of $\mathbb{R}^n$, the elements of which are denoted $(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n)$. $T^*\mathbb{R}^n$ is a symplectic manifold, endowed with the symplectic form $dq \wedge dp = \sum_{j=1}^n dq_j \wedge dp_j$. Any smooth function $H : T^*\mathbb{R}^n \to \mathbb{R}$ now induces the Hamiltonian vector field X_H given by the defining relation $\iota_{X_H}(dq \wedge dp) = dH$. In other words, we have the system of ordinary differential equations $\dot{q}_j = \frac{\partial H}{\partial p_j}$, $\dot{p}_j = -\frac{\partial H}{\partial q_j}$. The periodic FPU chain with n particles is the special Hamiltonian system on $T^*\mathbb{R}^n$ corresponding to the real analytic Hamiltonian

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

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

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

The $\alpha, \beta, \ldots$ are real parameters measuring the nonlinearity in the forces between the particles in the chain.

Numerically, the FPU system was first studied by E. Fermi, J. Pasta and S. Ulam [5]. These authors used the chain to model a nonlinear string. They expected that in the presence of small nonlinearities, the chain would show ergodic behaviour, meaning that almost all orbits densely fill up an energy levelset of the Hamiltonian. Ergodicity would eventually lead to an equal distribution of energy between the various Fourier modes of the system, a concept called *thermalisation*. FPU's nowadays famous numerical experiment was intended to investigate at what time scale thermalisation would take place. The result was astonishing: it turned out that there was no sign of thermalisation at all. Putting initially all the energy in one Fourier mode, they observed that this energy was shared by only a few other modes, the remaining modes were hardly excited. Additionally, within a not too long time the system returned close to its initial state.

In 1965 an article of Zabuski and Kruskal [15] appeared. These authors considered the Korteweg-de Vries equation as a continuum limit of the FPU chain and numerically found the first indications for the stable behaviour of solitary waves. We now know that the Korteweg-de Vries equation is integrable [9]. This clearly suggests an explanation for FPU's observations, although the relation between the FPU chain and its infinite dimensional limits has never been understood.

Another, possibly correct explanation for the quasiperiodic behaviour of the FPU system, is based on the Kolmogorov-Arnol'd-Moser theorem. As is well-known [2], the solutions of an n degrees of freedom Liouville integrable Hamiltonian system are constrained to move on n-dimensional tori and are not at all ergodic but periodic and quasiperiodic. The KAM theorem states that most of the invariant tori of this integrable system persist under small Hamiltonian perturbations, if the unperturbed integrable system satisfies a certain nondegeneracy condition. This nondegeneracy condition states that the frequency map, which assigns to each n-dimensional invariant torus of the integrable system the n-dimensional vector of frequencies of the (quasi)periodic motion on this torus, be a local diffeomorphism. Although several authors, starting with Izrailev and Chirikov [7], have stated that the KAM theorem explains the observations of the FPU experiment, it is still completely unclear how the FPU system can be seen as a perturbation of a nondegenerate integrable system. One could only view it as a perturbation of a harmonic oscillator, but the frequency map of the harmonic oscillator is constant and hence degenerate. This gap in the theory was recently mentioned again in the review article of Ford [6] and the book of Weissert [14].

The only serious attempt to overcome this problem was made in 1971 in a paper by Nishida [8]. Unlike us, this author considers an FPU chain with fixed endpoints. Under a rather strong nonresonance condition on the linear frequencies of his system, he shows that there is a nonlinear symplectic near-identity transformation of phase space, the 'Birkhoff transformation', with the following property: written out in the new coordinates, the Hamiltonian function of the FPU chain turns out to be a perturbation of a nondegenerate integrable system. And hence the KAM theorem can be applied. The weakness of this argument lies of course in the fact that the linear frequencies actually do not satisfy the imposed nonresonance condition.

Sanders [13] does a similar thing for FPU chains with periodic boundary conditions and an odd number of particles. Assuming a nonresonance condition, he observes that the normal form is again integrable, but he does not verify the KAM nondegeneracy condition.

In this short paper I shall give a summary of the results that F. Verhulst and I [11] [12] obtained in trying to generalise the work of Nishida and Sanders. In particular, we computed all the lower order resonance relations in the eigenvalues of the linearized FPU chain. And secondly, we exploited the discrete symmetries of the periodic FPU chain to show that its Birkhoff normal form has some very special properties. In a lot of the cases, one can actually prove that it is integrable or even satisfies the KAM nondegeneracy condition. We do not impose any nonresonance condition. For more details concerning the calculation, the reader should of course consult the original references [11] and [12].

2 The linear system

One would like to view the solutions of the equations induced by (1.1) as a superposition of sine and consine wave forms. Therefore, one usually applies a Fourier transformation $(q,p) \mapsto (\bar{q},\bar{p})$. The new coordinates $(\bar{q},\bar{p})$ are called 'phonons' or 'quasi-particles'. The transformation to phonons is a linear symplectic point transformation. We omit the transformation matrix here. See [11] or [12] for the exact formulas. The transformation is such that when written out in phonon-coordinates, the FPU Hamiltonian reads

$$H = \sum_{j=1}^{n-1} \frac{1}{2}(\bar{p}_j^2 + \omega_j^2 \bar{q}_j^2) + H_3(\bar{q}_1, \ldots, \bar{q}_{n-1}) + H_4(\bar{q}_1, \ldots, \bar{q}_{n-1}) + \ldots \qquad (2.1)$$

where H_k ($k = 2, 3, \ldots$) denotes the k-th order part of H. For $j = 1, \ldots, n-1$, the numbers ω_j are the eigenvalues of the linear periodic FPU problem:

$$\omega_j := 2 \sin(\frac{j\pi}{n}) \ . \tag{2.2}$$

Expressions for H_3 and H_4 in terms of the $\bar{q}_j$ can be found in the literature, cf. [10]. We do not repeat them.

Note that the new Hamiltonian has $n-1$ degrees of freedom instead of n, because simultaneously with introducing the phonons, we divided out the symmetry induced by the flow of the total momentum $p_1 + \ldots + p_n$, which is a constant of motion. More details can be found in [11]. The Hamiltonian (2.1) on $T^*\mathbb{R}^{n-1}$ represents the periodic FPU system from which the centre of mass motion has been eliminated.

Since $\omega_j^2 > 0$ ($1 \leq j \leq n-1$), using the Morse-Lemma [1] we conclude that the level sets of H are $2n-3$ dimensional spheres around the origin of $T^*\mathbb{R}^{n-1}$. Since H is a constant of motion for the flow of X_H, the origin is a stable stationary point for the system induced by (2.1). It corresponds to an equidistant configuration of the particles.

3 Birkhoff normalisation

From (2.1) we see that the solutions of the linearized FPU system are simply superpositions of pulsating wave forms. But in the full nonlinear system the Fourier modes can exchange energy. We shall study this much harder system using Birkhoff normalisation, hoping to be able to apply KAM theory and bifurcation methods.

The setting of normalisation is the following. Let P_k be the space of homogeneous polynomials of degree k in the canonical variables ($\bar{q}_1, \ldots, \bar{q}_{n-1}, \bar{p}_1, \ldots, \bar{p}_{n-1}$). The space of all convergent power series without linear part is denoted $P \subset \bigoplus_{k \geq 2} P_k$. P is a Lie-algebra under the usual Poisson bracket $\{f, g\} = dq \wedge dp(X_f, X_g)$. Finally, for each $f \in P$ one defines the adjoint operator $\mathrm{ad}_f : P \to P$ which maps $\mathrm{ad}_f : g \mapsto \{f, g\}$. Note that when $\mathrm{ad}_f(g) = \{f, g\} = 0$, then the flows of X_f and X_g commute. The following result is well-known:

Theorem 3.1 (Birkhoff) *Let $r > 2$ be a given natural number. Assume that $H = \sum_{k=2}^{\infty} H_k \in P$ is such that for each $3 \leq k \leq r$, $\mathrm{ad}_{H_2} : P_k \to P_k$ is semisimple, i.e. complex diagonalisable. Then there is an open neighborhood $U \in T^*\mathbb{R}^{n-1}$ of the origin and an analytic symplectic diffeomorphism $\Psi : U \to \Psi(U) \subset T^*\mathbb{R}^{n-1}$ such that $\Psi(0) = 0$, $D\Psi(0) = Id$ and $\overline{H} := H \circ \Psi =$*

$\sum_{k=2}^{\infty} \overline{H}_k \in P$ *has the properties that* $\overline{H}_2 = H_2$ *and* $ad_{H_2}(\overline{H_k}) = \{H_2, \overline{H}_k\} = 0$ *for all* $2 \leq k \leq r$.

The transformed Hamiltonian $\overline{H}$ is called a Birkhoff normal form for H of order r. It can be determined following a rather explicit procedure, which the reader can find in [3] and [11]. It is usually impossible to push r to infinity.

In the case of the periodic FPU Hamiltonian (2.1), $\mathrm{ad}_{H_2} : P_k \to P_k$ is indeed semisimple and its eigenvalues are the numbers

$$\sum_{j=1}^{n-1} i\omega_j(\eta_j - \theta_j) \quad . \tag{3.1}$$

where η, θ are $n-1$-dimensional multi-indices with the property that $|\eta| + |\theta| := \sum_{j=1}^{n-1} |\eta_j| + |\theta_j| = k$.

It is important to study the kernel of ad_{H_2} because this kernel contains all possible normal forms of the FPU chain. Therefore we wonder whether some of the eigenvalues (3.1) are zero. In this case we speak of 'resonance'. There are some trivial resonance relations: choose for instance $\eta_j = \theta_j$. Note also that from (2.2) it follows that $\omega_j = \omega_{n-j}$. This yields even more rather trivial 1:1 resonances.

Are there more resonance relations?

Nishida [8] and Sanders [13] had to make the assumption that weren't any, although in fact there are. Using Galois theory, we calculated all the resonance relations for which $|\eta| + |\theta| = 3, 4$. We got substantial help from Frits Beukers at this point. To give the reader some feeling for the type of resonance relations we found, we give two of them here:

$$2\sin\frac{\pi}{6} - \sin\frac{3\pi}{6} = 0 \quad \text{and} \quad \sin\frac{5\pi}{30} + \sin\frac{13\pi}{30} - \sin\frac{7\pi}{30} - \sin\frac{9\pi}{30} = 0 \ .$$

The first one is rather trivial, but the second is not. Nishida [8] and Sanders [13] were worried that this type of nontrivial resonances could spoil their normal form results. It is therefore very surprising that these resonances turn out to be completely harmless. This is caused by discrete symmetries.

4 Discrete symmetry

Consider the following maps in the space of positions of the particles:

$$T : \partial_{q_j} \mapsto \partial_{q_{j-1}} \quad \text{and} \quad S : \partial_{q_j} \mapsto -\partial_{q_{n-j}} \tag{4.1}$$

T and S represent permutations that rotate and flip the particles respectively. They can be extended to symplectic point transformations on $T^*\mathbb{R}^n$. These point transformations, which we shall also denote T and S, leave the Hamiltonian of the periodic FPU problem (1.1) invariant: $T^*H := H \circ T = H$ and $S^*H := H \circ S = H$. This implies that the Hamiltonian vector field X_H induced by H is equivariant under T and S. Therefore, T and S are called discrete symmetries of H. The group $\langle T, S \rangle$ generated by T and S is isomorphic to the n-th dihedral group, the symmetry group of the n-gon.

Finally, S and T project to symmetries of the reduced Hamiltonian (2.1).

5 The symmetric normal form

A crucial observation, which was brought to our attention by J.J. Duistermaat, is that one can construct Birkhoff normal forms, that respect these symmetries. In other words, one can choose to make normal forms that have the same symmetries as the Hamiltonian one started out with. For a proof of this statement, the reader can consult [3].

In the case of the FPU chain with periodic boundary conditions, this means that the nonquadratic terms of the normal form $H_2 + \overline{H}_3 + \overline{H}_4 + \ldots$ satisfy

$$\mathrm{ad}_{H_2}(\overline{H}_k) = 0 \ , \ (T^* - \mathrm{Id})(\overline{H}_k) = 0 \text{ and } (S^* - \mathrm{Id})(\overline{H}_k) = 0 \ . \qquad (5.1)$$

In other words, $\overline{H}_k$ is in the joint kernel of the linear operators $\mathrm{ad}_{H_2}, T^* - \mathrm{Id}$ and $S^* - \mathrm{Id}$ and it is our task to determine this joint kernel. This is the computation that constitutes the main part of [12]. Note that we already know what the kernel of ad_{H_2} is, as we have already calculated all the resonances. In the computation of the joint kernel one uses the fact that ad_{H_2} and $T^* - \mathrm{Id}$ commute to search inside the kernel of ad_{H_2} for degenerate directions of $T^* - \mathrm{Id}$. The invariance under S^* is then used to refine the results. I list the most important conclusions here:

1 The set of homogeneous third order polynomials that satisfy (5.1) is $\{0\}$. So $\overline{H}_3 = 0$ for the periodic FPU chain, independent of the number of particles n and the resonances in the eigenvalues.

2 If the number of particles n is odd, then the truncated normal form $H_2 + \overline{H}_4$ is Liouville integrable. The integrals are quadratic and constitute global action-angle coordinates. This is true for every homogeneous fourth order polynomial that satisfies (5.1), so we conclude it for the FPU chain without even calculating its normal form.

3 If the number of particles n is even, then we give a lot of integrals of the truncated normal form $H_2 + \overline{H}_4$, again without computing the normal form. But we can not prove Liouville integrability this way.

Just like Nishida [8] and Sanders [13], we explicitly calculated the normal form of the so-called β-chain, for which the nonlinearity-coefficient α is zero. This yields even more information:

4 If n is odd, then the truncated normal form $H_2 + \overline{H}_4$ of the β-chain satisfies the KAM nondegeneracy condition. Since the original system can be seen as a perturbation of this truncated normal form, the conclusions of the KAM theorem hold. We proved that most low energy solutions of the odd β-chain lie on tori.

5 If n is even, then the truncated normal form $H_2 + \overline{H}_4$ of the β-chain turns out to be Liouville integrable too. We have no explanation of this in terms of symmetries. It is very difficult to check the KAM condition in this case, since we have no expression for the action-angle coordinates. In fact, there are strong indications that global action-angle coordinates do not exist in this case. On the other hand, the integrability of the normal form makes one suspect that the KAM condition should actually hold.

Although we have a lot of results, there are obviously still many open questions.

6 Conclusion

The results of this paper might not immediately apply to the experiment of Fermi, Pasta and Ulam. First of all, these authors did not study a periodic chain. Secondly, it is not certain that the normal form approximation is still valid at the energy level they chose in their experiment.

But still, the special combination of the eigenvalues and discrete symmetries of the FPU problem might be the true reason for the observations that Fermi, Pasta and Ulam did.

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