# Symmetry and resonance in periodic FPU chains

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### 31st August 2000

### Abstract

The symmetry and resonance properties of the Fermi Pasta Ulam chain with periodic boundary conditions are exploited to construct a near-identity transformation bringing this Hamiltonian system into a particularly simple form. This 'Birkhoff-Gustavson normal form' retains the symmetries of the original system and we show that in most cases this allows us to view the periodic FPU Hamiltonian as a perturbation of a nondegenerate Liouville integrable Hamiltonian. According to the KAM theorem this proves the existence of many invariant tori on which motion is quasiperiodic. Experiments confirm this qualitative behaviour. We note that one can not expect it in lower-order resonant Hamiltonian systems. So the FPU chain is an exception and its special features are caused by a combination of special resonances and symmetries.

**Keywords:** periodic FPU chain, symmetry, resonance, Birkhoff-Gustavson normal form, near-integrability, KAM theorem

## 1 Introduction

The *n* particles FPU chain with periodic boundary conditions is a model for point masses moving on a circle with nonlinear forces acting between the nearest neighbours. It is in fact the *n* degrees of freedom Hamiltonian system on  $\mathbb{R}^{2n}$  induced by the real-analytic Hamiltonian

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

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

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

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

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Numerically, the FPU system was first studied by E. Fermi, J. Pasta and S. Ulam, see [4]. These authors used the chain as a model for a string of which the elements interact in a nonlinear way. 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-level set 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 timescale 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. On increasing the strength of the nonlinearity, this recurrence occurred even earlier. Later computations, e.g. described in [9], confirmed that the same phenomena can also be observed in very large periodic chains. Empirical evidence was found that for small total energy, normal mode energies are hardly shared. Ergodic behaviour can only be observed when the energy level passes a certain critical value.

In 1965 an article of Zabuski and Kruskal appeared, cf. [17]. 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, thereby suggesting an explanation for the striking data of the FPU experiment. In 1967, Gardner, Greene, Kruskal and Miura ([6]) discovered infinitely many conserved quantities for the KdV equation, which should account for the regular behaviour of its solutions. Reference [10] contains a good overview of these results. They are suggestive, but do not provide a full explanation of FPU's observations as the impact of the transition from a discrete to a continuous chain has never been analysed.

There is another, possibly correct explanation for the quasiperiodic behaviour of the FPU system. It is based on the Kolmogorov-Arnol'd-Moser (KAM) theorem (cf. [2]) and different from the Zabuski-Kruskal argument, it should work especially well for chains with a low number of particles. As is well-known (cf. [2]), the general solution of an n degrees of freedom Liouville integrable Hamiltonian system is constrained to move in an n-dimensional torus and is not at all ergodic but periodic or quasiperiodic. The KAM theorem states that most of the invariant tori of a nondegenerate integrable system persist under small Hamiltonian perturbations. Thus many authors, starting with Izrailev and Chirikov in [7], have stated that the KAM theorem explains the observations of the FPU experiment. This reasoning seems plausible, but, as was clearly pointed out by Ford in [5], it is still completely unclear why the FPU system should be a perturbation of such a nondegenerate integrable system. This gap in the theory was recently mentioned again in the book of Weissert ([16]).

What does 'nondegenerate' mean here? Let us consider the frequency map  $\omega$ , which assigns to each n-dimensional invariant torus of a Liouville integrable system the n-dimensional vector of frequencies of the (quasi)periodic motion on this torus. An integrable system is called 'nondegenerate' if  $\omega$  is a local diffeomorphism. The KAM theorem holds for perturbations of these nondegenerate integrable systems.

But it is no exception for an integrable system to be degenerate. A common example is the harmonic oscillator of which the frequency map is constant: the harmonic

oscillator is highly degenerate. And indeed, perturbations of it are known that are ergodic even on low-energy level sets of the Hamiltonian. Ford gives a nice example of such a perturbation in his review article [5]. We conclude that, although the FPU Hamiltonian can be considered as a perturbation of an integrable system -namely the harmonic oscillator-, the KAM theorem does not apply here!

The aim of this paper is to overcome this problem. The method we use to do so is called *Birkhoff-Gustavson normalisation* - it is sometimes also called *resonant normalisation*. It provides a transformation of phase space that in many cases enables us to write the periodic FPU Hamiltonian as a perturbation of a nondegenerate integrable Hamiltonian.

It must be stressed that it seems highly exceptional that one can do this for a resonant Hamiltonian system such as the periodic FPU chain. The current paper intends to make clear that the special symmetry, eigenvalue and resonance characteristics of the periodic FPU system play a crucial role in the construction of the near-identity transformation. It turns out that these characteristics cause the nondegenerate near-integrability of the chain. The conclusion is that the KAM theorem applies because of these resonance and symmetry properties: the quasiperiodic behaviour that Fermi, Pasta and Ulam observed is in some sense an exceptional feature of the FPU system.

## 1.1 Outline of the paper

This paper is a continuation of [12] in which normal forms of small chains are computed and the KAM theorem is verified. We generalize and explain the results of [12] in this paper.

In sections 2-6 the necessary theory is formulated. We start with an investigation of the eigenvalues (section 2) and the discrete symmetries (section 4) of the periodic FPU chain. The concept of a Birkhoff-Gustavson normal form as an approximation of a Hamiltonian system is explained in section 5. It will be shown that normal forms for the periodic FPU chain exist that inherit its symmetry properties.

In the appendix, which is based on notes of Beukers, number theory is used to compute all lower order resonances in the eigenvalues. We exploit this in sections 7 and 8 to prove theorem 8.2, which forms the core of this paper: it gives the restrictions that the Birkhoff-Gustavson normal form of any Hamiltonian with the same eigenvalues and symmetries as the periodic FPU chain, is subject to.

These restrictions on the normal form allow us to point out many near-integrals of the chain in section 9. We finish with an analysis of the  $\beta$ -chain, which is proved to be near-integrable in section 10. The KAM nondegeneracy condition can easily be checked when the  $\beta$ -chain contains an odd number of particles. Some open questions are formulated for the even  $\beta$ -chain.

# 1.2 Acknowledgement

The author thanks Frits Beukers, Richard Cushman, Hans Duistermaat, Reinout Quispel, Theo Tuwankotta and Ferdinand Verhulst for useful ideas, comments and discussions.

## 2 Phonons

To establish the sign conventions that we shall stick to during our analysis, some basic definitions follow here. For further reading on Hamiltonian systems and a thorough explanation of these concepts, the reader is referred to [1].

We shall be considering Hamiltonian systems of differential equations on  $\mathbb{R}^{2n}$ , the elements of which are denoted by  $(q,p)=(q_1,\ldots,q_n,p_1,\ldots,p_n)$ . On  $\mathbb{R}^{2n}$  the symplectic form  $\sigma:=\sum_{j=1}^n dq_j\wedge dp_j$  is defined. Endowed with this symplectic form  $\mathbb{R}^{2n}$  is a symplectic space. Any Hamiltonian function  $H:\mathbb{R}^{2n}\to\mathbb{R}$  induces a Hamiltonian vector field  $X_H$  on  $\mathbb{R}^{2n}$  which is defined by  $\sigma(X_H,\cdot)=dH$ . Furthermore, for any two Hamiltonians F and G the Poisson brackets are defined as  $\{F,G\}:=\sigma(X_F,X_G)=dF\cdot X_G=-dG\cdot X_F$ .

Keeping these definitions in mind, we now start our analysis of the periodic FPU chain:

In order to facilitate the equations of motion induced by the periodic FPU Hamiltonian (1.1), we apply a well-known Fourier transformation  $(q,p) \mapsto (\bar{q},\bar{p})$ . For  $1 \leq j < \frac{n}{2}$  define

$$\bar{q}_{j} = \sqrt{\frac{2}{n}} \sum_{k=1}^{n} \cos(\frac{2jk\pi}{n}) q_{k} , \quad \bar{p}_{j} = \sqrt{\frac{2}{n}} \sum_{k=1}^{n} \cos(\frac{2jk\pi}{n}) p_{k} ,$$

$$\bar{q}_{n-j} = \sqrt{\frac{2}{n}} \sum_{k=1}^{n} \sin(\frac{2jk\pi}{n}) q_{k} , \quad \bar{p}_{n-j} = \sqrt{\frac{2}{n}} \sum_{k=1}^{n} \sin(\frac{2jk\pi}{n}) p_{k} . \tag{2.1}$$

Furthermore, define

$$\bar{q}_n = \frac{1}{\sqrt{n}} \sum_{k=1}^n q_k \ , \quad \bar{p}_n = \frac{1}{\sqrt{n}} \sum_{k=1}^n p_k \ ,$$
 (2.2)

and if n is even,

$$\bar{q}_{\frac{n}{2}} = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} (-1)^k q_k , \quad \bar{p}_{\frac{n}{2}} = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} (-1)^k p_k .$$
(2.3)

The new coordinates  $(\bar{q}, \bar{p})$  are known as 'phonons'. The transformation to phonons is symplectic, that is  $\sigma = \sum_{j=1}^{n} d\bar{q}_j \wedge d\bar{p}_j$ . For a proof, cf. [11] or [12]. In phonon-coordinates, the Hamiltonian reads

$$H = \sum_{j=1}^{n} \frac{1}{2} (\bar{p}_{j}^{2} + \omega_{j}^{2} \bar{q}_{j}^{2}) + H_{3}(\bar{q}_{1}, \dots, \bar{q}_{n-1}) + H_{4}(\bar{q}_{1}, \dots, \bar{q}_{n-1}) + \dots ,$$
(2.4)

in which  $H_k$  (k=2,3,...) denotes the k-th order part of H; for j=1,...,n, the numbers  $\omega_j$  are the eigenvalues of the linear periodic FPU problem:

$$\omega_j := 2\sin(\frac{j\pi}{n}) \ . \tag{2.5}$$

Exact expressions for  $H_3$  and  $H_4$  in terms of the  $\bar{q}_j$  can be found in the literature, cf. [11]. We do not repeat them.

The linearised equations are the equations induced by  $H_2$ . They read:

$$\bar{q}_{j}' = \bar{p}_{j}, \bar{p}_{j}' = -\omega_{j}^{2} \bar{q}_{j}.$$
 (2.6)

The  $\bar{q}_j, \bar{p}_j$   $(1 \leq j \leq n-1)$  are harmonics with frequency  $\omega_j$ ;  $\bar{p}_n$  is constant, whereas  $\bar{q}_n$  increases with constant speed -note that  $\omega_n = 0$ . In fact, the linearised equations are Liouville integrable, with integrals  $E_j := \frac{1}{2}(\bar{p}_j^2 + \omega_j^2 \bar{q}_j^2)$ . The nonlinear equations ( $\alpha$  or  $\beta$  unequal to zero) are much harder to analyse. The  $E_j$  are for instance no longer constants of motion.

# 3 Reduction of a continuous symmetry group

From (2.4) we see that H is independent of  $\bar{q}_n$ , even if  $\alpha, \beta, \ldots \neq 0$ . This implies that  $\bar{p}_n$  is an integral of H. The set  $\bar{p}_n^{-1}(\{0\})$  defines a 2n-1 dimensional hyperplane in  $\mathbb{R}^{2n}$ , invariant under the flow of both  $X_H$  and  $X_{\bar{p}_n}$ . The flow of  $X_{\bar{p}_n} = \frac{\partial}{\partial \bar{q}_n}$  induces a symplectic  $\mathbb{R}$ -action on this hyperplane. The time-t flow  $e^{tX_{\bar{p}_n}}$  is actually given by

$$e^{tX_{\bar{p}_n}}: \sum_{j=1}^n \left( \bar{q}_j \frac{\partial}{\partial \bar{q}_j} + \bar{p}_j \frac{\partial}{\partial \bar{p}_j} \right) \mapsto \sum_{j=1}^n \left( \bar{q}_j \frac{\partial}{\partial \bar{q}_j} + \bar{p}_j \frac{\partial}{\partial \bar{p}_j} \right) + t \frac{\partial}{\partial \bar{q}_n} , \qquad (3.1)$$

or written out in the original coordinates:

$$e^{tX_{\frac{1}{\sqrt{n}}\sum p_k}}: \sum_{j=1}^n \left(q_j \frac{\partial}{\partial q_j} + p_j \frac{\partial}{\partial p_j}\right) \mapsto \sum_{j=1}^{n-1} \left((q_j + \frac{t}{\sqrt{n}}) \frac{\partial}{\partial q_j} + p_j \frac{\partial}{\partial p_j}\right) . \tag{3.2}$$

The orbits of this flow are the lines  $(\bar{q},\bar{p})+\mathbb{R}\frac{\partial}{\partial \bar{q}_n}$ . It is clear that the 2n-2 dimensional hyperplane  $\bar{q}_n^{-1}(\{0\})\cap\bar{p}_n^{-1}(\{0\})\cong\mathbb{R}^{2n-2}$  is transversal to these orbits. Therefore,  $\mathbb{R}^{2n-2}$  is a model for the space  $\bar{p}_n^{-1}(\{0\})/\mathbb{R}$  of  $X_{\bar{p}_n}$ -orbits lying in  $\bar{p}_n^{-1}(\{0\})$ .  $\mathbb{R}^{2n-2}$  inherits the symplectic structure  $\tilde{\sigma}:=\sum_{j=1}^{n-1}d\bar{q}_j\wedge d\bar{p}_j$  from  $\mathbb{R}^{2n}$ . And since the FPU Hamiltonian H is constant on the orbits of the flow of  $X_{\bar{p}_n}$ , H reduces to a Hamiltonian on  $\mathbb{R}^{2n-2}$  given by

$$H = \sum_{j=1}^{n-1} \frac{1}{2} (\bar{p}_j^2 + \omega_j^2 \bar{q}_j^2) + H_3(\bar{q}_1, \dots, \bar{q}_{n-1}) + H_4(\bar{q}_1, \dots, \bar{q}_{n-1}) + \dots$$
(3.3)

The reduced Hamiltonian (3.3) represents the periodic FPU system from which the centre of mass motion has been eliminated.

Since  $\omega_j^2 > 0$   $(1 \le j \le n-1)$ , we conclude with the Morse-Lemma (cf. [1]) that the level sets of H are 2n-3 dimensional spheres around the origin of  $\mathbb{R}^{2n-2}$ . And since H is a constant of motion for the flow of  $X_H$ , we see that the origin is a stable stationary point for the reduced system induced by the reduced Hamiltonian (3.3).

# 4 Discrete symmetries

Apart from the continuous family of symmetries of the previous section, the FPU Hamiltonian has some discrete symmetries. These have important dynamical consequences.

The first discrete symmetry is a rotation symmetry. Let  $T: \mathbb{R}^{2n} \to \mathbb{R}^{2n}$  denote the circle permutation, the unique linear mapping defined by

$$T: \frac{\partial}{\partial q_j} \mapsto \frac{\partial}{\partial q_{j-1}} , \quad \frac{\partial}{\partial p_j} \mapsto \frac{\partial}{\partial p_{j-1}} .$$
 (4.1)

T is symplectic:  $T^*\sigma = \sigma$ . Furthermore, note that T leaves H invariant:  $T^*H := H \circ T = H$ . This implies that the Hamiltonian vector field  $X_H$  induced by H is equivariant under  $T: DT \cdot X_H = X_H \circ T$ . In other words: if  $\gamma: \mathbb{R} \to \mathbb{R}^{2n}$  is an integral curve of  $X_H$ , then  $T \circ \gamma: \mathbb{R} \to \mathbb{R}^{2n}$  is an integral curve of  $X_H$ . This is why we call T a symmetry of T. The same thing holds for the powers of T. The group T is a discrete symmetry group of T.

We can point out another discrete symmetry, namely the reflection  $S: \mathbb{R}^{2n} \to \mathbb{R}^{2n}$  which is the unique linear mapping sending

$$S: \frac{\partial}{\partial q_j} \mapsto -\frac{\partial}{\partial q_{n-j}} , \quad \frac{\partial}{\partial p_j} \mapsto -\frac{\partial}{\partial p_{n-j}} . \tag{4.2}$$

S is again a symplectic symmetry:  $S^*\sigma = \sigma$  and  $S^*H = H$ . The group  $\langle S \rangle := \{ \mathrm{Id}, S \} \cong \mathbb{Z}/_{2\mathbb{Z}}$ , whereas the full discrete symmetry group  $\langle T, S \rangle := \{ \mathrm{Id}, T, T^2, \ldots, T^{n-1}, S, ST^2, \ldots, ST^{n-1} \} \cong D_n$  is called the 'n-th dihedral group'; its group structure is determined by the relation  $ST = T^{n-1}S$ . The vector field  $X_H$  is equivariant under the elements of  $\langle T, S \rangle$ , that is  $\langle T, S \rangle$  maps integral curves of  $X_H$  to integral curves of  $X_H$ .

The reader should note that T and S leave  $\overline{q_n}^{-1}(\{0\}) \cap \overline{p_n}^{-1}(\{0\})$  invariant. Therefore, T and S reduce to linear symplectic mappings on  $\mathbb{R}^{2n-2}$  that leave the reduced Hamiltonian invariant<sup>1</sup>.

## 5 Normalisation

We shall study the reduced FPU system (3.3) using Birkhoff-Gustavson normalisation. In fact, we shall construct a near-identity transformation of phase-space allowing us to write the FPU Hamiltonian in 'normal form', meaning that it can be seen as a perturbation of a rather simple system. The study of the truncated normal form that is this simpler system-leads to important conclusions for the original FPU system. For instance, the solutions of the truncated normal form are approximations of low-energetic solutions of the original system valid on a long time-scale. Integrals of the truncated normal form are near-integrals of the original system: on orbits of low

$$R: \frac{\partial}{\partial q_i} \mapsto \frac{\partial}{\partial q_i} , \frac{\partial}{\partial p_i} \mapsto -\frac{\partial}{\partial p_i} . \tag{4.3}$$

R leaves the FPU Hamiltonian invariant, i.e.  $R^*H = H$ . R is anti-symplectic in the sense that  $R^*\sigma = -\sigma$ . This implies that the vector field  $X_H$  is anti-equivariant under  $R: DR \cdot X_H = -X_H \circ R$ . In other words: if  $\gamma: \mathbb{R} \to \mathbb{R}^{2n}$  is an integral curve of  $X_H$ , then  $R \circ \gamma \circ (-\mathrm{Id}): \mathbb{R} \to \mathbb{R}^{2n}$  is an integral curve of  $X_H$ . Since R leaves  $\bar{q}_n^{-1}(\{0\}) \cap \bar{p}_n^{-1}(\{0\})$  invariant, R reduces to an anti-symplectic mapping on  $\mathbb{R}^{2n-2}$  leaving the reduced Hamiltonian invariant. More information on reversing symmetries can be found in [8].

<sup>&</sup>lt;sup>1</sup>The FPU Hamiltonian also has a reversing symmetry, namely the mapping  $R: \mathbb{R}^{2n} \to \mathbb{R}^{2n}$  given by

energy, they are almost conserved for a long time. See [14] for an explanation and explicit statements. Furthermore, the truncated normal form can help us understanding bifurcation phenomena. And last but not least, if the truncated normal form of the FPU chain is integrable in a nondegenerate way, then the FPU chain is a perturbation of a nondegenerate integrable system. We may apply the KAM theorem then and conclude that almost all low-energetic solutions of (3.3) are quasiperiodic and move on tori. Conclusions of this type were drawn for the first time in [12].

The setting of normalisation is the following:

Let  $P_k$  be the set of all homogeneous k-th degree polynomials in  $(\bar{q}_1, \ldots, \bar{q}_{n-1}, \bar{p}_1, \ldots, \bar{p}_{n-1})$ . The set of all power series without linear part,  $P := \bigoplus_{k \geq 2} P_k$ , is a Lie-algebra with the Poisson bracket. For each  $h \in P$  the adjoint representation  $\mathrm{ad}_h : P \to P$  is the linear operator defined by  $\mathrm{ad}_h(H) = \{h, H\}$ . Note that whenever  $h \in P_k$ , then  $\mathrm{ad}_h : P_l \to P_{k+l-2}$ .

The flow  $e^{tX_h}$  of a Hamiltonian vector field  $X_h$  induced by  $h \in P - P_2$  is a symplectic near-identity transformation in  $\mathbb{R}^{2n-2}$ . For its action on an arbitrary Hamiltonian  $H \in P$  we have  $\frac{d}{dt}(e^{tX_h})^*H = dH \cdot X_h = -\mathrm{ad}_h(H)$ . This is a linear differential equation in P of which the solution is  $(e^{tX_h})^*H = e^{-t\mathrm{ad}_h}H$ . In particular the near-identity 'Lie-transformation'  $e^{-X_h} = \mathrm{Id} - X_h + \ldots$  transforms H into

$$H' := (e^{-X_h})^* H = e^{\operatorname{ad}_h} H = H + \{h, H\} + \frac{1}{2} \{h, \{h, H\}\} + \dots$$
 (5.1)

Let us denote the k-th order part of the Hamiltonian H -that is the projection of H on  $P_k$ - by  $H_k$ . If for instance  $h \in P_3$ , then we obtain the formula  $H'_k = \sum_{m=0}^{k-2} \frac{1}{m!} (\operatorname{ad}_h)^m (H_{k-m})$ . We just gathered all terms of equal degree in formula (5.1).

Assume now, as is the case for the reduced FPU Hamiltonian, that  $ad_{H_2}: P_k \to P_k$  is semisimple (i.e. complex-diagonalisable) for every  $k \geq 2$ . Then  $P_k = \ker \operatorname{ad}_{H_2} \oplus$ 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  $h_3\in P_3$  such that  $\mathrm{ad}_{H_2}(h_3)=g_3$ . One could for example choose  $h_3 = \tilde{g}_3 := (\operatorname{ad}_{H_2}|_{\operatorname{im ad}_{H_2}})^{-1}(g_3)$ . But clearly the choice  $h_3 = \tilde{g}_3 + p_3$ suffices for any  $p_3 \in \ker \operatorname{ad}_{H_2} \cap P_3$ . For the new Hamiltonian H' we calculate from (5.1) that  $H'_2 = H_2$ ,  $H'_3 = f_3 \in \ker \operatorname{ad}_{H_2}$ ,  $H'_4 = H_4 + \{h_3, H_3 - \frac{1}{2}g_3\}$ , etc. But now we can again write  $H'_4 = f_4 + g_4$  with  $f_4 \in \ker \operatorname{ad}_{H_2}, g_4 \in \operatorname{im} \operatorname{ad}_{H_2}$  and it is clear that by a suitable choice of  $h_4 \in P_4$  the Lie-transformation  $e^{-X_{h_4}}$  transforms our H' into H''for which  $H_2'' = H_2$ ,  $H_3'' = f_3 \in \ker \operatorname{ad}_{H_2}$  and  $H_4'' = f_4 \in \ker \operatorname{ad}_{H_2}$ . 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  $l \geq k$ , whereas the composition  $e^{-X_{h_r}} \circ \ldots \circ e^{-X_{h_3}}$  transforms H into  $\overline{H}$  with the property that  $\overline{H}_k$  Poisson commutes with  $H_2$  for every  $2 \leq k \leq r$ .  $\overline{H}$  is called a normal form of H of order r. Its study can give us useful information on low-energetic solutions of the original Hamiltonian H. More on normalisation by Lie-transformations can be found in [3].

# 6 Normal forms and discrete symmetry

In section 4 we investigated the discrete symmetries of the periodic FPU Hamiltonian. We saw that they reduce to symmetries of the reduced FPU system on  $\mathbb{R}^{2n-2}$ . In this section we show how one can construct normal forms of the reduced FPU Hamiltonian that have the same symmetry properties as the reduced 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. We shall see that it does so in section 8 and further.

The symmetry properties are captured in the definition of the symmetric subspace of P:

$$P^{ST} := \{ f \in P | S^*f = f, T^*f = f \}$$
.

Note that the FPU Hamiltonian is in  $P^{ST}$ .

The next observation is that  $S^*$  and  $T^*$  are Lie-algebra automorphisms of P:

$$S^*\{f,g\} = \{S^*f, S^*g\} , \quad T^*\{f,g\} = \{T^*f, T^*g\} . \tag{6.1}$$

simply because T and S are symplectic. Now take  $f \in P^{ST}$  and  $g \in P^{ST}$ . Then from (6.1) it follows that  $S^*\{f,g\} = \{S^*f,S^*g\} = \{f,g\}$  and  $T^*\{f,g\} = \{T^*f,T^*g\} = \{f,g\}$ . This means that  $P^{ST}$  is a Lie-subalgebra of P: if  $f,g \in P^{ST}$ , then  $\{f,g\} \in P^{ST}$ . Alternatively stated: if  $h \in P^{ST}$ , then  $\mathrm{ad}_h : P^{ST} \to P^{ST}$ . In particular,  $e^{\mathrm{ad}_h} : P^{ST} \to P^{ST}$ .

Since  $\operatorname{ad}_{H_2}$  leaves  $P^{ST}$  invariant, we know that  $P^{ST} = (\ker \operatorname{ad}_{H_2} \cap P^{ST}) \oplus (\operatorname{im} \operatorname{ad}_{H_2} \cap P^{ST})$ . So if we decompose the third order part of the FPU Hamiltonian as  $H_3 = f_3 + g_3$  with  $f_3 \in \ker \operatorname{ad}_{H_2}$ ,  $g_3 \in \operatorname{im} \operatorname{ad}_{H_2}$ , then  $f_3$ ,  $g_3 \in P_3^{ST}$  automatically.  $h_3 = \tilde{g}_3 = (\operatorname{ad}_{H_2}|_{\operatorname{im} \operatorname{ad}_{H_2}})^{-1}(g_3)$  is the unique element of  $\operatorname{im} \operatorname{ad}_{H_2} \cap P_3^{ST}$  for which  $\operatorname{ad}_{H_2}(h_3) = g_3$ . But since  $\tilde{g}_3 \in P_3^{ST}$ , we find that  $H' = (e^{-X_{\tilde{g}_3}})^*H = e^{\operatorname{ad}_{\tilde{g}_3}}H \in P^{ST}$ . Of course the choice  $h_3 = \tilde{g}_3 + p_3$  also suffices for any  $p_3 \in \ker \operatorname{ad}_{H_2} \cap P_3^{ST}$ .

It should be clear that continuing this procedure, we can produce normal forms  $\overline{H} \in P^{ST}$  of H up to any finite order<sup>2</sup>.

# 7 Simultaneous diagonalisation

From (6.1) we infer that

$$(T^* \circ \operatorname{ad}_{H_2})(f) = T^* \{ H_2, f \} = \{ T^* H_2, T^* f \} = \{ H_2, T^* f \} = (\operatorname{ad}_{H_2} \circ T^*)(f) .$$

$$(7.1)$$

So  $\operatorname{ad}_{H_2}$  and  $T^*$  commute on  $P_k$ . Therefore  $\operatorname{ad}_{H_2}$  leaves the eigenspaces of  $T^*$  invariant and we can diagonalise  $\operatorname{ad}_{H_2}$  and  $T^*$  simultaneously. This allows us to calculate the subspace  $P_k \cap \ker \operatorname{ad}_{H_2} \cap \ker (T^* - \operatorname{Id}) \subset P_k$  in which  $\overline{H}_k$  is contained and helps us

<sup>&</sup>lt;sup>2</sup>Although the bookkeeping is a bit harder, one can extend the previous argument to prove that the normal forms can also be chosen invariant under  $R^*$ . For a complete proof, cf. [3].

formulate some important restrictions on the normal form of the FPU Hamiltonian.

In order to perform this simultaneous diagonalisation, we introduce the 'super-phonons'  $(z,\zeta)$ . For  $1 \leq j < \frac{n}{2}$ , define:

$$z_{j} := \frac{1}{2}(\bar{p}_{j} - i\bar{p}_{n-j}) + \frac{i\omega_{j}}{2}(\bar{q}_{j} - i\bar{q}_{n-j}) = \frac{1}{\sqrt{2n}} \sum_{k=1}^{n} e^{-\frac{2\pi i j k}{n}} (p_{k} + i\omega_{j} q_{k})$$

$$\zeta_{j} := \frac{1}{2i\omega_{j}}(\bar{p}_{j} + i\bar{p}_{n-j}) - \frac{1}{2}(\bar{q}_{j} + i\bar{q}_{n-j}) = \frac{1}{i\omega_{j}} \sum_{k=1}^{n} e^{\frac{2\pi i j k}{n}} (p_{k} - i\omega_{j} q_{k})$$

$$z_{n-j} := -\frac{1}{2}(\bar{p}_{j} - i\bar{p}_{n-j}) + \frac{i\omega_{j}}{2}(\bar{q}_{j} - i\bar{q}_{n-j}) = -\frac{1}{\sqrt{2n}} \sum_{k=1}^{n} e^{-\frac{2\pi i j k}{n}} (p_{k} - i\omega_{j} q_{k})$$

$$\zeta_{n-j} := \frac{1}{2i\omega_{j}}(\bar{p}_{j} + i\bar{p}_{n-j}) + \frac{1}{2}(\bar{q}_{j} + i\bar{q}_{n-j}) = \frac{1}{i\omega_{j}\sqrt{2n}} \sum_{k=1}^{n} e^{\frac{2\pi i j k}{n}} (p_{k} + i\omega_{j} q_{k})$$

and if n is even:

$$z_{\frac{n}{2}} := \frac{1}{\sqrt{2}i\omega_{\frac{n}{2}}} (\bar{p}_{\frac{n}{2}} + i\omega_{\frac{n}{2}}\bar{q}_{\frac{n}{2}}) = \frac{1}{i\omega_{\frac{n}{2}}\sqrt{2n}} \sum_{k=1}^{n} (-1)^{k} (p_{k} + i\omega_{\frac{n}{2}}q_{k})$$

$$\zeta_{\frac{n}{2}} := \frac{1}{\sqrt{2}} (\bar{p}_{\frac{n}{2}} - i\omega_{\frac{n}{2}}\bar{q}_{\frac{n}{2}}) = \frac{1}{\sqrt{2n}} \sum_{k=1}^{n} (-1)^{k} (p_{k} - i\omega_{\frac{n}{2}}q_{k})$$

$$(7.3)$$

One checks that  $\{z_j, z_k\} = \{\zeta_j, \zeta_k\} = 0$  and  $\{z_j, \zeta_k\} = \delta_{jk}$ , the Kronecker delta. So our superphonons define canonical coordinates, i.e.  $\tilde{\sigma} = \sum_{j=1}^{n-1} z_j \wedge \zeta_j$ .

From (4.1) we infer that  $T^*q_j = q_{j+1}$  and  $T^*p_j = p_{j+1}$ , where  $q_j, p_j : \mathbb{R}^{2n} \to \mathbb{R}$  are the coordinate functions. So from (7.2) we see that

$$T^*: z_j \mapsto e^{\frac{2\pi i j}{n}} z_j, \quad \zeta_j \mapsto e^{-\frac{2\pi i j}{n}} \zeta_j, \quad z_{n-j} \mapsto e^{\frac{2\pi i j}{n}} z_{n-j}, \quad \zeta_{n-j} \mapsto e^{-\frac{2\pi i j}{n}} \zeta_{n-j}, \quad z_{n-j} \mapsto e^{-\frac{2\pi i j}{n}} \zeta$$

We conclude that  $T^*$  acts diagonally on  $(z,\zeta)$ -coordinates. And it acts diagonally on monomials in  $(z,\zeta)$ : if  $\Theta,\theta\in\{0,1,2,\ldots\}^{n-1}$  are multi-indices, then

$$T^*: z^{\Theta} \zeta^{\theta} \mapsto e^{\frac{2\pi i \mu(\Theta, \theta)}{n}} z^{\Theta} \zeta^{\theta} , \qquad (7.5)$$

 $\mu$  being defined as:

$$\mu(\Theta, \theta) := \sum_{1 \le j < \frac{n}{2}} j \left(\Theta_j + \Theta_{n-j} - \theta_j - \theta_{n-j}\right) + \frac{n}{2} \left(\Theta_{\frac{n}{2}} - \theta_{\frac{n}{2}}\right) \mod n . \tag{7.6}$$

On the other hand one calculates:

$$H_2 = \sum_{1 \le j < \frac{n}{2}} i\omega_j (z_j \zeta_j - z_{n-j} \zeta_{n-j}) + i\omega_{\frac{n}{2}} z_{\frac{n}{2}} \zeta_{\frac{n}{2}} .$$
 (7.7)

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

$$\operatorname{ad}_{H_2}: z^{\Theta} \zeta^{\theta} \mapsto \nu(\Theta, \theta) z^{\Theta} \zeta^{\theta} , \qquad (7.8)$$

in which  $\nu$  is defined as

$$\nu(\Theta, \theta) := \sum_{1 \le j < \frac{n}{2}} i\omega_j (\theta_j - \theta_{n-j} - \Theta_j + \Theta_{n-j}) + i\omega_{\frac{n}{2}} (\theta_{\frac{n}{2}} - \Theta_{\frac{n}{2}}) . \tag{7.9}$$

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.

# 8 Restrictions for symmetric normal forms

From section 6 we know that we can transform the periodic FPU Hamiltonian into a discrete symmetric normal form of any desired order. Suppose we did so up to order r. Then  $\overline{H}_k \in P_k \cap \ker \operatorname{ad}_{H_2} \cap \ker (T^* - \operatorname{Id})$  for any  $2 \le k \le r$ . But since both  $T^*$  and  $\operatorname{ad}_{H_2}$  act diagonally in  $(z,\zeta)$ -coordinates, we know that this  $\overline{H}_k$  must be a linear combination of monomials  $z^{\Theta}\zeta^{\theta}$  for which

$$|\Theta| + |\theta| = k$$
,  $\mu(\Theta, \theta) = 0 \mod n$  and  $\nu(\Theta, \theta) = 0$ . (8.1)

Extra restrictions on  $\overline{H}_k$ , with which we shall deal later, arise from the fact that  $\overline{H}_k$  can be chosen in the even smaller set  $P^{ST-3}$ . But first we investigate which  $\Theta$  and  $\theta$  satisfy (8.1). Because the  $\omega_j$  in (7.9) are of the form  $2i\sin(\frac{j\pi}{n})$ , this is actually a number-theoretical question that we shall solve for  $|\Theta| + |\theta| = 2, 3, 4$ .

The quadratic case - i.e.  $|\Theta| + |\theta| = 2$  - is easy: since all the  $\omega_j$  are different, we find from  $\nu(\Theta, \theta) = 0$  that the Lie-subalgebra  $P_2 \cap \ker \operatorname{ad}_{H_2} \subset P_2$  is spanned by the monomials

$$z_j\zeta_j, \ z_{n-j}\zeta_{n-j}, \ z_jz_{n-j}, \ \zeta_j\zeta_{n-j} \ (1 \le j < \frac{n}{2}) \text{ and } z_{\frac{n}{2}}\zeta_{\frac{n}{2}}.$$
 (8.2)

 $T^*$  acts diagonally on these basis-elements as follows:

$$T^*: z_j \zeta_j \mapsto z_j \zeta_j, \ z_{n-j} \zeta_{n-j} \mapsto z_{n-j} \zeta_{n-j}, \ z_{\frac{n}{2}} \zeta_{\frac{n}{2}} \mapsto z_{\frac{n}{2}} \zeta_{\frac{n}{2}},$$

$$z_j z_{n-j} \mapsto e^{\frac{4\pi i j}{n}} z_j z_{n-j}, \ \zeta_j \zeta_{n-j} \mapsto e^{-\frac{4\pi i j}{n}} \zeta_j \zeta_{n-j}.$$

$$(8.3)$$

The Lie-subalgebra  $P_2 \cap \ker \operatorname{ad}_{H_2} \cap \ker (T^* - \operatorname{Id}) = \operatorname{span}\{z_j \zeta_j, z_{n-j} \zeta_{n-j}, z_{\frac{n}{2}} \zeta_{\frac{n}{2}}\}$  is abelian. From (4.2) and (7.2) we calculate the action of  $S^*$  on the coordinate-functions:

$$S^*: z_j \mapsto -i\omega_j \zeta_{n-j}, \ \zeta_j \mapsto \frac{1}{i\omega_j} z_{n-j}, \ z_{n-j} \mapsto i\omega_j \zeta_j, \ \zeta_{n-j} \mapsto \frac{-1}{i\omega_j} z_j, \ z_{\frac{n}{2}} \mapsto -z_{\frac{n}{2}}, \ \zeta_{\frac{n}{2}} \mapsto -\zeta_{\frac{n}{2}}. \tag{8.4}$$

<sup>&</sup>lt;sup>3</sup>and invariant under  $R^*$ 

So the action on the basis-elements reads:

$$S^*: z_j \zeta_j \mapsto -z_{n-j} \zeta_{n-j}, \ z_{n-j} \zeta_{n-j} \mapsto -z_j \zeta_j, \ z_{\frac{n}{2}} \zeta_{\frac{n}{2}} \mapsto z_{\frac{n}{2}} \zeta_{\frac{n}{2}},$$

$$z_j z_{n-j} \mapsto \omega_j^2 \zeta_j \zeta_{n-j}, \ \zeta_j \zeta_{n-j} \mapsto \frac{1}{\omega_j^2} z_j z_{n-j}.$$

$$(8.5)$$

We conclude that the Lie-subalgebra  $P_2^{ST} \cap \ker \operatorname{ad}_{H_2}$  is spanned by the quadratics  $z_j\zeta_j - z_{n-j}\zeta_{n-j}$  and  $z_{\frac{n}{2}}\zeta_{\frac{n}{2}}$ . Note that  $H_2$  itself is indeed a linear combination of these quadratics.

The analysis is harder if we consider the cases  $|\Theta| + |\theta| = 3$ , 4. With the use of number theory, the proof of the following theorem is given in the appendix.

### Theorem 8.1

- i) The set of multi-indices  $(\Theta, \theta) \in \{0, 1, 2, ...\}^{2n-2}$  for which  $|\Theta| + |\theta| = 3$ ,  $\mu(\Theta, \theta) = 0$  mod n and  $\nu(\Theta, \theta) = 0$  is empty.
- ii) The set of multi-indices  $(\Theta, \theta) \in \{0, 1, 2, ...\}^{2n-2}$  for which  $|\Theta| + |\theta| = 4$ ,  $\mu(\Theta, \theta) = 0$  mod n and  $\nu(\Theta, \theta) = 0$  is contained in the set given by the relations  $\theta_j \theta_{n-j} \Theta_j + \Theta_{n-j} = \theta_{\frac{n}{2}} \Theta_{\frac{n}{2}} = 0$ .

Theorem 8.1 has some major implications. We shall investigate these now and they will be summarised in theorem 8.2.

From i) we see that  $P_3^{ST} \cap \ker \operatorname{ad}_{H_2} \subset P_3 \cap \ker \operatorname{ad}_{H_2} \cap \ker (T^* - \operatorname{Id}) = \{0\}.$ 

First of all, this implies that we can always transform away  $H_3$  from the periodic FPU Hamiltonian:  $\overline{H}_3=0$ . This is an unexpected result. Consider for example the chain with 6 particles, which satisfies a third order resonance relation:  $\omega_1:\omega_3:\omega_5=1:2:1$ . For systems with a third order resonance relation one can generally not expect  $\overline{H}_3$  to be trivial. But, as was observed for the first time in [12], it is trivial for the 6 particles chain. One could say that the 1:2:1-resonance is not active at  $H_3$ -level. We now know that for the periodic FPU chain no resonance will ever be active at  $H_3$ -level. This simplification is caused by the symmetries of the FPU system.

Secondly, we conclude from i) that the  $h_3$  of section 6 is uniquely determined by the requirement that it be in  $P_3^{ST}$ . This in turn uniquely determines  $\overline{H}_4$ .

From ii) we infer that any element of  $P_4 \cap \ker \operatorname{ad}_{H_2} \cap \ker (T^* - \operatorname{Id})$  must be a linear combination of products of two of the basis-elements in (8.2).

Note however that not all these products are really  $T^*$ -invariant and that the full normal form is even invariant under  $S^*$ . We work out these extra restrictions now.

The question which products of the basis-elements (8.2) are invariant under  $T^*$  is easy to answer with help of the formulas (8.3). Clearly, all products of  $z_j\zeta_j$ ,  $z_{n-j}\zeta_{n-j}$  and  $z_{\frac{n}{2}}\zeta_{\frac{n}{2}}$  are.  $T^*$  multiplies the terms  $(z_j\zeta_j)(z_kz_{n-k}), (z_j\zeta_j)(\zeta_k\zeta_{n-k}), (z_{n-j}\zeta_{n-j})(z_kz_{n-k}), (z_{n-j}\zeta_{n-j})(z_kz_{n-k}), (z_{n-j}\zeta_{n-j})(\zeta_k\zeta_{n-k}), (z_{\frac{n}{2}}\zeta_{\frac{n}{2}})(z_kz_{n-k})$  and  $(z_{\frac{n}{2}}\zeta_{\frac{n}{2}})(\zeta_k\zeta_{n-k})$  with a factor  $e^{\pm\frac{4\pi ik}{n}}\neq 1$ , so these terms are not invariant under  $T^*$ .  $T^*$  multiplies  $(z_jz_{n-j})(\zeta_k\zeta_{n-k})$  by  $e^{\frac{4\pi i(j-k)}{n}}$  which is 1 if and only if 2(j-k)=0 mod n. But because  $1\leq j,k<\frac{n}{2}$ , the

condition is 2(j-k)=0, i.e. j=k. Thus we end up with a term that we already had:  $(z_jz_{n-j})(\zeta_j\zeta_{n-j})=(z_j\zeta_j)(z_{n-j}\zeta_{n-j})$ . Finally, the terms  $(z_jz_{n-j})(z_kz_{n-k})$  and  $(\zeta_j\zeta_{n-j})(\zeta_k\zeta_{n-k})$  are multiplied by a factor  $e^{\pm\frac{4\pi i(j+k)}{n}}$  which is 1 if and only if 2(j+k)=0 mod n. But since  $1\leq j,k<\frac{n}{2}$ , the only possibility is that 2(j+k)=n, that is n must be even and  $j+k=\frac{n}{2}$ . This concludes our search for fourth order monomials invariant under  $T^*$  and Poisson commuting with  $H_2$ .

We shall check now which combinations of these terms are also invariant under  $S^*$ . The action of  $S^*$  on  $P_2 \cap \ker$  ad<sub> $H_2$ </sub> can be diagonalised in real coordinates. For this purpose, besides our familiar complex basis, we also define the following real basis-elements for  $P_2 \cap \ker$  ad<sub> $H_2$ </sub>. For  $1 \leq j < \frac{n}{2}$ , let

$$a_{j} := i(z_{j}\zeta_{j} - z_{n-j}\zeta_{n-j}) = \frac{1}{2\omega_{j}}(\bar{p}_{j}^{2} + \bar{p}_{n-j}^{2} + \omega_{j}^{2}\bar{q}_{j}^{2} + \omega_{j}^{2}\bar{q}_{n-j}^{2}) ,$$

$$b_{j} := i(z_{j}\zeta_{j} + z_{n-j}\zeta_{n-j}) = \bar{p}_{j}\bar{q}_{n-j} - \bar{p}_{n-j}\bar{q}_{j} , \qquad (8.6)$$

$$c_{j} := \frac{1}{\omega_{j}}(\omega_{j}^{2}\zeta_{j}\zeta_{n-j} + z_{j}z_{n-j}) = \frac{1}{2\omega_{j}}(\bar{p}_{n-j}^{2} - \bar{p}_{j}^{2} + \omega_{j}^{2}\bar{q}_{n-j}^{2} - \omega_{j}^{2}\bar{q}_{j}^{2}) ,$$

$$d_{j} := \frac{i}{\omega_{j}}(\omega_{j}^{2}\zeta_{j}\zeta_{n-j} - z_{j}z_{n-j}) = \frac{1}{\omega_{j}}(\bar{p}_{j}\bar{p}_{n-j} + \omega_{j}^{2}\bar{q}_{j}\bar{q}_{n-j}) ,$$

and if n is even

$$a_{\frac{n}{2}} := i z_{\frac{n}{2}} \zeta_{\frac{n}{2}} = \frac{1}{2\omega_{\frac{n}{2}}} (\bar{p}_{\frac{n}{2}}^2 + \omega_{\frac{n}{2}}^2 \bar{q}_{\frac{n}{2}}^2) .$$

Note that these basis-elements are subject to the relation

$$a_j^2 = b_j^2 + c_j^2 + d_j^2 (8.7)$$

and that  $H_2$  can easily be expressed as

$$H_2 = \sum_{1 \le j \le \frac{n}{2}} \omega_j a_j . \tag{8.8}$$

Our definitions diagonalise the action of  $S^*$ :

$$S^*: a_j \mapsto a_j, \ a_{\frac{n}{2}} \mapsto a_{\frac{n}{2}}, \ b_j \mapsto -b_j, \ c_j \mapsto c_j, \ d_j \mapsto -d_j \ . \tag{8.9}$$

The products  $a_j a_k$ ,  $a_{\frac{n}{2}} a_j$  and  $b_j b_k$  are invariant under  $S^*$  and  $T^*$ . The products  $a_j b_k$  and  $a_{\frac{n}{2}} b_k$  are not invariant under  $S^*$ , although they are under  $T^*$ . It is left as an easy excercise for the reader to prove that the only configuration for other terms to appear is  $d_j d_{\frac{n}{2} - j} - c_j c_{\frac{n}{2} - j}$ .

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

**Theorem 8.2** Let H be the reduced periodic FPU Hamiltonian (3.3). There is a fourth order normal form  $\overline{H}$  of H which is invariant under  $T^*$  and  $S^{*-4}$ . For this normal form we have  $\overline{H}_3 = 0$ , whereas  $\overline{H}_4$  is a linear combination of the fourth order terms  $a_j a_k$ ,  $b_j b_k$   $(1 \le j, k < \frac{n}{2})$  and if n is even  $a_{\frac{n}{2}} a_j$   $(1 \le j \le \frac{n}{2})$  and  $d_j d_{\frac{n}{2}-j} - c_j c_{\frac{n}{2}-j}$   $(1 \le j \le \frac{n}{4})$ .

 $<sup>^4</sup>$ and  $R^*$ 

# 9 Near-integrals or integrals of the truncated normal form

In the previous section we proved that the truncated fourth order normal form of the periodic FPU Hamiltonian is subject to many restrictions, as indicated in theorem 8.2. This enables us to point out some integrals for the truncated normal form. These are near-integrals of the periodic FPU chain: quantities that are nearly conserved by the flow of the original chain (3.3) for a long time, cf. [14].

In order to be able to compute these integrals, we first write down the commutation relations between the real basis-elements (8.6). They are given by

$$\{b_j, c_j\} = 2d_j , \{b_j, d_j\} = -2c_j , \{c_j, d_j\} = 2b_j .$$
 (9.1)

All the other Poisson brackets between basis-elements give 0. These relations lead to the following conclusions:

### 9.1 The odd chain

**Corollary 9.1** If n is odd, then the truncated normal form  $H_2 + \overline{H}_4$  of the periodic FPU chain is Liouville integrable with the quadratic integrals  $a_j, b_j$   $(1 \le j \le \frac{n-1}{2})$ .

**Proof:**  $H_2$  is a linear combination of the quadratics  $a_j$  and  $\overline{H}_4$  is a linear combination of the fourth order terms  $a_j a_k$  and  $b_j b_k$ . The  $a_j$  and  $b_k$  Poisson commute with all these terms and with each other.

It is well-known (cf. [2]), that the integrals of a 2n-2-dimensional Liouville integrable Hamiltonian system generally define n-1-dimensional invariant tori. Let's see what these tori look like here and analyse the integral map  $F: \mathbb{R}^{2n-2} \to \mathbb{R}^{n-1}$  that maps  $(\bar{q}, \bar{p}) \mapsto (a, b)$ :

### Proposition 9.2

$$im \ F = \{(a,b) \in \mathbb{R}^{n-1} | a_i \ge 0, |b_i| \le a_i \} \ .$$
 (9.2)

For  $(a,b) \in (im\ F)^{int} = \{(a,b) \in \mathbb{R}^{n-1} | a_j > 0, |b_j| < a_j\}, \ F^{-1}(\{(a,b)\})$  is a smooth n-1-dimensional torus .

**Proof:** Clearly, im  $a_j = [0, \infty)$ . The level set of  $a_j$  is, for  $a_j > 0$ , the cartesian product of  $\mathbb{R}^{2n-6}$  and a 3-dimensional sphere in  $\mathbb{R}^4$  with radius  $\sqrt{2a_j}$ . Let us consider  $b_j$  restricted to the level set of  $a_j$ . To compute its critical points, we use the method of Lagrange multipliers:  $(\bar{q}, \bar{p})$  is a critical point iff there is a constant  $\lambda$  such that  $Da_j(\bar{q}, \bar{p}) = \lambda Db_j(\bar{q}, \bar{p})$ , that is  $(\omega_j \bar{q}_j, \omega_j \bar{q}_{n-j}, \frac{1}{\omega_j} \bar{p}_j, \frac{1}{\omega_j} \bar{p}_{n-j}) = \lambda(-\bar{p}_{n-j}, \bar{p}_j, \bar{q}_{n-j}, -\bar{q}_j)$ . From this we infer that  $\lambda = \pm 1$ . For  $\lambda = 1$ , we find  $\bar{p}_{n-j} = -\omega_j \bar{q}_j$ ,  $\bar{p}_j = \omega_j \bar{q}_{n-j}$ . In these points we have  $b_j = a_j$ .  $\lambda = -1$  gives  $\bar{p}_{n-j} = \omega_j \bar{q}_j$ ,  $\bar{p}_j = -\omega_j \bar{q}_{n-j}$ , so  $b_j = -a_j$ . These are the extreme values of  $b_j$  on the level set of  $a_j$ , giving (9.2). We also learn from this that if  $a_j > 0$  and  $|b_j| < a_j$ , then  $Da_j$  and  $Db_j$  are independent. So if  $(a,b) \in (\operatorname{im} F)^{int}$ , then all  $Da_j$  and  $Db_k$  are independent on  $F^{-1}(\{(a,b)\})$ . According to a theorem of Arnol'd (cf. [2]) such a level set must be a torus.

In order to compute the flow on these tori, we make the explicit transformation to action-angle coordinates  $(\bar{q},\bar{p}) \mapsto (a,b,\phi,\psi)$  as follows. Let  $\arg: \mathbb{R}^2 - \{(0,0)\} \to \mathbb{R}/2\pi\mathbb{Z}$  be the argument function,  $\arg: (r\cos\Phi,r\sin\Phi) \mapsto \Phi$ . Then, for  $1 \leq j \leq \frac{n-1}{2}$ , define

$$a_{j} := \frac{1}{2\omega_{j}} (\bar{p}_{j}^{2} + \bar{p}_{n-j}^{2} + \omega_{j}^{2} \bar{q}_{j}^{2} + \omega_{j}^{2} \bar{q}_{n-j}^{2}) ,$$

$$b_{j} := \bar{p}_{j} \bar{q}_{n-j} - \bar{p}_{n-j} \bar{q}_{j} ,$$

$$\phi_{j} := \frac{1}{2} \arg(-\bar{p}_{n-j} - \omega_{j} \bar{q}_{j}, \bar{p}_{j} - \omega_{j} \bar{q}_{n-j}) + \frac{1}{2} \arg(\bar{p}_{n-j} - \omega_{j} \bar{q}_{j}, \bar{p}_{j} + \omega_{j} \bar{q}_{n-j}) ,$$

$$\psi_{j} := \frac{1}{2} \arg(-\bar{p}_{n-j} - \omega_{j} \bar{q}_{j}, \bar{p}_{j} - \omega_{j} \bar{q}_{n-j}) - \frac{1}{2} \arg(\bar{p}_{n-j} - \omega_{j} \bar{q}_{j}, \bar{p}_{j} + \omega_{j} \bar{q}_{n-j}) .$$

$$(9.3)$$

Note that these are well-defined as long as  $(a,b) \in (\operatorname{im} F)^{int}$ . With the formula  $d \operatorname{arg}(x,y) = \frac{xdy - ydx}{x^2 + y^2}$ , one can verify that the  $(a,b,\phi,\psi)$  are canonical coordinates:  $\tilde{\sigma} = \sum_{j=1}^{n-1} d\bar{q}_j \wedge d\bar{p}_j = \sum_{1 \leq j \leq \frac{n-1}{2}} d\phi_j \wedge da_j + d\psi_j \wedge db_j$ .

The truncated normal form  $H_2 + \overline{H}_4$  is a function of the actions  $a_j, b_j$ . Its induced equations of motion therefore read:

$$\dot{a}_{j} = \dot{b}_{j} = 0 , \qquad (9.4)$$

$$\dot{\phi}_{j} = \omega_{j} + \frac{\partial \overline{H}_{4}}{\partial a_{i}}(a, b) , \quad \dot{\psi}_{j} = \frac{\partial \overline{H}_{4}}{\partial b_{i}}(a, b) ,$$

which are very simple. In order to verify that that the truncated normal form  $H_2 + \overline{H}_4$  is nondegenerate, we examine the frequency map  $\omega$  which adds to each invariant torus the frequencies of the flow on it:

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

 $\omega$  is a local diffeomorphism iff both the constant derivative matrices  $\frac{\partial^2 \overline{H}_4}{\partial a_j \partial a_k}$  and  $\frac{\partial^2 \overline{H}_4}{\partial b_j \partial b_k}$  are invertible. We will explicitly check this for the odd  $\beta$ -chain in section 10.

The situation is more difficult in the case of

### 9.2 The even chain

**Corollary 9.3** If n is even, then the truncated normal form  $H_2 + \overline{H}_4$  of the periodic FPU chain has the quadratic integrals  $a_j$   $(1 \le j \le \frac{n}{2})$  and  $b_j - b_{\frac{n}{2}-j}$   $(1 \le j < \frac{n}{4})$ .

**Proof:**  $H_2$  is a linear combination of the quadratics  $a_j$   $(1 \le j \le \frac{n}{2})$ , whereas  $\overline{H}_4$  is a linear combination of the fourth order terms  $a_j a_k$   $(1 \le j, k \le \frac{n}{2}), b_j b_k$   $(1 \le j < \frac{n}{2})$  and  $d_j d_{\frac{n}{2} - j} - c_j c_{\frac{n}{2} - j}$   $(1 \le j \le \frac{n}{4})$ . The  $a_j$  clearly commute with all these terms. So do the terms  $b_j - b_{\frac{n}{2} - j}$ :  $\{b_j - b_{\frac{n}{2} - j}, b_k\} = \{b_j - b_{\frac{n}{2} - j}, a_k\} = \{b_j - b_{\frac{n}{2} - j}, a_{\frac{n}{2}}\} = 0$ . But one also verifies from (9.1) that  $\{b_j - b_{\frac{n}{2} - j}, c_j c_{\frac{n}{2} - j} - d_j d_{\frac{n}{2} - j}\} = c_{\frac{n}{2} - j} \{b_j, c_j\} - c_j \{b_{\frac{n}{2} - j}, c_{\frac{n}{2} - j}\} - d_{\frac{n}{2} - j} \{b_j, d_j\} + d_j \{b_{\frac{n}{2} - j}, d_{\frac{n}{2} - j}\} = 2c_{\frac{n}{2} - j} d_j - 2c_j d_{\frac{n}{2} - j} + 2d_{\frac{n}{2} - j} c_j - 2d_j c_{\frac{n}{2} - j} = 0$ .  $\square$ 

If n is even, then the n-1-degrees of freedom Hamiltonian  $H_2 + \overline{H}_4$  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 chain (3.3). We have not yet found a complete system of integrals for the truncated normal form though. We will do so for the even  $\beta$ -chain in section 10.2.

# 10 The normal form of the $\beta$ -chain

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 (1.1). This chain, that has no cubic terms, is usually referred to as the  $\beta$ -chain. 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 tedious though and that is why we do not present it. The reader can find an example of a similar computation in [12]. The following theorem is a major generalisation of the result in [12], which in turn is a restatement -with a much more efficient proof- of a theorem in the PhD thesis of Sanders ([13]).

**Theorem 10.1** If  $\alpha = 0$ , then in the periodic FPU chain one has

$$\overline{H}_{4} = \frac{\beta}{n} \left\{ \sum_{0 < k < l < \frac{n}{2}} \frac{\omega_{k} \omega_{l}}{4} a_{k} a_{l} + \sum_{0 < k < \frac{n}{2}} \frac{\omega_{k}^{2}}{32} (3a_{k}^{2} - b_{k}^{2}) + \frac{1}{4} a_{\frac{n}{2}}^{2} + \frac{1}{2} a_{\frac{n}{2}} \sum_{0 < k < \frac{n}{2}} \omega_{k} a_{k} + \frac{1}{8} \sum_{0 < k < \frac{n}{4}} \omega_{2k}^{2} (d_{k} d_{\frac{n}{2} - k} - c_{k} c_{\frac{n}{2} - k}) + \frac{1}{16} (d_{\frac{n}{4}}^{2} - c_{\frac{n}{4}}^{2}) \right\}.$$

$$(10.1)$$

In formula (10.1) it is understood that terms with the subscript  $\frac{n}{2}$  and  $\frac{n}{4}$  only appear if 2 respectively 4 divides n.

# 10.1 The odd $\beta$ -chain

In formula (10.1) we see again what was already predicted in theorem 8.2, namely that  $\overline{H}_4$  is a linear combination of the terms  $a_j a_k$  and  $b_j b_k$   $(1 \le j, k \le \frac{n-1}{2})$ . According to corollary 9.1 this normal form is integrable, the  $a_j$  and  $b_j$  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  $a_j$  and  $b_j$ :

$$\frac{\partial^{2}\overline{H}_{4}}{\partial a_{j}\partial a_{k}} = \frac{\beta}{16} n \begin{pmatrix}
3\omega_{1}^{2} & 4\omega_{1}\omega_{2} & \cdots & 4\omega_{1}\omega_{\frac{n-1}{2}} \\
4\omega_{2}\omega_{1} & 3\omega_{2}^{2} & \cdots & 4\omega_{2}\omega_{\frac{n-1}{2}} \\
\vdots & & \ddots & \vdots \\
4\omega_{\frac{n-1}{2}}\omega_{1} & 4\omega_{\frac{n-1}{2}}\omega_{2} & \cdots & 3\omega_{\frac{n-1}{2}}^{2}
\end{pmatrix}, (10.2)$$

$$\frac{\partial^2 \overline{H}_4}{\partial b_j \partial b_k} = -\frac{\beta}{16 n} \begin{pmatrix} \omega_1^2 & & & \\ & \omega_2^2 & & \\ & & \ddots & \\ & & & \omega_{\frac{n-1}{2}}^2 \end{pmatrix}$$
(10.3)

 $\frac{\partial^2 \overline{H}_4}{\partial b_j \partial b_k}$  is clearly nondegenerate. But so is  $\frac{\partial^2 \overline{H}_4}{\partial a_j \partial a_k}$ . This can be proved by applying elementary row and column operations to (10.2), thus reducing it to upperdiagonal form. This yields an expression for the determinant that is unequal to 0. We conclude that the reduced periodic  $\beta$ -chain 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 (cf. [2]) applies:

**Theorem 10.2** If n is odd,  $\alpha = 0$  and  $\beta \neq 0$ , then almost all low-energy solutions of the reduced periodic FPU chain (3.3) are periodic or quasiperiodic 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  $\varepsilon$  goes to 0.

It should also be possible to write down an expression for the normal form if  $\alpha \neq 0$ . The nondegeneracy condition can be checked again then. But the computation of this normal form is very nasty - transforming away  $H_3$  we obtain the transformed  $H_4' = H_4 + \frac{1}{2}\{(\mathrm{ad}_{H_2}|_{\mathrm{im ad}_{H_2}})^{-1}(H_3), H_3\}$  which thereafter has to be normalised to produce  $\overline{H}_4$ . The result is most likely that for almost all  $\alpha$  and  $\beta$  the nondegeneracy condition holds and the KAM theorem applies. Without computation this is clear for  $|\alpha| \ll |\beta|$ , because in this situation the coefficients of the normal form (10.1) change only slightly and the invertible matrices form an open set in the set of all matrices.

### 10.2 The even $\beta$ -chain

It is a surprise that in the normal form of the even  $\beta$ -chain no terms  $b_j b_k$   $(j \neq k)$  arise, see formula (10.1). This leads to the following remarkable conclusion:

Corollary 10.3 If n is even and  $\alpha = 0$ ,  $\beta \neq 0$ , then the truncated normal form  $H_2 + \overline{H}_4$  of the reduced periodic FPU chain (3.3) is Liouville integrable. The integrals are the quadratics  $a_j$   $(1 \leq j \leq \frac{n}{2})$ ,  $b_j - b_{\frac{n}{2} - j}$   $(1 \leq j < \frac{n}{4})$  and  $d_{\frac{n}{4}}$  (if n is a multiple of 4) and the fourth order terms  $\omega_k^2 b_k^2 + \omega_{\frac{n}{2} - k}^2 b_{\frac{n}{2} - k}^2 + 4\omega_{2k}^2 (c_k c_{\frac{n}{2} - k} - d_k d_{\frac{n}{2} - k})$   $(1 \leq j < \frac{n}{4})$ .

**Proof:** This follows from simply computing all the Poisson brackets, using (9.1) and the fact that the Poisson brackets form a derivation.

Only the  $a_j, b_j - b_{\frac{n}{2}-j}$  and  $d_{\frac{n}{4}}$  induce a  $2\pi$ -periodic flow and can therefore be seen as actions after some symplectic action-angle transformation. It is an open problem to construct the remaining action variables. Thereafter one could differentiate  $\overline{H}_4$  with respect to them and verify the KAM nondegeneracy condition.

One exceptional case is easier: the  $\beta$ -problem with 4 particles. Its truncated normal form reads:

$$H_2 + \overline{H}_4 = \sqrt{2}a_1 + 2a_2 + \frac{\beta}{4} \left( \frac{1}{8}a_1^2 + \frac{1}{4}a_2^2 + \frac{\sqrt{2}}{2}a_1a_2 + \frac{1}{8}d_1^2 \right) ,$$
 (10.4)

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

$$\omega: (a_1, a_2, d_1) \mapsto (\sqrt{2} + \frac{\beta}{16}a_1 + \frac{\sqrt{2}\beta}{8}a_2, 2 + \frac{\beta}{8}a_2 + \frac{\sqrt{2}\beta}{8}a_1, \frac{\beta}{16}d_1) . \tag{10.5}$$

 $\omega$  is nondegenerate, since

$$\frac{\partial \omega}{\partial (a_1, a_2, d_1)} = \frac{\beta}{4} \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{2}}{2} & 0\\ \frac{\sqrt{2}}{2} & \frac{1}{2} & 0\\ 0 & 0 & \frac{1}{4} \end{pmatrix}$$
 (10.6)

is invertible. So a similar theorem as 10.2 holds for the  $\beta$ -chain with 4 particles.

It is unclear what happens for the even chain if  $\alpha \neq 0$ . The truncated normal form might not be integrable. On the other hand we already found about  $\frac{3n}{4}$  integrals. And in [12] it was already shown that the normal forms of the  $\alpha$ - $\beta$ -chain with up to 6 particles are Liouville integrable.

## 11 Discussion

The lesson that we can learn from this analysis is that the characteristic features of the Fermi-Pasta-Ulam chain, such as quasiperiodicity and nonergodicity, are not just a property shared by all low-energy solutions of resonant Hamiltonian systems. On the contrary: the periodic FPU chain is a rather special system possessing particular symmetries and eigenvalues. These cause or may cause nondegenerate integrability of the Birkhoff-Gustavson normal form of the chain, which in turn implies that the KAM theorem (cf. [2]) is applicable. Still, some questions remain unanswered:

- 1. From corollary 9.1 we know that the truncated normal form of the odd FPU chain is integrable. In section 10.1 we checked a nondegeneracy condition for the odd  $\beta$ -chain and were able to apply the KAM theorem. Can the truncated normal form of the odd chain explicitly be computed also if  $\alpha \neq 0$ ? Is it really nondegenerate, as we are tempted to assume?
- **2.** What is the reason that the truncated normal form of the even  $\beta$ -chain is integrable as we know from corollary 9.3? Is there some hidden symmetry-like property of the FPU chain that prevents terms  $b_j b_k$   $(j \neq k)$  from appearing in the truncated normal form, thus causing the integrability?
- 3. Is it possible to explicitly construct action-angle coordinates for the truncated normal form of the even  $\beta$ -problem, globally or locally, and verify the KAM nondegeneracy condition?
- 4. What about the even  $\alpha$ - $\beta$  chain? As indicated in corollary 9.3 its truncated 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. And otherwise: can we find a counterexample of an even  $\alpha$ - $\beta$  chain with many ergodic orbits of low energy?

Where the second question is of a rather philosophical nature, the other three involve tough computations. Answers might be given in a subsequent paper.

## A Proof of theorem 8.1

This appendix is based on notes of Frits Beukers. Its main intention is to prove theorem 8.1. Some algebra is used that might be uncommon to the reader, but fortunately the conclusions of theorem 8.1 and theorem 8.2 are easily understood.

## A.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  $\pm i\omega_j = \pm 2i\sin(\frac{j\pi}{n})$ . 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  $\zeta_1 + \zeta_2 + \cdots + \zeta_N = 0$  in the unknown roots of unity  $\zeta_i$ . 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 roots of unity. Let  $p^k$  be a prime power and let  $\zeta := e^{2\pi i/p^k}$ . Suppose  $\zeta \not\in K$  and  $\zeta^p \in K$ .

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

For the proof of this proposition we refer to [15], §60-61.

To return to our problem 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  $\zeta_1^{-1}$  and put  $\zeta_i = \zeta_i/\zeta_1$  we may as well assume that all  $\zeta_i$  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  $n_i \in \{0, 1, 2, \dots, p-1\}$ . Then, according to proposition A.1, the minimal polynomial of  $\zeta$  over K is  $X^p - \zeta^p$  if k > 2 and  $X^{p-1} + X^{p-2} + \cdots + X + 1$  if k = 1.

We now rewrite our relation in the following form

$$\sum_{s=0}^{p-1} \sum_{n:=s} \tilde{\zeta}_i \zeta^s = 0 \tag{R} .$$

If  $k \geq 2$  the minimal polynomial of  $\zeta$  over K is  $X^p - \zeta^p$ . In particular this means that there exist no non-trivial K-linear relations between  $1, \zeta, \ldots, \zeta^{p-1}$ . So the relation (R) implies that all coefficients are zero, hence  $\sum_{n_i=s} \tilde{\zeta}_i \zeta^s = 0$  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  $\zeta$  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

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

have the same value  $\sigma$ . 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.

### A.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  $\geq 5$  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  $\{i, j, k, l\} = \{1, 2, 3, 4\}$ .

# A.3 Sums of the $i\omega_i$

We are interested in vanishing sums of the eigenvalues  $\pm i\omega_j = \pm 2i\sin(\frac{j\pi}{n})$ . So we look for all solutions of  $\zeta_1 + \cdots + \zeta_N = 0$  such that together with each  $\zeta_i$ , minus its complex conjugate  $-\zeta_i^{-1}$  also occurs. Since we shall only be interested in sums of 3 or 4 eigenvalues  $i\omega_j$ , 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  $i\omega_j$ '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  $\zeta_1, \zeta_2$ 

arbitrary. It is necessary and sufficient to assume that  $\zeta_1\zeta_2 = -1$ . This means  $(\zeta - \zeta^{-1})(1 + \delta + \delta^2)$  where  $\zeta$  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  $\zeta_1,\zeta_2$  must be purely imaginary and have opposite sign. So we can take  $\zeta_1=-\zeta_2=i$ , hence

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

### A.4 Proof of theorem 8.1

We indicate how theorem 8.1 can be proved using the previous paragraphs.

From the first relation in section A.3 we infer that  $i\omega_{\frac{n}{6}} + i\omega_{\frac{n}{10}} - i\omega_{\frac{3n}{10}} = 0$  if n is a multiple of 30. So multi-indices  $\Theta$ ,  $\theta$  can be found such that  $|\Theta| + |\theta| = 3$  and  $\pm \nu(\Theta, \theta) = i\omega_{\frac{n}{6}} + i\omega_{\frac{n}{10}} - i\omega_{\frac{3n}{10}} = 0$ . But for this  $\Theta$  and  $\theta$ , we must have that  $\mu(\Theta, \theta) = \pm \frac{n}{6} \pm \frac{n}{10} \pm \frac{3n}{10}$  of which one easily verifies that it is unequal to 0 modulo n.

One finds the same result for the other third order relation of the previous section. The verification is not hard, but needs more bookkeeping because of the appearance of the arbitrary rational. The conclusion is that for all multi-indices  $\Theta$ ,  $\theta$  with  $|\Theta| + |\theta| = 3$  and  $\nu(\Theta, \theta) = 0$ , we have that  $\mu(\Theta, \theta) \neq 0 \mod n$ . This proves the first part of theorem 8.1, which actually states that  $P_3 \cap \ker \operatorname{ad}_{H_2}$  is too small to have a nontrivial intersection with  $\ker(T^* - \operatorname{Id})$ .

The proof of the second part of theorem 8.1 is not harder. For  $|\Theta| + |\theta| = 4$ , there are a number of trivial solutions to the equation  $\nu(\Theta,\theta) = 0$ , namely those of the form  $i\omega_j - i\omega_j + i\omega_k - i\omega_k = 0$ . These give rise to the  $\Theta$  and  $\theta$  mentioned in theorem 8.1. All the other solutions to  $\nu = 0$  must be of the form mentioned in section A.3 under the item 'N = 8'. From the first relation we see for instance that  $i\omega_{\frac{n}{6}} + i\omega_{\frac{3n}{14}} - i\omega_{\frac{5n}{14}} = 0$  if n is a multiple of 42. So multi-indices  $\Theta, \theta$  with  $|\Theta| + |\theta| = 4$  can be found such that  $\pm \nu(\Theta, \theta) = i\omega_{\frac{n}{6}} + i\omega_{\frac{3n}{14}} - i\omega_{\frac{n}{14}} - i\omega_{\frac{5n}{14}} = 0$ . But for these multi-indices, one must have that  $\mu(\Theta, \theta) = \pm \frac{n}{6} \pm \frac{3n}{14} \pm \frac{n}{14} \pm \frac{5n}{14} \neq 0$  mod n. One finds the same conclusion for the other relations under the item 'N = 8'. This poves the second part of theorem 8.1.

# References

- [1] Abraham, R., Marsden, J.E., Foundations of Mechanics. The Benjamin/Cummings Publ. Co., Reading, Mass., 1987.
- [2] Arnol'd, V.I., Avez, A., Ergodic problems of classical mechanics. Benjamin, 1968.
- [3] Churchill, R.C., Kummer, M., Rod, D.L. On averaging, reduction, and symmetry in hamiltonian systems. J. Diff. Eq. 49, 359-414, 1983.
- [4] Fermi, E., Pasta, J., Ulam S., Los Alamos Report LA-1940, in 'E. Fermi, Collected Papers', 2, 977-988, 1955.
- [5] Ford, J., The Fermi-Pasta-Ulam problem: paradox turns discovery. Phys. Rep., **213**, 271-310, 1992.
- [6] Gardner, C.S., Greene, J.M., Kruskal, M.D., Miura, R.M., Method for solving the Korteweg-de Vries equation. Physics Rev. Lett. 19, 1095-1097, 1967.
- [7] Izrailev, F.M., Chirikov, B.V., Statistical properties of a nonlinear string. Sov. Phys. Dokl. 11 No. 1, 30-32, 1966.
- [8] Lamb, J.S.W., Roberts, J.A.G., *Time-reversal symmetry in dynamical systems: a survey.* Phys. D **112**, 1-39, 1998.
- [9] Livi, R., Pettini, M., Ruffo, S., Sparpaglione, M., Equipartition threshold in nonlinear large Hamiltonian systems: The Fermi-Pasta-Ulam model. Phys. Rev. A, **31**, 1039-1045, 1985.
- [10] Palais, R.S., The symmetries of solitons. Bull. Amer. Math. Soc. 34, 339-403, 1997.
- [11] Poggi, P., Ruffo, S., Exact solutions in the FPU oscillator chain. Phys. D, **103**, 251-272, 1997.
- [12] Rink, B., Verhulst, F., Near-integrability of periodic FPU-chains. Accepted for publication in Phys. A.
- [13] Sanders, J. A., On the theory of nonlinear resonance. Thesis, University of Utrecht, 1979.
- [14] Verhulst, F., Symmetry and integrability in Hamiltonian normal forms. in "Symmetry and Perturbation Theory", Bambusi, D., Gaeta, G. (eds.), Quaderni GNFM, Firenze, 1998.
- [15] Van der Waerden, B.L., Algebra I. Heidelberger Taschenbücher, Springer, 1966.
- [16] Weissert, T.W., The genesis of simulation in dynamics; pursuing the FPU problem. Springer, New York, 1997.
- [17] Zabuski, N.J., Kruskal, M.D., Interaction of "Solitons" in a collisionless plasma and the recurrence of initial states. Phys. Rev. Lett., 15, 240-243, 1965.