

Explorations for alternating FPU-chains with large mass

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ABSTRACT

We show interaction between high- and low-frequency modes in periodic α -FPU chains with alternating large masses. This high-low frequency interaction is known if the number of particles N is a 4-fold, our treatment discusses the difficult case where the number of particles $N = 2p$ involves p prime. A key role is played by identifying symmetric invariant manifolds, thus reducing the dimension of the problems drastically, and a MATHEMATICA programme focused on these systems. We show explicitly high-low frequency interaction for systems with $2pn$ particles where $2 \leq p \leq 47$ is prime and n is an arbitrary natural number. In addition we have strong arguments for interactions in arbitrary large chains.

My ideas and my opinions feel like groping their way, faltering, stumbling and making false steps; and when I have gone as far as is possible for me, I am not satisfied at all: I see more fields after this, vaguely and in a haze that I cannot clear up.

[Michel de Montaigne, Essais vol. I (1580)]

1. Introduction

The present paper is a sequel to [1]. In large nonlinear chains and in nonlinear wave theory one of the basic questions is whether interaction between very different parts of the spectrum are of importance, see for an example [2]. Fermi–Pasta–Ulam (FPU) chains play a paradigmatic part in discussions of particle interactions, see the surveys [3,4] and for a nice introduction to FPU-like models [5]. Originally FPU chains were studied to understand fundamental questions (ergodicity) in statistical mechanics but the perspective has changed to bifurcations, periodic solutions and waves in nonlinear chains. As usual in theoretical physics and dynamical systems theory in such studies symmetry considerations are basic. It came as a surprise that for certain FPU-like chains widely separate parts of the spectrum can interact at the nonlinear level. For periodic FPU-chains with N alternating large masses it was shown in [1], see also [6], that for α -chains with $N = 2n$ particles, in particular if n is even (N a 4-fold), we have significant interactions caused by external forcing of the low-frequency acoustic modes by a stable or unstable high-frequency optical normal mode. In the case of n prime

the analysis was restricted to the examples $N = 6, 10$; this was caused by the formidable problems posed by linear algebra manipulations to transform to quasi-harmonic (normal mode) equations. For the present paper a special MATHEMATICA programme was developed and used to extend the analysis to periodic chains with many more particles.

It was shown in [1] that in the case $N = 2p$ with p odd invariant manifolds exist allowing drastic reduction of the number of degrees-of-freedom (dof) to $p - 1$. The dynamics is more complicated than in the case N with p even. The novel results in the present paper are both quantitative and qualitative. For p odd and $3 \leq p \leq 47$ we can extend the analysis to find significant interactions between widely different parts of the spectrum, but even more interestingly, we find a surprising circular dependence of the equations of motion involving the interactions.

In general the existence and use of invariant manifolds for FPU-chains is very important because it produces insight in the global dynamics of FPU-chains and enables us to replace the problems by studying submanifolds with less degrees-of-freedom (dof). In a number of seminal papers Czechin et al. identified *bushes* of solutions forming submanifolds for classical (equal masses) FPU-chains; see [7] and further references there; the paper also generalised the results found for two-mode invariant manifolds in [8]. Our analysis is related to this approach, also to “localisation analysis” for FPU-chains in [9]. See also the analysis of acoustic and optical vibrations for a monatomic lattice in [10].

The spatially periodic FPU-chain with N particles where the first oscillator is connected with the last one can be described by the

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Hamiltonian

$$H(p, q) = \sum_{j=1}^N \left(\frac{1}{2m_j} p_j^2 + V(q_{j+1} - q_j) \right). \quad (1)$$

For a general introduction to Hamiltonian dynamics see [11]. Following [12], we choose the number $N = 2n$ of particles even and take the odd masses m_{2j+1} equal to 1, the much larger even masses $m_{2j} = m = \frac{1}{a}$, where $a > 0$ is small. This chain is an example of an alternating FPU-chain. With this choice of the masses, 1 and m , the eigenvalues of the FPU equations of motion near equilibrium split in 2 groups of n eigenvalues with size resp. $O(a)$ (the acoustic group) and size $2 + O(a)$ (the optical group). The cases of $O(1)$ choices of mass m was discussed in [13].

We consider the Hamiltonian near stable equilibrium $p = q = 0$, and use a potential V of the form

$$V(z) = \frac{1}{2} z^2 + \frac{\alpha}{3} z^3 + \frac{\beta}{4} z^4,$$

and speak of an α -chain if $\alpha \neq 0$, $\beta = 0$ and of a β -chain if $\alpha = 0$, $\beta \neq 0$. In this study we will discuss only α -chains.

1.1. Two reduction methods

It was shown in [13] and used in [1] that an *embedding theorem* is useful.

Theorem 1.1. *Consider the equations of motion induced by Hamiltonian (1) for $\alpha \neq 0$ and α - or β -chains, with alternating masses 1, $m > 0$ and n (even) particles. Suppose k is a multiple of n and consider the equations of motion induced by Hamiltonian (1) with identical α , β , m and $2kn$ dof, then there exists a restriction of this larger Hamiltonian system that is equivalent to the first system with $2n$ dof.*

So we have that each alternating periodic FPU-chain with $2n \geq 4$ particles occurs isomorphically as an invariant submanifold in all subsystems with $2kn$ particles ($k = 2, 3, \dots$). This makes the study of small alternating FPU-chains relevant for larger alternating systems.

If we have studied for instance an alternating chain with 6 particles, we will find the dynamics of this chain in a submanifold of alternating chains with $N = 12, 18, 24$ etc. particles. From a reverse point of view, if we study an alternating chain with 32 particles we can at least expect to find invariant manifolds with dynamics of 4, 8 and 16 particles.

For $N = 4$ high-low frequency interaction was shown in [1], so we will have this interaction in all alternating FPU-chains with N a 4-fold. What remains are the infinite number of cases where $N = 2p$ with p odd. If p is odd we can factorise in a product of prime numbers. Showing interaction for one of these prime numbers implies interaction for this odd p because of the embedding theorem. So we have to consider only the cases of p prime.

To understand more of the dynamics in the case $N = 2p$ with p prime we have a second reduction method based on the existence of certain lower-dimensional invariant manifolds derived in [1]. As we will show in Section 2 in this case there exist 2 symmetric invariant manifolds corresponding with $(p-1)$ dof. Using this reduction we will study high-low frequency interaction in alternating chains for $4 \leq N \leq 104$.

1.2. Set-up of the paper

As mentioned above it was shown in [1] that with N a 4-fold and $N = 2p$, $p = 3, 5$, there is considerable interaction between the acoustic and optical group; the analysis was mainly based on asymptotics (averaging). The embedding Theorem 1.1 implies that this high-low frequency interaction holds in system with N a multiple of these values. In Sections 3–4 we extend this analysis with stability considerations and aspects of normal modes.

In Section 5 we consider $p = 9$ (18 particles chain) to obtain insight in the case where p is odd but not prime. Interestingly we find after reduction to symmetric invariant manifolds eight 2nd order equations with the following dependence:

$$x_1 \rightarrow x_8 \rightarrow x_5 \rightarrow x_2 \rightarrow x_7 \rightarrow x_6 \rightarrow x_1,$$

meaning that acoustic x_1^2 forces optical x_8 , x_8^2 forces acoustic x_5 etc.

For $N = 2p$ with $5 \leq p \leq 47$ (p prime and odd) we will consider the results of interaction in Section 6 using a MATHEMATICA programme without giving technical details.

One remarkable feature is that applying the reduction method for the problem with $(p-1)$ dof, we obtain as in the case $p = 9$ “forcing squares” as nonlinearities with one of the acoustic group and one optical. This involves a surprising circular dependence of the equations of motion on each other as shown explicitly for $p = 9$. For the discussion see Section 6.2, where we also consider forcing of optical by optical or acoustic by acoustic, which hides the circularity a bit. Finally two cartoon problems are discussed to demonstrate the influence of mixed quadratic terms on the right-hand sides of the equations of motion.

The figures were produced by using the programme MATCONT under MATLAB; the numerics utilises ode78 with (usually) absolute and relative accuracy 10^{-10} . The MATHEMATICA notebook performing the transformations from equations of motion to quasi-harmonic equations for normal modes is described in Section 6 and [14].

2. Models with p prime

From [1] we have that we can apply symmetries to the system induced by Hamiltonian (1) with $2p$ particles, $p \geq 3$ prime. We assume:

$$\begin{cases} q_p(t) = q_{2p}(t) = 0, \\ q_2(t) = -q_{2p-2}(t), \quad q_4(t) = -q_{2p-4}(t), \dots, q_{p-1}(t) = -q_{p+1}(t), \\ q_1(t) = -q_{2p-1}(t), \quad q_3(t) = -q_{2p-3}(t), \dots, q_{p-2}(t) = -q_{p+2}(t). \end{cases} \quad (2)$$

The symmetry assumptions imply that the value of the momentum integral (see [1]) vanishes. The Hamiltonian system with $2p$ dof contains a submanifold of $2p-2$ dof which is a 4-fold; we are left with two $(p-1)$ dof systems with identical dynamics, quite a reduction. The $(p-1)$ dof system is of the form:

$$\ddot{q} + Bq = \alpha N(q)$$

with $q = (q_1, \dots, q_{p-1})^T$, B is a $(p-1) \times (p-1)$ matrix and $N(q)$ a homogeneous vector, quadratic in the q variables. Explicitly for $p > 5$:

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_2 &= \alpha(q_2^2 - 2q_1q_2), \\ m\ddot{q}_2 + 2q_2 - q_1 - q_3 &= \alpha(q_3^2 - 2q_2q_3 + 2q_1q_2 - q_1^2), \\ \ddot{q}_3 + 2q_3 - q_2 - q_4 &= \alpha(q_4^2 - 2q_3q_4 + 2q_2q_3 - q_2^2), \\ m\ddot{q}_4 + 2q_4 - q_3 - q_5 &= \alpha(q_5^2 - 2q_4q_5 + 2q_3q_4 - q_3^2), \\ \dots &= \alpha(\dots), \\ m\ddot{q}_{p-1} + 2q_{p-1} - q_{p-2} &= \alpha(2q_{p-1}q_{p-2} - q_{p-2}^2). \end{cases} \quad (3)$$

The normal mode frequencies of system (3) are derived from the single eigenvalues of B , resp. $\sqrt{2+O(a)}$ and $O(\sqrt{a})$. To put the system in quasi-harmonic form we use a linear transformation that diagonalises B and puts the eigenvalues on the diagonal. The linear transformation of q keeps the nonlinearities quadratic, resulting in interactions. In [1] the cases $p = 2, 3, 5$ were discussed and consequently chains with $4n, 6n, 10n$ particles, n a natural number.

3. Periodic FPU α -chain with 6 particles

The invariant manifolds described by (2) can be used to consider systems with 6 particles ($p = 3$). Interactions of this chain were studied in [1] using averaging, we add an analysis of the symmetric invariant manifolds, their stability in 12-dimensional phase-space and some new aspects of the general dynamics. The stability analysis of invariant manifolds is not easy in the case of high dimensions; we will use the stability results of individual modes and in addition we obtain insight from application of the Poincaré recurrence theorem. The eigenvalues, producing squared frequencies of the linearised system are:

$$\omega_1^2 = 2(1+a), \quad \omega_{2,3}^2 = a+1+\sqrt{a^2-a+1}, \quad \omega_{4,5}^2 = a+1-\sqrt{a^2-a+1}, \quad \omega_6^2 = 0. \quad (4)$$

For $a = 0.01$ the corresponding eigenvalues are 2.02, 2.00504, 0.0149623, 0.

3.1. Stability of symmetric invariant manifolds

The equations of motion induced by Hamiltonian (1) contain symmetric invariant manifolds described by system (3). In the general case with the number of particles $N = 2p$ with p odd, we have that $q_p(t) = q_{2p}(t) = 0$, $t \geq 0$. In the case $p = 3$ we have:

$$q_3(t) = q_6(t) = 0, \quad q_2(t) = -q_4(t), \quad q_1(t) = -q_5(t). \quad (5)$$

It is clear from system (3) that on breaking the symmetry conditions, in the case $p = 3$, the modes q_3, q_6 (in general q_p, q_{2p}) are forced. So the solutions $q_3 = q_6 = 0$ will not persist, the symmetric invariant manifolds are expected to be unstable. Instead of explicit matrix calculations we can demonstrate the instability by high precision numerical analysis as indicated in the Introduction. We show this explicitly for the case of 6 particles in Fig. 1.

A related criterion is using the Poincaré recurrence theorem. Hamiltonian flow on a bounded energy manifold will after some time return arbitrarily close to the initial value. Of course the time for this return will depend on our definition of closeness and the particular system studied, see for discussion and Refs. [15]. The computation illustrated in Fig. 1 should lead after some time to $q_3(t), q_6(t)$ simultaneously approaching zero arbitrarily close but this takes longer than 16000 timesteps. The dynamics shows more complexity than expected.

3.2. Symmetric invariant manifold

If $2p = 6$ the dynamics in the symmetric invariant manifold for q_1, q_2 is described by:

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_2 &= \alpha(q_2^2 - 2q_1q_2), \\ m\ddot{q}_2 + 2q_2 - q_1 &= \alpha(2q_1q_2 - q_1^2). \end{cases} \quad (6)$$

System (6) has 4 critical points (we take $\alpha = 1$): $(q_1, q_2, \dot{q}_1, \dot{q}_2) = (1, 2, 0, 0)$, $(1, -1, 0, 0)$, $(-2, -1, 0, 0)$ and the origin. The first three are indicated by C_1, C_2, C_3 . The eigenvalues near the origin are $-a - 1 \pm \sqrt{a^2 - a + 1}$ corresponding with the frequencies $\omega_{2,3}, \omega_{4,5}$. For the normal modes in system (6) we have one optical, and one acoustic. For $a = 0.01$ the eigenvalues (frequencies squared) are:

$$\omega_1^2, \omega_2^2 = 0.0149623, 2.00504$$

Denoting the critical points by (q_1, q_2) we find the eigenvalues: $(1, 2) \rightarrow \pm 2.4525i, \pm 0.1223$, $(1, -1) \rightarrow \pm 0.5477i, \pm 0.5477$, $(-2, -1) \rightarrow \pm 0.5758i, \pm 0.5211$. We conclude that for each of the nontrivial equilibria we have a centre manifold corresponding with 2 purely imaginary eigenvalues, one stable manifold and one unstable manifold. All nontrivial equilibria are unstable and may produce unbounded solutions.

Note that the full 6 dof Hamiltonian system contains system (6) supplemented by the (mirrored) modes q_4, q_5 . The symmetry assumptions reduce the 6 dof system to two equivalent 2 dof systems. Using the eigenvalues and eigenvectors for system (6) we can construct a 2 dof system in quasi-harmonic form with dynamics described by:

$$\begin{cases} \ddot{x}_1 + 0.0149623x_1 &= \alpha(0.0074805894x_1^2 + 0.0004488580x_1x_2 \\ &\quad - 0.0395000057x_2^2), \\ \ddot{x}_2 + 2.00504x_2 &= \alpha(0.0056956264x_1^2 - 2.0048858034x_1x_2 \\ &\quad - 0.0300748059x_2^2). \end{cases} \quad (7)$$

The 2 frequencies ω_1, ω_2 are not resonant; according to Lyapunov we can continue the linear normal modes in a neighbourhood of the origin. It is straightforward to obtain a convergent series approximation of the normal modes by the Poincaré-Lindstedt method.

3.3. Interactions in a neighbourhood of the origin

System (7) is, apart from the coefficients, symmetric in x_1, x_2 showing similar forcing of acoustic modes by optical ones and vice versa. In the equation for x_1 the square x_2^2 will be forcing, in the equation for x_2 this will be x_1^2 . Starting with initial zero values in the optical mode the normal mode $x_1(t)$ shows interactions with the optical mode. Continuing the optical mode with zero acoustic initial values we find small interactions.

An asymptotic approximation scheme runs as follows. Near the origin we rescale the coordinates $x \mapsto \varepsilon x$ and divide the resulting equations by ε . We may replace $\varepsilon\alpha$ by ε in system (7). The lowest order normal form is easy to obtain, see for the procedure [16]. The normal form has 3 integrals, the Hamiltonian

$$H = \frac{1}{2}(\dot{x}_1^2 + \omega_1^2 x_1^2) + \frac{1}{2}(\dot{x}_2^2 + \omega_2^2 x_2^2) - \varepsilon 0.00249x_1^3 + \varepsilon 0.001x_2^3, \quad (8)$$

and the 2 actions $\frac{1}{2}(\dot{x}_j^2 + \omega_j^2 x_j^2)$, $j = 1, 2$. Quasiperiodic interaction will show at the next order of approximation. A more direct and easier approach runs as follows.

To approximate the quasi-periodic flow we use the lowest order $\varepsilon = 0$ approximations:

$$x_1^0(t) = a_0 \cos \omega_1 t + b_0 \sin \omega_1 t, \quad x_2^0(t) = c_0 \cos \omega_2 t + d_0 \sin \omega_2 t. \quad (9)$$

Introducing the zero order approximation (9) in the right-hand sides of system (7) we obtain an approximation of first order; as the modes are not resonant we get no secular terms.

Some numerical experiments for $\alpha = 1$ are shown in Fig. 2 where we abbreviate in the caption $\dot{x} = v$. In Fig. 2 we have $a = 0.01$, $x_2(0) = 0.2$ and the other initial values zero. We find interaction in the form of excitation of the acoustic mode x_1 .

Consider now the first order approximation of $x_1(t)$ described above, If we start with the initial values used in Fig. 2 we have for $t \geq 0$, $x_1^0(t) = 0$, $x_2^0(t) = 0.2 \cos \omega_2 t$. The next step is solving an inhomogeneous linear equation to find the excitation of the acoustic mode $x_1(t)$ from:

$$\ddot{x}_1 + 0.0149623x_1 = -0.0395000057(0.2 \cos \omega_2 t)^2.$$

Comparing $x_1^1(t)$ with the result in Fig. 2 we find on 200 timesteps the same behaviour with error 0.02. Extending the Poincaré expansion procedure we can extend the accuracy and/or the time interval. Another possibility is to use 2nd order averaging.

In the case of 2 dof with resonant frequencies the phase-space dynamics near stable equilibrium is more interesting. In our case of widely separated frequencies we find quasiperiodic solutions corresponding with families of tori but as prominent feature significant interaction of modes.

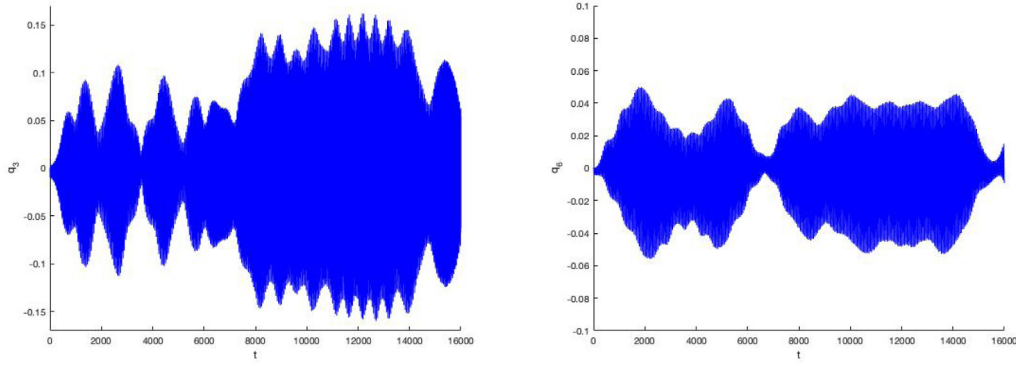


Fig. 1. Solutions in the case of $N = 6$ ($p = 3$) described by the chain induced by Hamiltonian (1) close to the symmetric invariant manifolds for 16000 timesteps; $a = 0.01$, $\alpha = 1$. The initial values close to symmetry are: $q_1(0) = 0.08$, $q_2(0) = -0.085$, $q_3(0) = 0$, $q_4(0) = 0.075$, $q_5(0) = -0.07$, $q_6(0) = 0$ and initial velocities zero. We observe forcing of the modes q_3 , q_6 showing instability of the symmetric invariant manifolds.

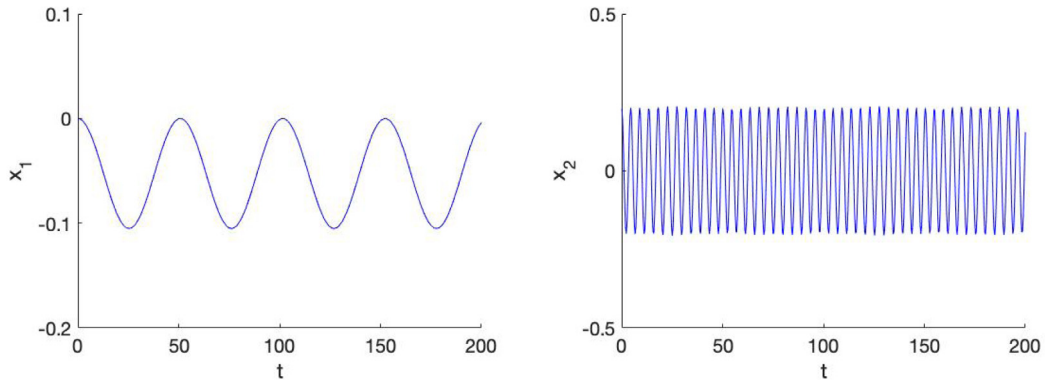


Fig. 2. Solutions within the symmetric invariant manifold in the case $p = 3$ described by Eq. (7), $a = 0.01$, $\alpha = 1$. The coordinates are $x_1, v_1 = \dot{x}_1$ (acoustic) and $x_2, v_2 = \dot{x}_2$ (optical) of the α -chain with 6 particles in 200 timesteps. The initial values are $x_1(0) = v_1(0) = 0$, $x_2(0) = 0.2$, $v_2(0) = 0$. We observe forcing of the acoustic mode.

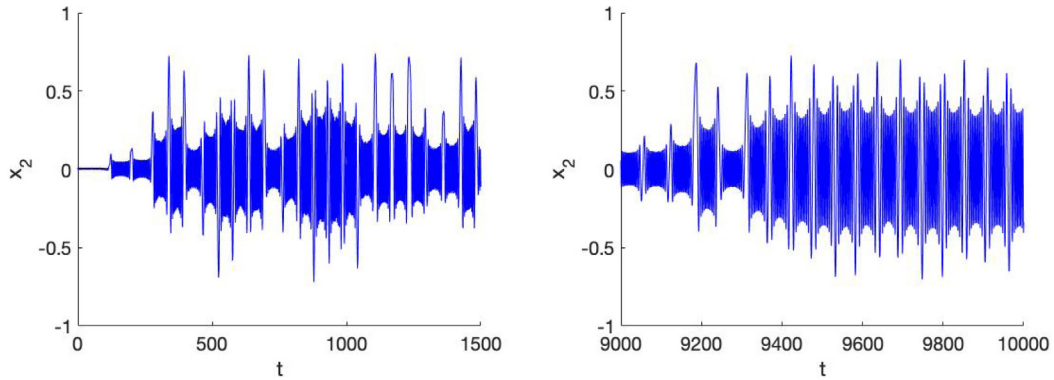


Fig. 3. Solutions in the case $p = 3$ described by Eq. (7), $a = 0.01$, $\alpha = 1$. The coordinates are $x_1, v_1 = \dot{x}_1$ (acoustic) and $x_2, v_2 = \dot{x}_2$ (optical) of the α -chain with 6 particles; left $x_2(t)$ in 1500 timesteps, right the time series from 9k till 10k. The initial values are $x_1(0) = 2$, $v_1(0) = 0$, $x_2(0) = 0.01$, $v_2(0) = 0$ near unstable equilibrium. We observe forcing of the optical mode x_2 .

3.4. Interactions near unstable equilibria

The general dynamics merits closer attention, we perform calculations for larger initial values, take $\alpha = 1$. As an example we consider the dynamics near equilibrium C_1 with coordinate values $(1, 2, 0, 0)$ in system (6). The equilibrium is unstable and although we can approximate the centre manifold with high accuracy, we cannot be certain to start exactly in this submanifold. Using system (7) we start with

initial conditions $(2, 0, 0, 0)$. Inverting our transformations we find that for system (6) this implies $q_1(0) = 1.00754$, $q_2(0) = 2$ so we start close to equilibrium C_1 . The numerical solutions increase rapidly to very large numbers, suggesting unbounded behaviour.

Next we choose initial conditions $(2, 0.01, 0, 0)$ corresponding in system (6) with $q_1(0) = 0.98768$, $q_2(0) = 2.0001$, again close to C_1 . The numerics shown in Fig. 3 suggest that the initial values are located in a stable centre manifold; the time series $x_1(t)$ (not shown) shows

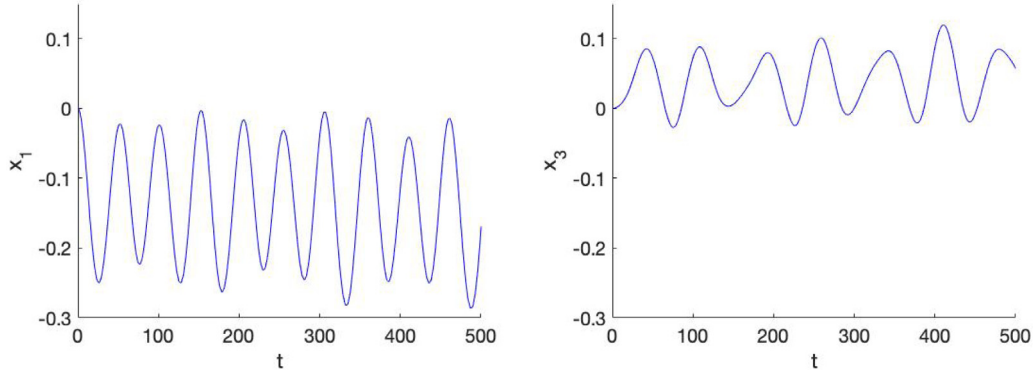


Fig. 4. Solutions of system (12) (case $p = 5$) producing 2 invariant manifolds with 4 dof and equivalent dynamics, $a = 0.01$. Initial values $x_1(0), x_3(0) = 0$ (acoustic) and $x_2(0), x_4(0) = 0.15$ (optical) in 500 timesteps. The initial velocities are zero. We observe forcing of the acoustic modes and recurrence.

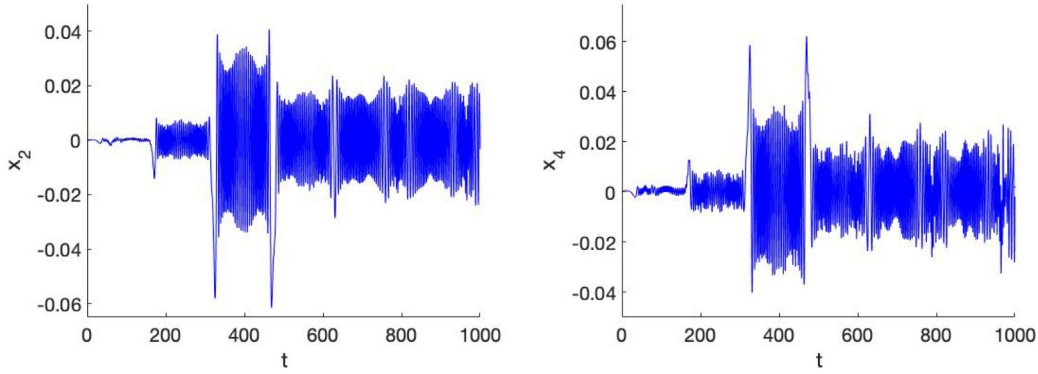


Fig. 5. Solutions in the case $p = 5$ starting near the unstable x_1 normal mode in system (12). The initial conditions are $x_1(0) = 0.25$, $\dot{x}_1(0) = 0.065$, $x_3(0) = 0.01$, $\dot{x}_3 = 0.01$. The initial x_2, x_4 positions and velocities are zero. We observe excitation of the optical modes x_2, x_4 .

oscillations between -1 and 2 . We have strong excitation of the optical mode. The stable and unstable manifolds of the 4-dimensional equilibrium are outside the centre manifold, but can still be near the orbits. The light-grey vertical segments show relatively fast motion away from these 2-dimensional saddle structures.

4. Periodic FPU α -chain with 10 particles

As the next case we consider $N = 10$. With $p = 5$ the symmetry assumptions (2) produce invariant manifolds with dynamics described by 2 equivalent 4 dof systems. We have for the 1st system:

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_2 &= q_2^2 - 2q_1q_2, \\ m\ddot{q}_2 + 2q_2 - q_1 - q_3 &= q_3^2 - 2q_2q_3 + 2q_1q_2 - q_1^2, \\ \ddot{q}_3 + 2q_3 - q_2 - q_4 &= q_4^2 - 2q_3q_4 + 2q_2q_3 - q_2^2, \\ m\ddot{q}_4 + 2q_4 - q_3 &= 2q_3q_4 - q_3^2. \end{cases} \quad (10)$$

The first two equations are identical to the first two of the general case in system (3), but the linear transformation to quasi-harmonic equations will be different in the general case. The eigenvalues of the linear part on the left-hand side are:

$$a + 1 \pm \sqrt{1 - \frac{1}{2}(1 + \sqrt{5})a + a^2}, \quad a + 1 \pm \sqrt{1 - \frac{1}{2}(1 - \sqrt{5})a + a^2}, \quad (11)$$

4.1. Equilibria

Equilibria correspond with critical points of the vector field describing system (10). To find the equilibria we have to solve 4 quadratic algebraic equations. Apart from the trivial solution (the origin of phase-space) there are at most 15 different solutions. With velocities zero

we find easily: $(q_1, q_2, q_3, q_4) = (2, -1, 1, -2), (2, -1, 1, 3), (3, -1, 1, -1), (3, -1, 1, 3)$; more equilibria can be obtained by considering the cases $2q_1 = q_2$ and $2q_3 = q_4$.

4.2. Dynamics and interaction near the origin

The origin corresponds with stable equilibrium. After transformation to quasi-harmonic form we consider the dynamics described by the system:

$$\begin{cases} \ddot{x}_1 + 0.0180728x_1 &= -0.04x_4^2 - 0.13x_2x_4 + 0.018x_1x_3 \\ &\quad + 0.00065x_2x_3 + 0.009x_3^2 + \\ &\quad 0.0004x_1x_4 + 0.00025x_3x_4, \\ \ddot{x}_2 + 2.00193x_2 &= +0.0063x_1x_3 - 0.0019x_3^2 - 2.0018x_2x_3 \\ &\quad - 1.251x_1x_4 - 0.045x_2x_4 + \\ &\quad 1.251x_3x_4 + 0.0086x_4^2, \\ \ddot{x}_3 + 0.00686474x_3 &= -0.039x_2^2 + 0.049x_2x_4 + 0.00025x_1x_2 \\ &\quad + 0.0069x_1x_3 - 0.00015x_2x_3 + \\ &\quad 0.00009x_1x_4 + 0.0034x_1^2, \\ \ddot{x}_4 + 2.01314x_4 &= 0.0051x_1^2 + 0.0062x_1x_3 - 3.22x_1x_2 - 0.05798x_2^2 \\ &\quad + 3.22x_2x_3 - \\ &\quad 2.013x_1x_4 + 0.0443x_2x_4. \end{cases} \quad (12)$$

The modes x_1, x_3 belong to the acoustic group, x_2, x_4 are optical. The largest coefficients of the quadratic terms are found in the optical group x_2, x_4 . This will also influence the dynamics.

A difference with the case $p = 3$ is that within the acoustic and optical group we have a detuned 1 : 1 resonance. In [17] the 1 : 1 resonance is studied with results on in-phase and out-of-phase periodic solutions; in [18] (sections 1.3 and 3) a systematic study was set up, for instance regarding the 1 : 1 : 1 : 1 resonance. We note that the optical modes in system (12) are closer to exact resonance than the acoustic ones. For each equation we have 2 forcing terms, for x_1 they are x_4^2 and x_2x_4 ; for x_2 we have x_3^2 and x_1x_3 . Terms like x_2x_3 or x_1x_4 have initially less influence as can be shown by averaging.

In Fig. 4 we start with nonzero optical modes x_2, x_4 leading to significant $x_1(t)$ oscillations.

Invariant manifolds and normal modes

As the two 1 : 1 resonances are detuned we can apply Lyapunov continuation, the normal modes exist. However, all the normal modes are unstable because of the high-low frequency interaction.

System (12) contains 2 invariant manifolds described by the systems:

$$\begin{aligned}\ddot{x}_1 + 0.01807x_1 &= -0.04x_4^2 + 0.0004x_1x_4, \quad \ddot{x}_4 + 2.01314x_4 \\ &= -0.0051x_1^2 - 2.013x_1x_4,\end{aligned}\quad (13)$$

$$\begin{aligned}\ddot{x}_2 + 2.00193x_2 &= -0.0019x_3^2 - 2.0018x_2x_3, \quad \ddot{x}_3 + 0.00686474x_3 \\ &= -0.039x_2^2 - 0.00015x_2x_3.\end{aligned}\quad (14)$$

Within these invariant manifolds the normal modes are harmonic and unstable but on long intervals of time. Because of the recurrence theorem for measure-preserving maps, in particular Hamiltonian systems on a bounded energy manifold, high frequency modes that excite low frequency modes imply that the reverse will also happen, except that the energy stored in low frequency modes is much less than in high frequency modes. We demonstrate this for the submanifold consisting of the (x_1, x_4) modes of system (13). In Fig. 5 we show excitation of mode 4 when starting close to the unstable x_1 normal mode.

5. Periodic FPU α -chain with 18 particles (p not prime)

The motivation to study briefly the case $p = 9$ is to compare with the results in [1] where after the case $N = 4$ the case $N = 8$ keeps the interaction of the chain with 4 particles but also shows new phenomena, in particular new invariant manifolds. In the case of 18 particles we expect from the embedding theorem a submanifold corresponding with 6 particles ($p = 3$).

We will use now the theory of symmetric invariant manifolds from Section 2. Transforming the 18 equations of motion induced by Hamiltonian (1) to quasi-harmonic form by $q \mapsto x$ we find 2 symmetric invariant manifolds with 8 2nd order equations. The 8 eigenvalues λ_j are:

$$\begin{aligned}0.019391, 2.00061, 0.0149623, 2.00504, 0.00821511, 2.01178, \\ 0.00231905, 2.01768.\end{aligned}\quad (15)$$

The acoustic group corresponds with indices $j = 1, 3, 5, 7$, the optical group with even indices. Note that from the embedding theorem we expect submanifolds corresponding with 6 and 12 particles, but now we are working in the subsystem (3) corresponding with $p - 1 = 8$ particles.

5.1. The reduced system

The system in x -coordinates becomes:

$$\begin{cases} \ddot{x}_1 + \lambda_1 x_1 = 0.00970x_5^2 + 0.0194x_3x_5 + 0.000490x_4x_5 \\ \quad + 0.000320x_6x_5 - 0.0401x_6^2 \\ \quad + 0.000434x_3x_6 - 0.0906x_4x_6 + 0.0194x_1x_7 \\ \quad + 0.000746x_2x_7 + 0.0194x_3x_7 \\ \quad + 0.000259x_4x_7 + 0.000404x_1x_8 \\ \quad - 0.352x_2x_8 + 0.000354x_3x_8 - 0.140x_4x_8, \\ \ddot{x}_2 + \lambda_2 x_2 = -0.00140x_5^2 + 0.00380x_3x_5 - 0.794x_4x_5 + 0.703x_6x_5 \\ \quad + 0.00579x_6^2 - 0.703x_3x_6 - 0.0177x_4x_6 + 0.00229x_1x_7 \\ \quad - 2.00x_2x_7 - 0.00201x_3x_7 + 0.794x_4x_7 - 1.08x_1x_8 \\ \quad - 0.0417x_2x_8 + 1.08x_3x_8 + 0.0145x_4x_8, \\ \ddot{x}_3 + \lambda_3 x_3 = 0.00748x_5^2 + 0.000449x_4x_3 - 0.0395x_4^2 + 0.0150x_1x_5 \\ \quad + 0.000953x_2x_5 + 0.000335x_1x_6 - 0.176x_2x_6 + 0.0150x_1x_7 \\ \quad - 0.000504x_2x_7 + 0.0150x_5x_7 + 0.000114x_6x_7 + 0.000273x_1x_8 \\ \quad + 0.272x_2x_8 + 0.000176x_5x_8 - 0.0954x_6x_8, \\ \ddot{x}_4 + \lambda_4 x_4 = 0.00570x_3^2 - 2.00x_4x_3 - 0.0301x_4^2 + 0.00959x_1x_5 \\ \quad - 5.05x_2x_5 - 1.78x_1x_6 - 0.113x_2x_6 + 0.00507x_1x_7 \\ \quad + 5.05x_2x_7 - 0.00327x_5x_7 + 1.78x_6x_7 - 2.74x_1x_8 \\ \quad + 0.0921x_2x_8 + 2.74x_5x_8 + 0.0209x_6x_8, \\ \ddot{x}_5 + \lambda_5 x_5 = 0.00411x_7^2 + 0.00822x_3x_7 - 0.0000708x_4x_7 + 0.0000377x_8x_7 \\ \quad - 0.0404x_8^2 + 0.00821x_1x_3 + 0.000523x_2x_3 + 0.000208x_1x_4 \\ \quad - 0.109x_2x_4 + 0.00821x_1x_5 - 0.000386x_2x_5 + 0.000135x_1x_6 \\ \quad + 0.0968x_2x_6 + 0.0000967x_3x_8 + 0.0592x_4x_8, \\ \ddot{x}_6 + \lambda_6 x_6 = -0.000724x_7^2 + 0.00371x_3x_7 + 2.27x_4x_7 + 3.10x_8x_7 \\ \quad + 0.00711x_8^2 + 0.0109x_1x_3 - 5.73x_2x_3 - 2.27x_1x_4 \\ \quad - 0.145x_2x_4 + 0.00801x_1x_5 + 5.73x_2x_5 - 2.01x_1x_6 \\ \quad + 0.0944x_2x_6 - 3.10x_3x_8 + 0.0267x_4x_8, \\ \ddot{x}_7 + \lambda_7 x_7 = 0.00116x_1^2 + 0.0000892x_2x_1 + 0.00232x_3x_1 + 0.0000310x_4x_1 \\ \quad - 0.0389x_2^2 - 0.0000781x_2x_3 + 0.0309x_2x_4 + 0.00232x_3x_5 \\ \quad - 0.0000200x_4x_5 + 0.0000177x_3x_6 + 0.0108x_4x_6 + 0.00232x_5x_7 \\ \quad - (6.91 \times 10^{-6})x_6x_7 + 0.0000106x_5x_8 + 0.0148x_6x_8, \\ \ddot{x}_8 + \lambda_8 x_8 = 0.00214x_1^2 - 3.73x_2x_1 + 0.00374x_3x_1 - 1.48x_4x_1 \\ \quad - 0.0717x_2^2 + 3.73x_2x_3 + 0.0498x_2x_4 + 0.00242x_3x_5 \\ \quad + 1.48x_4x_5 - 1.31x_3x_6 + 0.0113x_4x_6 + 0.000942x_5x_7 \\ \quad + 1.31x_6x_7 - 2.02x_5x_8 + 0.00601x_6x_8.\end{cases}\quad (16)$$

A first consequence of the forcing is that the acoustic and optical groups do not exist as separate invariant manifolds. To be explicit: each equation in system (16) contains one quadratic forcing term of the other group and 3 quadratic mixed forcing terms of the other group, for instance for the first equation x_6^2 and x_4x_6, x_2x_8, x_4x_8 . The largest coefficients of the quadratic terms are found in the optical group for the x_6, x_8 equations. Analogous to the case of $p = 3$ we have detuned (1 : 1 : 1 : 1) resonances that will affect the dynamics.

The (x_3, x_4) invariant manifold.

There is an invariant submanifold given by $x_1 = x_2 = x_5 = x_6 = x_7 = x_8 = 0$. The system is:

$$\begin{cases} \ddot{x}_3 + 0.01496x_3 = 0.00748x_3^2 + 0.000449x_4x_3 - 0.0395x_4^2, \\ \ddot{x}_4 + 2.00504x_4 = 0.00570x_3^2 - 2.00x_4x_3 - 0.0301x_4^2. \end{cases} \quad (17)$$

The system (17) is identical (modulo numeric abbreviations) to system (7) for $p = 3$. The presence of system (17) as a submanifold in the case $p = 9$ is predicted by the embedding theorem of [13], see also [1]. We found only 1 invariant manifold for system (16).

Normal modes

As the $1 : 1 : 1 : 1$ resonances are all detuned we can apply Lyapunov continuation, the normal modes exist. Even when using normal forms, applying detuned resonance, we can use the Weinstein [19] theorem for periodic normal mode solutions. However, all the normal modes are unstable because of the high-low frequency interaction. From system (16) we can list the quadratic forcing of each mode between brackets; we have

$$x_1(x_6), x_2(x_5), x_3(x_4), x_4(x_3), x_5(x_8), x_6(x_7), x_7(x_2), x_8(x_1).$$

So acoustic x_1 excites optical x_6 , x_6 excites acoustic x_7 etc. This circularity of excitations persists for more than 18 dof, it will be an important aspect of further study.

6. Alternating FPU-chains with many particles

Our MATHEMATICA programme described below produces by suitable linear transformations quasi-harmonic systems of equations where the normal modes can be identified. As in our studies of the cases $p = 3, 5$, but considering now all cases p prime, $p \leq 47$ we find out again whether for instance quadratic optical terms x_i^2 arise as forcing terms in the quasi-harmonic form of the acoustic part of the system. This turns out to be the case for all prime numbers $p = 3, 5, 7, \dots, 47$. We conclude that we have interaction between the acoustic and optical group for the alternating FPU-chain with large mass up to 104 particles and all multiples of these cases.

6.1. The notebook `plotinteractionp.nb`

We developed and used a Mathematica notebook `plotinteractionp.nb`, see for details [14]. Given an odd p it first sets up the system in q -variables (3) in symbolic form. As described in Section 2 it is of the form $\ddot{q} + Bq = \alpha N(q)$ with B a $(p-1) \times (p-1)$ matrix and $N(q)$ a quadratic vector function. We need to get to quasiharmonic form. We know the eigenvalues in symbolic form of the matrix B , but the notebook finds them anyway, also in symbolic form. Finding the corresponding matrix of eigenvectors takes longer. As the matrix that is found becomes singular for $a = 0$, we rescale the offending rows by a factor $1/a$. Then we substitute high precision numbers before inverting the matrix. We are ready to produce the system in quasiharmonic form in x -variables and can start plotting solutions.

6.2. Forcing squares on the right-hand sides

When checking where the squares occur on the right-hand sides of a system in x -coordinates like system (12), a remarkable pattern arises. To study this pattern we considered in detail chains with $N = 2p$ particles for odd p , $p \leq 47$. Recall that the modes come in pairs consisting of an acoustic mode with variable x_{2j-1} and an optical mode with variable x_{2j} . The modes $2j-1$ and $2j$ belong together in the sense that $\lambda_{2j-1}, \lambda_{2j}$ are the eigenvalues of a matrix

$$\begin{pmatrix} 2a & 2a \cos\left(\frac{\pi j}{p}\right) \\ 2 \cos\left(\frac{\pi j}{p}\right) & 2 \end{pmatrix}.$$

Note that $\lambda_{2j} + \lambda_{2j-1} = 2 + 2a$. Compare with (7). Now if one makes MATHEMATICA look where x_{2i-1}^2, x_{2i}^2 occur, then one finds that there is exactly one j so that they both occur in the right-hand side of the equations for $\ddot{x}_{2j-1} + \lambda_{2j-1}x_{2j-1}$ and $\ddot{x}_{2j} + \lambda_{2j}x_{2j}$. And x_{2i-1}^2, x_{2i}^2 occur nowhere else. Explicit examples are systems (12) and (16).

Let us write $j = \rho(i)$, so that ρ is the permutation of $\{1, \dots, (p-1)/2\}$ that associates j to i . We have MATHEMATICA determine ρ for all odd p up to 47. As pointed out to us by Stienstra [20] one has

$$\rho(i) = \min(2i, p - 2i) \quad (18)$$

in all these cases. If p is prime, $5 \leq p \leq 47$, then ρ has no fixed points. On the other hand, when p is divisible by three, we may have $i = j = \rho(i)$ as in system (17). But notice that in (15) the eigenvalues are ordered differently, making the formula $\rho(i) = \min(2i, p - 2i)$ less apparent. MATHEMATICA computes the cycle decomposition of ρ . There is a connection between the cycle structure of ρ and the existence of certain invariant submanifolds of phase space. Indeed if $Y \subset \{1, \dots, p-1\}$ is a nonempty proper subset of indices such that

$$V(Y) = \{x_i = \dot{x}_i = 0 \text{ for } i \in Y\}$$

is an invariant submanifold of phase space, then $2i-1 \notin Y$ implies $2\rho(i)-1 \notin Y$. So $\{i \mid 2i-1 \in Y\}$ is a union of cycles of ρ . (We consider fixed points as cycles too.) Observe that $\{i \mid 2i-1 \in Y\} = \{i \mid 2i \in Y\}$. Not every union Y of cycles will give an invariant manifold, as one must also take mixed terms into account. But the cycle decomposition of ρ greatly simplifies the search for Y with $V(Y)$ invariant.

One may also use plotting to search experimentally for suitable subsets Y . Simply take initial values such that initially a single mode is active and then look at the plots of all modes. Clearly it suffices to try one initially mode for each cycle of ρ .

For instance, when $p = 17$ the permutation ρ has two cycles and none of them yields an invariant proper submanifold. In fact we did not find any invariant manifold of type $V(Y)$ for primes $3 \leq p \leq 47$. We present a few results without technical details.

Multiples of $p = 3$

If $p = 9$ (18 particles), see also Section 5, ρ has cycles of length 1, 3 and we recover subsystem (7) with 2 modes.

If $p = 15$ (30 particles) we recover the submanifolds with 2 modes and 4 modes respectively; in this case 5 is also a divisor.

For $p = 27$ (54 particles) we find one $V(Y)$ with 8 modes, containing another one with 2 modes.

For $p = 45$ we find four different invariant $V(Y)$. They have 2, 4, 8 or 14 modes, corresponding with the respective divisors 3, 5, 9, 15 of 45. There are four containments: The one with 14 modes contains both the one with 2 modes and the one with 4 modes. The one with 2 modes is contained in both the one with 8 modes and the one with 14 modes. We recognise the divisor relations between 3, 5, 9, 15.

Multiples of $p = 5$

The case $p = 5$ (10 particles) is discussed in Section 4.

The case $p = 15$ has also 3 as a divisor, see above.

If $p = 25$ (50 particles) we find a $V(Y)$ with 4 modes.

More generally, if q is a proper divisor of an odd p , $p \leq 47$, we find a subsystem of $(q-1)$ modes inside the system in x -coordinates that has $(p-1)$ modes. More specifically, the $(q-1)$ modes that remain are the ones involving x_i whose λ_i is an eigenvalue of a matrix

$$\begin{pmatrix} 2a & 2a \cos\left(\frac{\pi j}{q}\right) \\ 2 \cos\left(\frac{\pi j}{q}\right) & 2 \end{pmatrix}$$

with $1 \leq j \leq (q-1)/2$. So that is the form that the embedding Theorem 1.1 now takes.

For odd p , $p \leq 47$, we find no $V(Y)$ that are not explained by the embedding theorem.

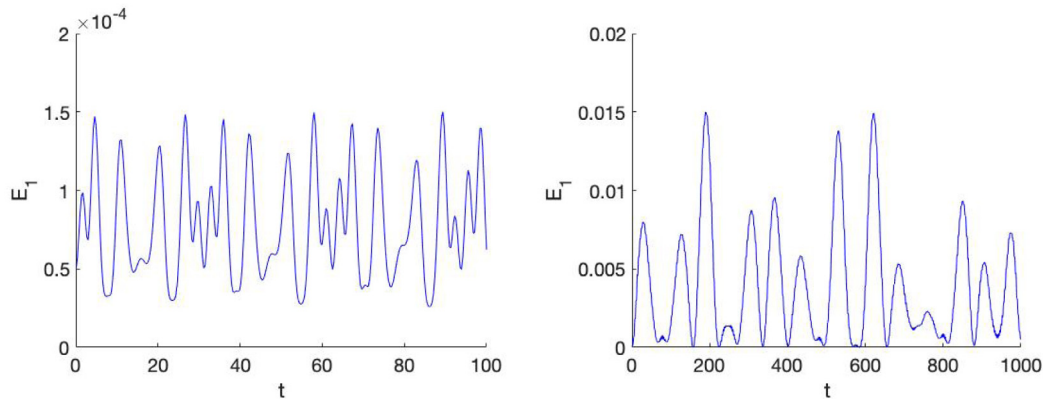


Fig. 6. The action $E_1(t)$ for 2 cartoon problems. Left the behaviour in system (19) where $\omega_1 = 0.1$, $\omega_2 = 1$, $x(0) = 0.1$, $y(0) = 0.1$, $E_1(0) = 0.00005$ and initial velocities zero. Right the behaviour in system (20) where $\omega_1 = 0.1$, $\omega_2 = 1$, $\omega_3 = 1.05$, $x(0) = 0.1$, $y(0) = 0.3$, $z(0) = 0.3$, $E_1(0) = 0.00005$ and initial velocities zero.

6.3. Quadratic terms and normal forms

Near stable equilibrium it is natural to apply normal form analysis to the systems. Apart from forcing squares we have mixed terms of the acoustic and optical groups but these terms are non-resonant; they will appear in the normal form at very high order and have little influence. Forcing quadratic terms consisting of only mixed acoustic or only mixed optical contributions will have forcing influence as they are in detuned resonance. For instance in the case of system (16) a calculation shows that we are still left with 8 quadratic terms on the right-hand side of each equation. Analysing the normal form poses a formidable problem.

Instead of normalising the systems obtained in the preceding sections we demonstrate the influence of mixed quadratic terms by integrating 2 typical Hamiltonian cartoon problems. In both cases we have coupled oscillators with widely separated frequencies; see [21] for an introduction and references. The standard procedure would be to introduce slowly-varying variables, for instance amplitude-phase or action-angle variables, see [16], to compute by averaging-normalisation an approximating normal form system. We leave out these technical details and will discuss the numerical results shown in Fig. 6. The first cartoon is the system:

$$\begin{cases} \ddot{x} + \omega_1^2 x = xy, \\ \ddot{y} + \omega_2^2 y = \frac{1}{2}x^2. \end{cases} \quad (19)$$

We introduce the action $E_1 = 0.5(\dot{x}^2 + \omega_1^2 x^2)$. In Fig. 6 (left) we have $0 < \omega_1 \ll \omega_2$. As predicted by normalisation the action $E_1(t)$ shows only small variations around its initial value. In the 2nd cartoon we have detuned forcing:

$$\begin{cases} \ddot{x} + \omega_1^2 x = 0.2yz, \\ \ddot{y} + \omega_2^2 y = 0.2xz + 0.25(z^2 + 2yz), \\ \ddot{z} + \omega_3^2 z = 0.2xy + 0.25(y^2 + 2yz), \end{cases} \quad (20)$$

where $\omega_1 \ll \omega_2$ and ω_2 is close to ω_3 . The x normal mode is harmonic. The y, z oscillators are in detuned resonance and are strongly forcing the x -oscillator, see Fig. 6 (right).

7. Conclusions

1. We have demonstrated interaction between acoustic and optical modes for periodic FPU-chains with alternating large mass up to 104 particles and their multiples.
2. It was shown in section 5 of [13] that if $N = 8$ we find 3 invariant manifolds with 3 dof in the case of the periodic FPU α -chain with alternating masses. One of them corresponds with the

dynamics of an alternating FPU-chain with 4 particles. The case $N = 18$ in our Section 5 shows a different structure of invariant manifolds.

Considering the case of $N = 2p$ particles with p prime or odd we have obtained some general insight in the existence and structure of the invariant manifolds in the systems described by system (3).

3. An open problem was formulated in Section 6 regarding the presence of quadratic terms in the quasi-harmonic form of the FPU-chains considered here. The circularity of exciting quadratic terms noted in Section 5 plays probably an essential part. A general solution to this problem might answer the interaction question for systems with an arbitrary number of even particles.
4. An interesting open problem is the high-low frequency interaction problem for $N = 2p$ with p prime, $p \geq 53$. The form of the invariant manifolds described by system (3) in Section 2 suggest that such interactions take place.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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