

# High–low frequency interaction in alternating FPU $\alpha$ -chains

Ferdinand Verhulst

University of Utrecht, Department of Mathematics, PO Box 80.010, 3508 TA Utrecht, The Netherlands

## ARTICLE INFO

MSC:  
37J20  
37J40  
34C20  
58K70  
37G05  
70H33  
70K30  
70K45

### Keywords:

Fermi–Pasta–Ulam chain  
Alternating mass  
High–low frequency interaction  
Invariant manifolds  
Symmetry

## ABSTRACT

One of the problems of periodic FPU-chains with alternating large masses is whether significant interactions exist between the so-called (high frequency) optical and (low frequency) acoustic groups. We show that for  $\alpha$ -chains with  $2n$  particles we have significant interactions caused by external forcing of the acoustic modes by a stable or unstable optical normal mode. In the proofs an embedding theorem plays a part; the analysis is straightforward in the case that  $n$  is even, a different approach using invariant manifolds with symmetry is needed if  $n$  is odd. For  $\beta$ -chains the interactions are characterised by parametric excitation, there are indications that interaction is negligible.

## 1. Introduction

In large nonlinear chains and in nonlinear wave theory one of the basic questions is whether interaction between very different parts of the spectrum plays a part. Such knowledge helps to reduce the often formidable size of the problem. For many applications, for example in Galerkin truncations of wave equations, this has strong implications for the selection of resonances and mode groups; see for many examples [1] ch. 7, for recent research and Ref. [2].

A classical problem of mathematical physics is the Fermi–Pasta–Ulam chain (FPU) that consists of a chain of nonlinearly coupled oscillators with equal masses and nearest-neighbour interaction only. It was formulated to show the thermalisation of interacting particles by starting with exciting one mode with the expectation that after some time the energy would spread out over all the modes. This is one of the basic ideas of statistical mechanics. In the first numerical experiment in 1955, 32 oscillators were used with the spectacular outcome that the dynamics was recurrent as after some time most of the energy returned to the chosen initial state. For the original report see Fermi et al. [3], recent references can be found in Christodoulidi et al. [4] or Bountis and Skokos [5]. Discussions can be found in Campbell et al. [6] and Galavotti (ed.) [7]. The recurrence problem is mainly solved now for low energy chains, see for Ref. [8].

We will study the alternating periodic FPU-chain, formulated in [9], for the special case of a large difference between the 2 alternating masses and for many particles; the general case of alternating masses was

studied in [10] but the problem is far from solved. If the 2 mass sizes are very different, we will see that the spectrum of the linear part can be divided into two groups, the optical group with relatively large frequencies, and the acoustic group with small frequencies. We will show that for FPU  $\alpha$ -chains energy exchanges can occur between the optical group and the acoustic group; this is quite unexpected as there is no frequency resonance. Because the system is Hamiltonian such exchanges will always be reversible.

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

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

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.

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  $\alpha$ -chain if  $\alpha \neq 0, \beta = 0$  and of a  $\beta$ -chain if  $\alpha = 0, \beta \neq 0$ .

E-mail address: [f.verhulst@uu.nl](mailto:f.verhulst@uu.nl).

We mention some facts concerning such systems, and refer to paper [10] for more details. The eigenvalues of the linear system for  $2n$  particles are given in [10], Proposition 3.2:

$$\lambda_j = 1 + a \pm \sqrt{1 + 2a \cos(2\pi \frac{j}{n}) + a^2}, \quad 0 \leq j \leq n. \quad (2)$$

As  $a \ll 1$  the eigenvalues are splitting naturally into 2 groups. With  $2n$  particles in the chain the optical group is characterised by  $n$  eigenvalues of size  $2 + O(a)$  and we have  $n$  eigenvalues of size  $O(a)$ , the acoustic group, which includes the eigenvalue 0 corresponding to the momentum integral:

$$\dot{q}_1 + m\dot{q}_2 + \dots + \dot{q}_{2n-1} + m\dot{q}_{2n} = L, \quad (3)$$

with  $L$  a constant. This integral enables us to reduce any FPU-chain with  $2n$  dof ( $2n$  particles) to  $(2n - 1)$  dof. It is remarkable that for  $a \ll 1$  both the optical and the acoustic group (excluding the case of eigenvalue zero) consist of detuned  $1 : 1 : \dots : 1$  resonances with nonlinear coupling between the 2 groups.

From section 2 of [10] we have some explicit results:

If  $N = 4n$  the system produces for  $j = 0, n$  the eigenvalues  $2(1 + a)$ , 2 (in the optical group), and  $2a, 0$  (in the acoustic group). For each of these non-zero eigenvalues we found periodic solutions, for the  $\alpha$ -chain as well as the  $\beta$ -chain.

In the more general case  $N = 2n$  we find a 2-parameter family of periodic solutions, determined by  $q_2 = q_4 = \dots = q_{2n}, q_1 = q_3 = \dots = q_{2n-1}$  with as an example:

$$q_1(t) = \cos \sqrt{2(1+a)t}, \quad q_2(t) = \frac{a}{\sqrt{2(1+a)}} \sin \sqrt{2(1+a)t}.$$

It is interesting that  $O(1)$  deviations of particles of mass 1 produce  $O(a)$  deviations of particles of mass  $m$ , see Section 4. In the case of  $O(1)$  initial conditions in the optical group and interaction  $O(a)$  with the acoustic group we will indicate this by *weak interaction*; an  $O(1)$  response in the acoustic group is called *strong interaction*.

Czechin et al. identified *bushes* of solutions forming submanifolds for classical (equal masses) FPU-chains; see [11] and further references there; the paper also generalised the results found for two-mode invariant manifolds in [12]. We will use related results for alternating FPU-chains. In our approach an important role will be played by Theorem 3.1 in [10] which is an embedding result that enables us to extend results obtained for chains with a small number of particles like 4 to systems with  $4n$  particles with  $n$  arbitrarily large. We formulate the theorem as follows:

**Theorem 1.1.** *Consider the equations of motion induced by Hamiltonian (1) for  $\alpha\beta \neq 0$  and  $\alpha$ - or  $\beta$ -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  $\alpha, \beta, m$  and  $2kn$  dof, then there exists a restriction of this larger Hamiltonian system that is equivalent to the first system with  $2n$  dof.*

The theorem states that each alternating periodic FPU-chain with  $2n \geq 4$  particles occurs isomorphically as an invariant submanifold in all subsystems with  $2kn$  particles ( $k = 2, 3, \dots$ ) with the same parameters  $a, \alpha$ , and  $\beta$ . So the study of small alternating FPU-chains is relevant for larger alternating systems.

Our basic question is whether there is energy exchange between the two groups or, formulated differently, can high frequency modes transfer energy to low frequency modes and vice versa? In [8] an affirmative answer was given for the special case of an  $\alpha$ -chain with 4 particles. Here we consider this question more generally for  $\alpha$ -chains but using the same dynamical mechanism.

The parameters  $\alpha, \beta$  scale the nonlinearities. To avoid the solutions of the acoustic group leaving the domain of stable equilibrium around the origin, we choose the initial values small or adjust  $\alpha, \beta$ . The techniques are equivalent. The interaction dynamics will be characterised by using actions  $E(t)$ , the traditional form of the quadratic part of

the energies, or by computing the Euclidean distance to the initial values as a function of time. The Euclidean distance is interesting as it gives information about the timescales and recurrence properties of the FPU-chain.

For the case of 4 and 8 particles the coefficients used for  $\alpha$ -chains can be found in [13] and [10] Table 1. The coefficients of the  $\beta$ -chain of the alternating FPU-chain discussed in Section 4 were listed in [14]. As usual we will use for the action  $E_i$  of normal mode  $i$  the expression:

$$E_i = \frac{1}{2}(\dot{x}_i^2 + \omega_i^2 x_i^2).$$

The approximation theory in the case of widely different frequencies shows special aspects.

### 1.1. The asymptotics

A typical example will show the interaction of Hamiltonian systems with widely different frequencies.

**Example 1.1.** Consider the Hamiltonian:

$$H = \frac{1}{2}(\dot{x}^2 + x^2) + \frac{1}{2}(y^2 + \epsilon^2 y^2) - \epsilon x^2 y,$$

with  $\epsilon$  a small positive parameter. The equations of motion are:

$$\ddot{x} + x = 2\epsilon xy, \quad \ddot{y} + \epsilon^2 y = \epsilon x^2. \quad (4)$$

Averaging, see [15], requires that the solutions are located in a bounded domain of phase-space and that the frequencies of the unperturbed solutions ( $\epsilon = 0$ ) are bounded from below and above by positive constants independent of  $\epsilon$ . Suppose that the initial values produce the value  $E \geq 0$  for the Hamiltonian. The energy manifold will be bounded and so the solutions will also be bounded if  $0 \leq E < 1/8$ . The frequency condition poses in this case a problem as there are at least 2 timelike variables  $t$  and  $\tau = \epsilon t$ . According to Lyapunov we can continue the normal modes in the non-resonant system (4), for instance  $x = a \cos t + \epsilon \dots$ . To approximate the solutions we write the system as 2 integral equations and apply contraction. We have with initial conditions  $x(0) = c (c^2 < 1/4), \dot{x}(0) = 0, y(0) = \dot{y}(0) = 0$ :

$$x(t) = c \cos t + 2\epsilon \int_0^t \sin(t-s)x(s)y(s)ds, \quad y(t) = \epsilon \int_0^t \sin(\epsilon t - \epsilon s)x^2(s)ds. \quad (5)$$

Starting iteration with  $x^{(0)}(t) = c \cos t, y^{(0)}(t) = 0$  produces

$$x^{(1)}(t) = c \cos t, \quad y^{(1)}(t) = c^2 \left( \frac{\epsilon}{8 - 2\epsilon^2} - \frac{1}{2\epsilon} \right) \cos \epsilon t + \frac{c^2}{2\epsilon} - \frac{c^2 \epsilon}{8 - 2\epsilon^2} \cos 2t$$

which is the beginning of a convergent series on intervals of time  $O(1)$ .

To perform asymptotics we choose  $c = \sqrt{\epsilon}$ ; we can easily solve the equation for  $y$  in this case to  $O(\epsilon)$ . Assuming that initially the  $y$ -mode is at rest we find considerable interaction:

$$y(t) = \frac{1}{2} - \frac{\epsilon^2}{2(4 - \epsilon^2)} \cos 2t + \left( \frac{\epsilon^2}{2(4 - \epsilon^2)} - \frac{1}{2} \right) \cos \epsilon t + \dots,$$

showing for this approximation oscillations with periods  $O(1)$  and  $O(1/\epsilon)$ .

We shall see that the quadratic forcing of the slowly varying  $y$ -component is typical for the interaction in FPU  $\alpha$ -chains where the optical normal modes are forcing the acoustic ones.

### 1.2. Set-up of the paper

In the sequel we will consider for Hamiltonian (1) interactions between optical and acoustic modes to show that optical modes may induce a nonzero response of one or more acoustic modes that start with zero or small initial conditions. Both the set of optical modes and the set of acoustic modes present detuned  $1 : 1 : \dots : 1$  resonances; Lyapunov–Weinstein results [16] give periodic solutions for these resonances. As we have seen in the example of Section 1.1  $O(\sqrt{\epsilon})$  forcings can already produce considerable perturbations; the example

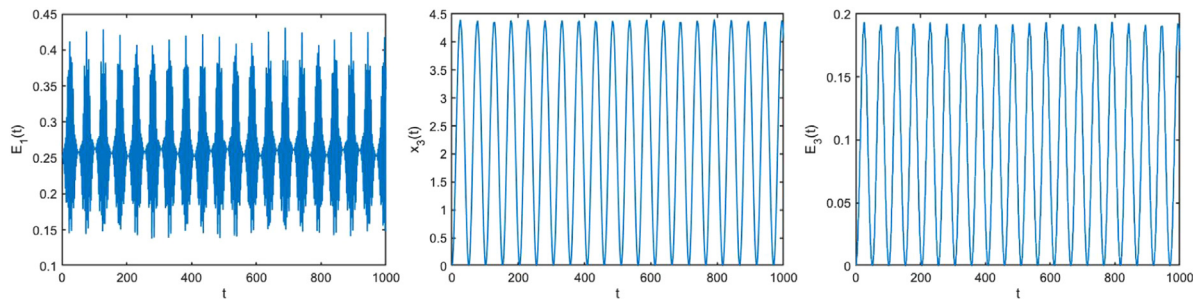


Fig. 1. We illustrate the interaction of the optical and acoustic groups of system (6) for  $a = 0.01$ . Initial positions  $x_1(0) = x_2(0) = 0.5, x_3(0) = 0$  and initial velocities zero. Left  $E_1(t)$  (optical group), middle the acoustic mode  $x_3(t)$  and right  $E_3(t)$  (acoustic group) (the scales for  $E_1$  and  $E_3$  are different). The action  $E_3(t)$  starts at  $E_3(0) = 0$  and oscillates between 0 and 0.2.

was inspired by [8] where for the case of an alternating FPU  $\alpha$ -chain with 4 particles interaction was shown.

Theorem 1.1 enables us to study FPU-chains with more general initial conditions and more particles. For an alternating system with  $N = 2n$  particles with  $n$  even, it is enough to show interaction in the case of 4 particles. The embedding theorem guarantees then interaction in any system generated by Hamiltonian (1) with the number of particles a 4-fold. We will study this case in Section 2. The case  $N = 8$  is considered to show that adding particles enriches and complicates the interactions.

We cannot simply apply Theorem 1.1 if the chain consists of  $2p$  particles where  $p$  is a prime number as there are an infinite number of prime numbers. In Section 3 we will consider the case of  $n = 3, N = 6$ . Showing interaction in systems with 6 particles implies interaction in systems with  $6n$  particles. The asymptotic analysis results here are more restricted as we have to rescale the optical modes, but on the other hand the asymptotics produces simple normal forms and provides inspiration for the study of special solutions and manifolds. More importantly, we can identify invariant manifolds in the case  $N = 6$  that can be found in generalised form for any  $p > 3$ .

To show interaction between optical and acoustic modes in the remaining cases of  $2p$  particles with  $p$  prime we will identify, inspired by the case  $N = 6$ , in Section 4 invariant manifolds with  $(p - 1)$  dof. On these lower-dimensional manifolds we can show interaction between the optical and acoustic modes. This is shown explicitly for  $N = 10$ . Section 5 contains a note on  $\beta$ -chains, in (Appendix) we list the coefficients for the case  $N = 6$ .

## 2. Periodic FPU $\alpha$ -chain with 4n particles

Systems with 4 particles are embedded in systems with  $4n$  particles. So the occurrence of interaction that we show to occur in a system of 4 particles, occurs in all systems where the number of particles is  $N = 2n$  with  $n$  even. We discuss the cases of 4 and 8 particles.

### 2.1. Periodic FPU $\alpha$ -chains with 4 particles (embedded in 4n particles)

In the case of 4 particles we find the eigenvalues (or squared frequencies):

$$\omega_1^2 = 2(1 + a), \omega_2^2 = 2, \omega_3^2 = 2a, \omega_4^2 = 0.$$

Reduction to 3 degrees-of-freedom (dof), see [13] and [8], produces for the  $\alpha$ -chain the following system:

$$\begin{cases} \ddot{x}_1 + 2(1 + a)x_1 &= 2\alpha\sqrt{a(1 + a)}x_2x_3, \\ \ddot{x}_2 + 2x_2 &= 2\alpha\sqrt{a(1 + a)}x_1x_3, \\ \ddot{x}_3 + 2ax_3 &= 2\alpha\sqrt{a(1 + a)}x_1x_2. \end{cases} \quad (6)$$

(The factor in the cubic term differs with a multiplicative factor from [10]; it depends on the choice of an eigenbasis.) We can choose  $\alpha = 1$  and suitable initial values. For system (6) the 3 normal modes exist and are harmonic functions with frequencies  $\sqrt{2(1 + a)}, 2, 2a$ .

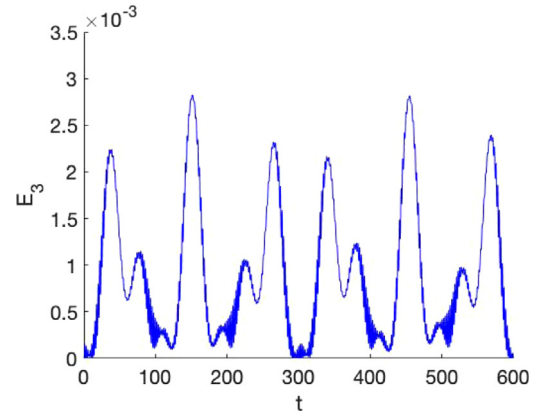


Fig. 2. We illustrate weak interaction of the optical and acoustic groups of system (6) for  $a = 0.01$  by plotting  $E_3(t)$ . Initial positions are  $x_1(0) = 0.5, \dot{x}_1(0) = \dot{x}_2(0) = 0, \dot{x}_3(0) = 1/\sqrt{2}$  (optical),  $x_3(0) = \dot{x}_3(0) = 0$  (acoustic). Because of the phase difference of the optical modes the forcing of the acoustic mode  $E_3(t)$  is small, less than 0.003, but still shows interesting dynamics. See also Section 2.3.

This problem for  $a$  small was studied in [8] with the conclusion that there exists strong interaction between the optical group (modes 1 and 2) and the acoustic group (mode 3) when starting in a neighbourhood of periodic solutions of the detuned resonance formed by the modes 1 and 2; this is illustrated in Fig. 1. When starting at initial conditions that are not close to a periodic solution in 1 : 1 resonance for modes  $x_1, x_2$ , the interaction is negligible; see Fig. 2.

The interaction is demonstrated in [8] by constructing normal forms for system (6), see for details Section 2.3. The asymptotic approximation to  $O(\sqrt{a})$  obtained in this way leads to a forced, linear equation for  $x_3(t)$ :

$$\ddot{x}_3 + 2ax_3 = 2\sqrt{a}r_0^2 \cos^2(\sqrt{2}t + \psi_0), \quad (7)$$

$\psi_0$  is the constant phase of the optical periodic solution,  $r_0$  the amplitude. The general solution with constants  $c_1, c_2$  is:

$$x_3(t) = \frac{r_0^2}{2\sqrt{a}} - \frac{r_0^2}{8r_0^2 - 2\sqrt{a}} \cos(2\sqrt{2}t + 2\psi_0) + c_1 \cos(\sqrt{2a}t) + c_2 \sin(\sqrt{2a}t). \quad (8)$$

Note the factor  $1/\sqrt{a}$ . To illustrate the interaction we use the actions

$$E_1(t) = \frac{1}{2}(\dot{x}_1^2 + 2(1 + a)x_1^2), \quad E_2(t) = \frac{1}{2}(\dot{x}_2^2 + 2x_2^2), \quad E_3(t) = \frac{1}{2}(\dot{x}_3^2 + 2ax_3^2).$$

The (constant) Hamiltonian is the sum of these three actions plus the cubic term, a multiple of  $x_1x_2x_3$ .

In Fig. 1 the initial values are  $E_1(0) \approx E_2(0) \approx 0.25$ , up to  $O(a)$ , and  $E_3(0) = 0$ . We see the interaction:  $E_3$  quickly rises almost immediately from 0 to a value comparable to the values of the other actions. It is interesting to compare with a case where the forcing is not resonant because of a phase difference. In Fig. 2 we take the initial values

$x_1(0) = 0.5$ ,  $x_2(0) = x_3(0) = 0$ ,  $\dot{x}_1(0) = \dot{x}_3(0) = 0$ ,  $\dot{x}_2(0) = 1/\sqrt{2}$ . There is no strong interaction due to the phase difference of the optical modes.

### 2.2. Periodic FPU $\alpha$ -chain with 8 particles (embedded in $8n$ particles)

We have demonstrated the interaction between acoustic and optical modes in the preceding subsection for the case of 4 particles; this result extends to  $4n$  particles because of [Theorem 1.1](#). However, there are some new aspects involving different interactions that are instructive.

We use system (23) and Table 1 of [\[10\]](#) to determine the 7 dof system describing the alternating FPU-chain with 8 particles. The eigenvalues and squared frequencies of the linearised system are:

$$\omega_1^2 = 2(a + 1), \omega_{2,3}^2 = 2\sqrt{a^2 + 1} + a + 1, \omega_4^2 = 2, \omega_5^2 = 2a, \omega_{6,7}^2 = -\sqrt{a^2 + 1} + a, \omega_8^2 = 0.$$

We number the eigenmodes according to the size of the eigenvalue. The relation between eigenmode variables in this system and the system with 4 particles is  $x_1 \leftrightarrow x_1$ ,  $x_4 \leftrightarrow x_2$ ,  $x_5 \leftrightarrow x_3$ .

For simplicity we leave out the complete form of the coefficients given in [\[10\]](#) for the reduced 7 dof system. To show the relative size of the terms in the equations of motion we include for the optical group (equations 1 – 4) from [\[10\]](#) the nonlinear terms to  $O(\sqrt{a})$ . We find for this group:

$$\begin{cases} \ddot{x}_1 + 2x_1 &= \alpha\sqrt{a}(2x_4x_5 + \sqrt{2}x_3x_6 + \sqrt{2}x_2x_7) + O(a^{\frac{3}{2}}), \\ \ddot{x}_2 + 2x_2 &= \alpha\sqrt{a}(\sqrt{2}x_7x_4 + x_2x_5 + \sqrt{2}x_1x_7) + O(a^{\frac{3}{2}}), \\ \ddot{x}_3 + 2x_3 &= \alpha\sqrt{a}(-\sqrt{2}x_6x_4 - x_3x_5 + \sqrt{2}x_1x_6) + O(a^{\frac{3}{2}}), \\ \ddot{x}_4 + 2x_4 &= \alpha\sqrt{a}(-\sqrt{2}x_6x_3 + 2x_1x_5 + \sqrt{2}x_2x_7) + O(a^{\frac{3}{2}}). \end{cases} \quad (9)$$

In the same way the acoustic group with nonlinear terms to  $O(\sqrt{a})$  becomes:

$$\begin{cases} \ddot{x}_5 + 2ax_5 &= \alpha\sqrt{a}(x_2^2 - x_3^2 + 2x_1x_4) + O(a^{\frac{3}{2}}), \\ \ddot{x}_6 + ax_6 &= \alpha\sqrt{2a}(x_1x_3 - x_4x_3) + O(a^{\frac{3}{2}}), \\ \ddot{x}_7 + ax_7 &= \alpha\sqrt{2a}(x_1x_2 + x_4x_2) + O(a^{\frac{3}{2}}). \end{cases} \quad (10)$$

For the  $\alpha$ -chain with 8 particles 3 invariant manifolds were found in [\[10\]](#); indicated by the mode numbers they are  $M_{145}, M_{256}, M_{357}$ . In manifold  $M_{145}$  we recognise the case of 4 particles. Considering possible interactions between optical and acoustic modes in these manifolds we find that in each case acoustic mode  $x_5$  is excited by an optical mode.

#### General initial conditions

As we can see by inspection of the Hamiltonian with coefficients given in table 1 of [\[10\]](#) there are terms outside the 3 invariant manifolds discussed above that may lead to interaction of the optical and acoustic group, for instance the terms  $x_3x_4x_6, x_2x_4x_7$ . We illustrate the interaction by choosing *nonzero* initial values in the optical group and zero initial values in the acoustic group, see [Fig. 3](#). We use the distance to the initial values of the optical and acoustic groups:

$$d_o(t) = \sqrt{\sum_{j=1}^4 ((x_j(t) - x_j(0))^2 + (\dot{x}_j(t) - \dot{x}_j(0))^2)}, \quad (11)$$

and

$$d_a(t) = \sqrt{\sum_{j=5}^7 ((x_j(t) - x_j(0))^2 + (\dot{x}_j(t) - \dot{x}_j(0))^2)}. \quad (12)$$

Without interactions  $d_a(t)$  would remain zero for  $t > 0$ . On a time interval of 1000 steps the interaction between the optical and acoustic groups is clear, it is dominated by  $x_5(t)$ ; for a more complete picture we also give  $d_a(t)$  for 50 000 timesteps in [Fig. 3](#). The numerics suggests that the dynamics becomes more complex on large intervals of time.

We conclude that in periodic  $\alpha$ -chains with  $4n$  particles we have *significant interaction between the optical and the acoustic groups*. In the case of 4 particles mode  $x_3$  and for 8 particles mode  $x_5$  play an important part.

### 2.3. Normal forms and the case of 4 particles

The dynamics of slow-fast Hamiltonian systems is usually non-hyperbolic so this necessitates a special approach. In this paper  $\sqrt{a}$  is a small parameter, we will use below the more usual  $\epsilon$ . We focus on FPU-chains with alternating large mass. The dynamics of the eigenmodes is described by the Hamiltonian:

$$H(x, y) = \sum_1^{2n-1} \frac{1}{2}(y_j^2 + \omega_j^2(\epsilon)x_j^2) + \epsilon H_3(x_1, \dots, x_{2n-1}). \quad (13)$$

$H_3$  is a homogeneous polynomial of degree 3, for  $j = 1, \dots, n, \omega_j^2 = 2 + O(\epsilon^2)$ , for  $j = n + 1, \dots, 2n - 1, \omega_j^2 = O(\epsilon^2)$ . A much simpler example of such systems is discussed in [Section 1.1](#); we will use and extend the same idea.

For a compact set of initial values containing the origin the solutions exist uniquely and are found on bounded energy manifolds that are topologically spheres ( $S^{2n-2}$ ). The equations of motion are for  $j = 1, \dots, n$  of the form:

$$\ddot{x}_j + 2x_j = -\epsilon \frac{\partial H_3}{\partial x_j} + O(\epsilon^2). \quad (14)$$

The usual transformation to slowly varying systems for amplitude  $r$  and phase  $\psi$  is:

$$x = r \cos(\omega t + \psi), \dot{x} = -\omega r \sin(\omega t + \psi). \quad (15)$$

The slowly varying system for  $j = 1, \dots, n$  (the optical group) contains terms  $x_j, j = n + 1, \dots, 2n - 1$  that are governed by perturbed, coupled harmonic equations with frequencies near  $\sqrt{2}$  and  $O(\epsilon)$ . We rescale the optical variables to localise near the origin, see the cases  $N = 4$  and 6. Introducing the timelike variable  $\tau = \epsilon t$  we average the slowly varying system of the optical group over  $t$  while keeping the terms  $x_{n+1}, \dots, x_{2n-1}$ . It turns out that because of the  $1, \dots, 1$  resonance it is easy to extract periodic solutions from the averaged system. They have validity  $O(\epsilon)$  on intervals of time  $O(1/\epsilon)$ . We sketch the analysis for FPU-chains with alternating large mass in the case  $N = 4$  and in [Section 3](#) for  $N = 6$ . A common feature will be that  $1 : \dots : 1$  resonances produce generally periodic solutions in general position, i.e. outside the normal mode planes.

The case  $N = 4$ .

In system (6) we put  $\sqrt{a} = \epsilon$ , rescale  $x_1 = \sqrt{\epsilon}\bar{x}_1, x_2 = \sqrt{\epsilon}\bar{x}_2$  and find after omitting the bars:

$$\begin{cases} \ddot{x}_1 + 2x_1 &= 2\epsilon\alpha x_2 x_3 + \dots, \\ \ddot{x}_2 + 2x_2 &= 2\epsilon\alpha x_1 x_3 + \dots, \\ \ddot{x}_3 + 2\epsilon^2 x_3 &= 2\alpha\epsilon^2 x_1 x_2 + \dots, \end{cases} \quad (16)$$

where the dots stand for higher order terms. The linear part of the equation for  $x_3$  yields timelike variable  $\epsilon t$ , terms dependent on  $t$  are present at order  $\epsilon^2$ . Transforming by Eqs. (15) we find from system (16) after averaging over  $t$ :

$$\begin{cases} \dot{r}_1 &= -\frac{\epsilon}{\sqrt{2}}\alpha r_2 \sin(\psi_1 - \psi_2)x_3, \dot{\psi}_1 = -\frac{\epsilon}{\sqrt{2}}\alpha \frac{r_2}{r_1} \cos(\psi_1 - \psi_2)x_3, \\ \dot{r}_2 &= \frac{\epsilon}{\sqrt{2}}\alpha r_1 \sin(\psi_1 - \psi_2)x_3, \dot{\psi}_2 = \frac{\epsilon}{\sqrt{2}}\alpha \frac{r_1}{r_2} \cos(\psi_1 - \psi_2)x_3. \end{cases} \quad (17)$$

We put  $\chi = \psi_1 - \psi_2$  to obtain the equation:

$$\dot{\chi} = -\sqrt{\frac{a}{2}}\alpha \left( \frac{r_2}{r_1} - \frac{r_1}{r_2} \right) \cos(\chi)x_3. \quad (18)$$

The averaged system has the first integral  $r_1^2 + r_2^2 = 2E_0$  with  $E_0$  a positive constant. The amplitudes  $r_1, r_2$  will be constant if  $\chi = 0, \pi$ ; from the equation for  $\chi$  we find this is the case if  $r_1 = r_2 = E_0$ . The results are valid on intervals of time  $O(1/\epsilon)$ . The 1-parameter family of solutions with constant amplitudes leads for  $x_3$  (replacing  $\epsilon^2$  by  $a$ ) to the equation:

$$\ddot{x}_3 + 2ax_3 = 2a\alpha E_0 \cos(\sqrt{2}t + \psi_1) \cos(\sqrt{2}t + \psi_2) = \pm 2a\alpha E_0 \cos^2(\sqrt{2}t + \psi_1) \quad (19)$$

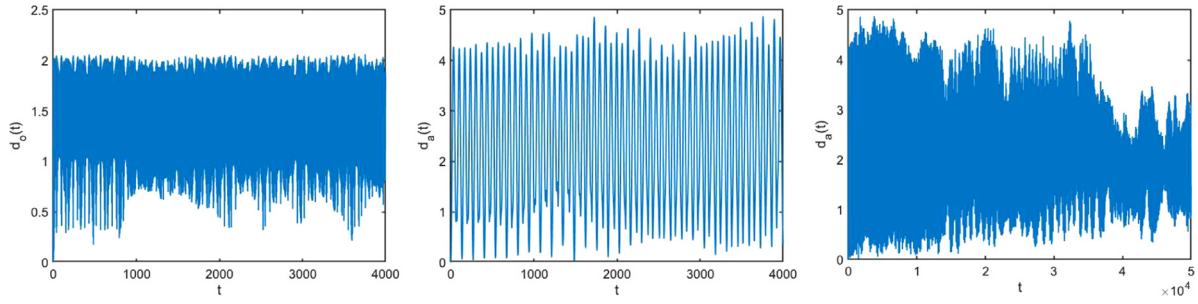


Fig. 3. We illustrate for  $a = 0.01$  the interaction of the optical and acoustic groups of system (23) in [10] (derived for  $\alpha$ -chains with 8 particles). Initial positions  $x_j(0) = 0.5, j = 1, \dots, 4$  (optical),  $x_j(0) = 0, j = 5, 6, 7$  (acoustic) and initial velocities zero. Left  $d_o(t)$  for 4000 timesteps. The distance  $d_o(t)$  to the zero initial values in the acoustic group grows from 0 to value nearly 5 and is mainly excited by  $x_5(t)$  (middle figure shows  $d_a(t)$  on 4000 timesteps). As an illustration  $d_o(t)$  is also shown for 50 000 timesteps.

with  $\psi_1 - \psi_2 = 0, \pi$ . This result is similar to Eq. (7) of Section 2.

If  $\sin(\psi_1 - \psi_2) \neq 0$  because of a phase difference as in Fig. 2 the forcing of the equation for  $x_2$  in system (16) remains small.

### 3. Periodic FPU $\alpha$ -chain with 6n particles

We start again with analysing the system after reduction using the momentum integral.

#### 3.1. The case of 6 particles

The eigenvalues, producing squared frequencies of the linearised system are:

$$\omega_1^2 = 2(1+a), \omega_{2,3}^2 = a+1 + \sqrt{a^2 - a + 1}, \omega_{4,5}^2 = a+1 - \sqrt{a^2 - a + 1}, \omega_6^2 = 0. \quad (20)$$

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

Using momentum integral (3) a symplectic transformation to 5 dof produces the Hamiltonian  $H_2 + H_3$  with:

$$H_3 = \sum_{i,j,k} d_{ijk} x_i x_j x_k.$$

The coefficients  $d_{ijk}$  are given in Table 1 of the appendix. For the interaction analysis the terms  $O(\sqrt{a})$  and  $O(a)$  are sufficient. The equations of motion for the optical group  $x_1, x_2, x_3$  and the acoustic group  $x_4, x_5$  become:

$$\begin{cases} \ddot{x}_1 + \omega_1^2 x_1 = -2\sqrt{a}x_2x_5 - 2\sqrt{a}x_3x_4 + O(a^{3/2}), \\ \ddot{x}_2 + \omega_2^2 x_2 = -2\sqrt{a}x_1x_5 - \frac{3}{\sqrt{2}}ax_2x_3 - \sqrt{2a}x_2x_5 + \sqrt{2a}x_3x_4 + O(a^{3/2}), \\ \ddot{x}_3 + \omega_3^2 x_3 = -2\sqrt{a}x_1x_4 - \frac{3}{4}\sqrt{2a}x_2^2 + \sqrt{2a}x_2x_4 + \frac{3}{4}\sqrt{2a}x_3^2 + \sqrt{2a}x_3x_5 + O(a^{3/2}), \\ \ddot{x}_4 + \omega_4^2 x_4 = -2\sqrt{a}x_1x_3 + \sqrt{2a}x_2x_3 + O(a^{3/2}), \\ \ddot{x}_5 + \omega_5^2 x_5 = -2\sqrt{a}x_1x_2 - \frac{1}{2}\sqrt{2a}x_2^2 + \frac{1}{2}\sqrt{2a}x_3^2 + O(a^{3/2}). \end{cases} \quad (21)$$

The optical group is in detuned 1 : 1 : 1 resonance, the detuning is  $O(\sqrt{a})$ . In system (21) we observe quadratic forcing terms for modes 4 and 5, similar to the case of  $4n$  particles, so we expect interaction of acoustic and optical modes. Fortunately we can identify an invariant manifold that is easier to study. In system (21), putting  $x_1 = x_2 = x_4 = 0$  we have an invariant manifold consisting of mode 3 and 5:

$$\ddot{x}_3 + 2x_3 = \sqrt{2a}x_3x_5, \quad \ddot{x}_5 + \frac{3}{2}ax_5 = \frac{1}{2}\sqrt{2a}x_3^2. \quad (22)$$

The dynamics is basically that of system (4) in Section 1.1, this clarifies the interaction.

Another invariant manifold, consisting of modes 1, 2 and 5 is analysed in the next subsection.

System (21) is a system with widely different frequencies and it merits a deeper analysis, but here we restrict ourselves to numerical demonstration of the interactions. We have  $a = 0.01$  in Fig. 4, we start with zero energy in the acoustic modes. In this example mode 4 shows more interaction than mode 5 but their role is reversed for other initial conditions.

#### 3.2. Normal forms in the case of 6 particles

For system (21) we put  $\sqrt{a} = \epsilon$ , rescale  $x_i = \sqrt{\epsilon}\tilde{x}_i, i = 1, 2, 3$  and leave out the bars. The dots stand for higher order terms in  $\epsilon$ .

$$\begin{cases} \ddot{\tilde{x}}_1 + 2\tilde{x}_1 = \epsilon(-2x_2x_5 - 2x_3x_4) + \dots, \\ \ddot{\tilde{x}}_2 + 2\tilde{x}_2 = \epsilon(-2x_1x_5 - \sqrt{2}x_2x_5 + \sqrt{2}x_3x_4) + \dots, \\ \ddot{\tilde{x}}_3 + 2\tilde{x}_3 = \epsilon(-2x_1x_4 + \sqrt{2}x_2x_4 + \sqrt{2}x_3x_5) + \dots, \\ \ddot{\tilde{x}}_4 + \frac{3}{2}\epsilon^2\tilde{x}_4 = \epsilon^2(-2x_1x_3 + \sqrt{2}x_2x_3) + \dots, \\ \ddot{\tilde{x}}_5 + \frac{3}{2}\epsilon^2\tilde{x}_5 = \epsilon^2(-2x_1x_2 - \frac{1}{2}\sqrt{2}x_2^2 + \frac{1}{2}\sqrt{2}x_3^2) + \dots \end{cases} \quad (23)$$

The linear part of the equations for  $x_4, x_5$  has timelike variable  $\sqrt{3/2}\epsilon t$ , terms dependent on  $t$  are present at higher order. We find after averaging of the 3 equations of the optical group:

$$\begin{cases} \dot{r}_1 = \epsilon\frac{1}{2}\sqrt{2}(r_2 \sin(\psi_1 - \psi_2)x_5 + r_3 \sin(\psi_1 - \psi_3)x_4), \\ \dot{\psi}_1 = \epsilon\frac{1}{2}\sqrt{2}(\frac{r_2}{r_1} \cos(\psi_1 - \psi_2)x_5 + \frac{r_3}{r_1} \cos(\psi_1 - \psi_3)x_4), \\ \dot{r}_2 = \epsilon(-\frac{1}{2}\sqrt{2}r_1 \sin(\psi_1 - \psi_2)x_5 + \frac{1}{2}r_3 \sin(\psi_2 - \psi_3)x_4), \\ \dot{\psi}_2 = \epsilon(\frac{1}{2}\sqrt{2}\frac{r_1}{r_2} \cos(\psi_1 - \psi_2)x_5 + \frac{1}{2}x_5 + \frac{1}{2}\frac{r_3}{r_2} \cos(\psi_2 - \psi_3)x_4), \\ \dot{r}_3 = \epsilon(-\frac{1}{2}\sqrt{2}r_1 \sin(\psi_1 - \psi_3)x_4 - \frac{1}{2}r_2 \sin(\psi_2 - \psi_3)x_4), \\ \dot{\psi}_3 = \epsilon(\frac{1}{2}\sqrt{2}\frac{r_1}{r_3} \cos(\psi_1 - \psi_3)x_4 - \frac{1}{2}\frac{r_2}{r_3} \cos(\psi_2 - \psi_3)x_4 - \frac{1}{2}x_5). \end{cases} \quad (24)$$

This is a more difficult system than obtained for  $N = 4$  as it is more asymmetric and it is more difficult to find from system (24) solutions with constant amplitude. We note a few aspects:

- We have the first integral of system (24)  $r_1^2 + r_2^2 + r_3^2 = 2E_0$  with  $E_0$  a positive constant. We know from Lyapunov–Weinstein theory (see [16]) that on a compact energy manifold system (23) contains at least 5 periodic solutions. However it is not easy to find all of them, even when considering the averaged system.
- In Section 3 we noted the presence of an invariant manifold consisting of mode 3 and 5 with modes 1, 2, 4 vanishing. The averaged system to be analysed from (24) is:

$$\dot{r}_3 = 0, \dot{\psi}_3 = -\frac{1}{2}x_5, \ddot{x}_5 + \frac{3}{2}\epsilon^2x_5 = \epsilon^2\frac{1}{2}\sqrt{2}x_3^2.$$

Integration shows again forcing of mode 5.

- A manifold consisting of modes 1, 2, 5 with vanishing modes 3, 4 contains 3 dof. From system (24) we have:

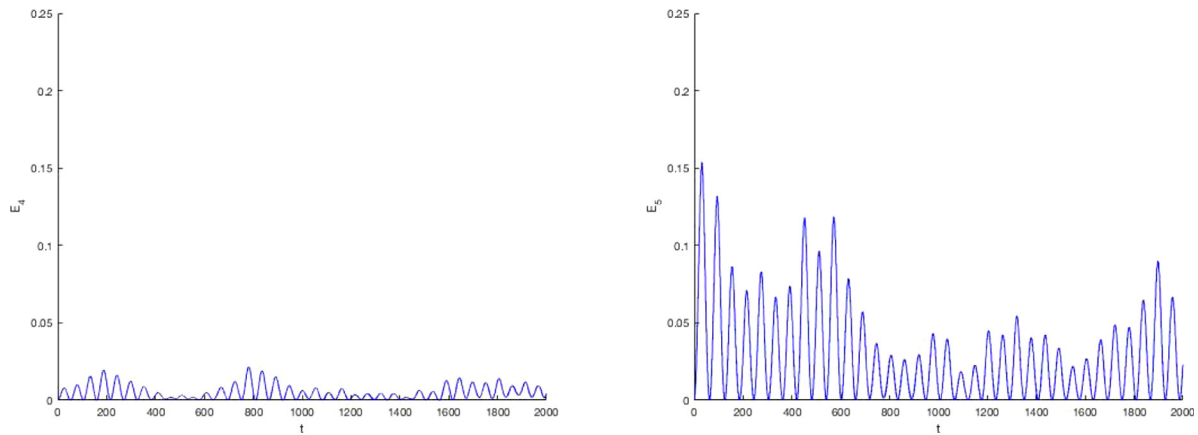


Fig. 4. Left the action  $E_4$ , right action  $E_6$  for the  $\alpha$ -chain with 6 particles in 2000 timesteps. The initial conditions are  $x_1(0) = 0.5, x_2(0) = 0.5, x_3(0) = 0.5, x_4(0) = x_5(0) = 0$  and all initial velocities zero so that  $E_1(0) = 0.25, E_2(0) = 0.25, E_3(0) = 0.25, E_4(0) = 0.0, E_5(0) = 0.0$ . We observe forcing of the acoustic modes with mode 5 most affected in this case.

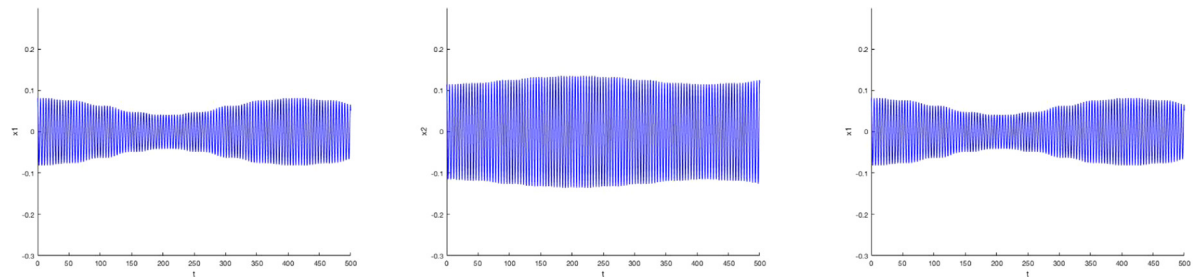


Fig. 5. From left to right  $x_1(t), x_2(t), x_5(t)$  for the invariant manifold of modes 1, 2, 5 of the  $\alpha$ -chain with 6 particles in 500 timesteps, see system (25). The initial values are chosen to obtain “constant” amplitudes with initial conditions  $x_1(0) = 0.8164966, x_2(0) = 1.154701, x_3(0) = x_4(0) = x_5(0) = 0$  and all initial velocities zero. We observe forcing of the acoustic mode 5.

$$\begin{cases} \dot{r}_1 &= \varepsilon \frac{1}{2} \sqrt{2} r_2 \sin(\psi_1 - \psi_2) x_5, \psi_1 = \varepsilon \frac{1}{2} \sqrt{2} \frac{r_2}{r_1} \cos(\psi_1 - \psi_2) x_5, \\ \dot{r}_2 &= -\varepsilon \frac{1}{2} \sqrt{2} r_1 \sin(\psi_1 - \psi_2) x_5, \psi_2 = \varepsilon (\frac{1}{2} \sqrt{2} \frac{r_1}{r_2} \cos(\psi_1 - \psi_2) x_5 \\ &\quad + \frac{1}{2} x_5), \\ \ddot{x}_5 + \frac{3}{2} \varepsilon^2 x_5 &= \varepsilon^2 (-2x_1 x_2 - \frac{1}{2} \sqrt{2} x_2^2). \end{cases} \quad (25)$$

For the combination angle  $\chi = \psi_1 - \psi_2$  we find:

$$\dot{\chi} = \frac{1}{2} \varepsilon (\sqrt{2} (\frac{r_2}{r_1} - \frac{r_1}{r_2}) \cos \chi - 1) x_5.$$

We have  $\dot{r}_1 = \dot{r}_2 = 0$  (solutions with constant amplitude) if  $\chi = 0, \pi$ . We find a solution for  $\chi = 0$ :  $r_2 = \lambda r_1$  with  $\lambda = \sqrt{2}$  so that  $r_1 = \sqrt{2/3} E_0, r_2 = \sqrt{4/3} E_0$ . The amplitudes of modes 1 and 2 are constant in Fig. 5 with error  $O(\varepsilon)$ .

#### 4. The cases of $2p$ alternating FPU-chains with $p$ prime

Inspired by Section 3 we will look for low-dimensional invariant manifolds that show interaction between acoustic and optical modes in the cases  $N = 2p$  with  $p \geq 5$  prime. We put  $\alpha = 1$  as we can adjust  $\alpha (\neq 0)$  by scaling of the coordinates. It is useful to write out the equations of

motion:

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_{2p} - q_2 &= (q_2 - q_1)^2 - (q_1 - q_{2p})^2, \\ m\ddot{q}_2 + 2q_2 - q_1 - q_3 &= (q_3 - q_2)^2 - (q_2 - q_1)^2, \\ \ddot{q}_3 + 2q_3 - q_2 - q_4 &= (q_4 - q_3)^2 - (q_3 - q_2)^2, \\ m\ddot{q}_4 + 2q_4 - q_3 - q_5 &= (q_5 - q_4)^2 - (q_4 - q_3)^2, \\ \dots &= \dots, \\ m\ddot{q}_{p-1} + 2q_{p-1} - q_{p-2} - q_p &= (q_p - q_{p-1})^2 - (q_{p-1} - q_{p-2})^2, \\ \ddot{q}_p + 2q_p - q_{p-1} - q_{p+1} &= (q_{p+1} - q_p)^2 - (q_p - q_{p-1})^2, \\ m\ddot{q}_{p+1} + 2q_{p+1} - q_p - q_{p+2} &= (q_{p+2} - q_{p+1})^2 - (q_{p+1} - q_p)^2, \\ \dots &= \dots, \\ \ddot{q}_{2p-1} + 2q_{2p-1} - q_{2p-2} - q_{2p} &= (q_{2p} - q_{2p-1})^2 - (q_{2p-1} - q_{2p-2})^2, \\ m\ddot{q}_{2p} + 2q_{2p} - q_{2p-1} - q_1 &= (q_1 - q_{2p})^2 - (q_{2p} - q_{2p-1})^2. \end{cases} \quad (26)$$

##### 4.1. A case of weak interaction

From system (26) we find the special manifold defined by:

$$q_1(t) = q_3(t) = \dots = q_{2p-1}(t), q_2(t) = q_4(t) = \dots = q_{2p}(t), \quad (27)$$

leading to the 2-dimensional system:

$$\begin{cases} \ddot{q}_1 + 2q_1 - 2q_2 &= 0, \\ m\ddot{q}_2 + 2q_2 - 2q_1 &= 0. \end{cases} \quad (28)$$

The characteristic equation is  $\lambda^4 + 2(a+1)\lambda^2 = 0$  producing the frequencies  $\sqrt{2(a+1)}, 0$ , the manifold is associated with the eigenvalues  $2(a+1), 0$  of (2) and contains a member of the optical group. A typical solution with  $q_1(t)$  equalling the odd modes,  $q_2(t)$  the even modes, is

$$q_1(t) = \cos \sqrt{2(a+1)t}, q_2(t) = -a \cos \sqrt{2(a+1)t}, \quad (29)$$

showing weak high-frequency interaction (small in parameter  $a$ ).

#### 4.2. Strong interaction for $N = 6$

The invariant manifolds we found for  $2p = 6$  in Section 3 inspire us to consider system (26) again. If  $2p = 6$  a special family of solutions, defining an invariant manifold, arises if for all time we have:

$$q_3(t) = q_6(t) = 0, \quad q_2(t) = -q_4(t), \quad q_1(t) = -q_5(t), \quad (30)$$

resulting in the system (similar for  $q_3, q_4$ ):

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_2 &= q_2^2 - 2q_1q_2, \\ m\ddot{q}_2 + 2q_2 - q_1 &= 2q_1q_2 - q_1^2. \end{cases} \quad (31)$$

The eigenvalues near the origin are  $-a - 1 \pm \sqrt{a^2 - a + 1}$ , see also eq. (20). Reversing the transformations  $q \rightarrow x$  in Section 3 we find that the invariant manifold described by assumptions (30) consists of the modes  $x_3, x_5$  (one optical, one acoustic).

Note that the full Hamiltonian system contains system (31) 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 (31) we can construct a 2 dof system in quasi-harmonic form with dynamics as in Section 3 for  $N = 6$ . The linear transformation of  $q_1, q_2$  produces quadratic terms for the nonlinearities as before with interaction of optical and acoustic modes.

#### 4.3. The general case with $p$ prime

We can apply similar symmetries to the general system (26) with  $2p$  particles. We assume:

$$\begin{cases} q_p(t) &= q_{2p}(t) = 0, \\ q_2(t) &= -q_{2p-2}(t), q_4(t) = -q_{2p-4}(t), \dots, q_{p-1}(t) = -q_{p+1}(t), \\ q_1(t) &= -q_{2p-1}(t), q_3(t) = -q_{2p-3}(t), \dots, q_{p-2}(t) = -q_{p+2}(t). \end{cases} \quad (32)$$

The symmetry assumptions imply that the value of the momentum integral (3) vanishes. System (26) with  $2p$  dof reduces to  $2p - 2$  dof which is a 4-fold; we are left with two  $(p-1)$  dof systems with identical dynamics. The  $(p-1)$  dof system is of the form:

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

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  $p > 5$ :

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_2 &= q_2^2 - 2q_1q_2, \\ m\ddot{q}_2 + 2q_2 - q_1 - q_3 &= q_3^2 - 2q_2q_3 + 2q_1q_2 - q_1^2, \\ \ddot{q}_3 + 2q_3 - q_2 - q_4 &= q_4^2 - 2q_3q_4 + 2q_2q_3 - q_2^2, \\ m\ddot{q}_4 + 2q_4 - q_3 - q_5 &= q_5^2 - 2q_4q_5 + 2q_3q_4 - q_3^2, \\ \dots &= \dots, \\ m\ddot{q}_{p-1} + 2q_{p-1} - q_{p-2} &= 2q_{p-1}q_{p-2} - q_{p-2}^2. \end{cases} \quad (33)$$

The normal mode frequencies of system (33) are derived from the single eigenvalues of  $B$ , again resp.  $\sqrt{2+O(a)}$  and  $O(\sqrt{a})$ . To put the system in quasi-harmonic form we use a linear transformation that diagonalises  $B$ . The linear transformation of  $q$  keeps the nonlinearities quadratic, resulting in interaction as before. We demonstrate the process for  $p = 5$ .

#### 4.4. Strong interaction for $N = 10$

As an illustration we consider the case  $N = 10$ . With  $p = 5$  the symmetry assumptions (33) produce invariant manifolds with dynamics described by 2 equivalent 4 dof systems. We have for the 1st system:

$$\begin{cases} \ddot{q}_1 + 2q_1 - q_2 &= q_2^2 - 2q_1q_2, \\ m\ddot{q}_2 + 2q_2 - q_1 - q_3 &= q_3^2 - 2q_2q_3 + 2q_1q_2 - q_1^2, \\ \ddot{q}_3 + 2q_3 - q_2 - q_4 &= q_4^2 - 2q_3q_4 + 2q_2q_3 - q_2^2, \\ m\ddot{q}_4 + 2q_4 - q_3 &= 2q_3q_4 - q_3^2. \end{cases} \quad (34)$$

The first two equations are identical to the first two of the general case in system (33), 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:

$$a + 1 \pm \sqrt{1 - \frac{1}{2}(1 + \sqrt{5})a + a^2}, \quad a + 1 \pm \sqrt{1 - \frac{1}{2}(1 - \sqrt{5})a + a^2}, \quad (35)$$

with approximate size  $O(a), 2+O(a), O(a), 2+O(a)$  so after transformation the 1st and 3rd modes are acoustic. The eigenvalues (35) are contained in Eq. (2) in the case  $N = 10$ . Carrying out the linear transformation for system (34) by MATHEMATICA we find that the 4 right-hand sides contain 10 quadratic terms and products of the variables of the system. We have again forcing of the acoustic modes as in the case of  $N = 6$ . We omit the general  $a$ -dependent (messy) expressions that arise by the transformations. For  $a = 0.01$  the right-hand sides are after rescaling the eigenvectors:

$$\begin{cases} \ddot{x}_1 + \omega_1^2 x_1 &= -0.04x_4^2 - 0.13x_2x_4 + R_1(x) \\ \ddot{x}_2 + \omega_2^2 x_2 &= 0.0063x_1x_3 - 0.0019x_3^2 + R_2(x), \\ \ddot{x}_3 + \omega_3^2 x_3 &= -0.039x_2^2 + 0.049x_2x_4 + R_3(x), \\ \ddot{x}_4 + \omega_4^2 x_4 &= 0.0051x_1^2 + 0.0062x_1x_3 + R_4(x). \end{cases} \quad (36)$$

$R_1(x), \dots, R_4(x)$  consist of quadratic terms that have no or less influence on the interaction between acoustic and optical modes (modes  $x_1, x_3$  are acoustic,  $x_2, x_4$  are optical). System (36) is typical for system (34) transformed to quasi-harmonic equations if  $0 < a \ll 1$ . We have checked that the same forcing of acoustic modes by optical ones takes place for  $N = 14$ . As we have seen in Sections 2 and 3 the forcing by the quadratic terms guarantees strong interaction.

### 5. Remark on periodic alternating FPU $\beta$ -chains

As stated in the Introduction the embedding Theorem 1.1 holds both for  $\alpha$ - and  $\beta$ -chains, but the interaction results for  $\beta$ -chains will be much more modest. To illustrate the difference with  $\alpha$ -chains we consider again the case of 4 (or  $4n$ ) particles. Using the momentum integral the reduction to 3 dof, choosing  $\beta = 1$ , becomes for 4 particles (see [13]):

$$\begin{cases} \ddot{x}_1 + 2(1+a)x_1 &= -x_1(x_1^2 + 3x_2^2) - ax_1(2x_1^2 + 3x_2^2 + 3x_3^2) \\ &\quad - a^2x_1(x_2^2 + 3x_3^2), \\ \ddot{x}_2 + 2x_2 &= -x_2(x_2^2 + 3x_1^2) - 3ax_2(x_1^2 + x_3^2), \\ \ddot{x}_3 + 2ax_3 &= -3ax_3(x_1^2 + x_2^2) - a^2x_3(x_2^2 + 3x_1^2). \end{cases} \quad (37)$$

As for  $a = 0$  system (37) is already nonlinear we use averaging-normalisation in the usual way, see [15]. Considering small  $O(a)$  initial values we put  $x_1 \mapsto ax_1, \dot{x}_1 \mapsto a\dot{x}_1$  etc. We summarise the results. The analysis leads to in-phase and out-of-phase periodic solutions for the detuned 1 : 1 resonance of the modes 1 and 2. The symmetry of the first two equations of system (37) can be used to put  $x_1(t) = \pm x_2(t)$ . To  $O(a)$  we find for these periodic solutions:

$$\ddot{x}_1 + 2x_1 = -4x_1^3, \quad x_1(t) = \pm x_2(t). \quad (38)$$

The equation for the acoustic mode  $x_3$  becomes in this  $O(a)$  approximation:

$$\ddot{x}_3 + 2a(1 + 3x_1^2(t))x_3 = 0, \quad (39)$$

with  $x_1(t)$  a periodic solution. For the Floquet exponents we have  $\lambda_1 + \lambda_2 = 0$ . Eq. (39) is an example of a parametrically excited oscillator with widely different frequencies, close to  $\sqrt{2a}$  and  $\sqrt{2}$ ; see for parametric excitation [17,18] or [1]. The Floquet instability tongues will be extremely narrow for  $a \rightarrow 0$ . Interactions between optical and acoustic modes are then negligible for the 4 particles  $\beta$ -chain. Numerical experiments confirm this.

We can repeat the analysis for a periodic FPU  $\beta$ -chain with 8 (or  $8n$ ) particles. Using [10] and the appendix of [14] we can write down the cubic part of the 7 dof Hamiltonian; it contains 49 terms dependent on  $a$ . As in the case of 4 particles we find parametrically excited systems

with widely different frequencies. This suggests that we can ignore interaction between optical and acoustic groups but as in the case of 4 particles, the analysis is not conclusive.

The case of 8 particles is more complicated as among the 49 coefficients of the Hamiltonian we have terms like  $x_1x_2x_3x_5$ ,  $x_1x_2x_3x_5$ ,  $x_1x_3x_4x_7$ ; in the equations of motion these terms will produce a certain forcing of the acoustic modes  $x_5, x_6, x_7$ . However, in all the cases of such forcing terms a closer analysis shows they have coefficients that are  $O(a^{3/2})$ , so they will have less influence.

**6. Conclusions and discussion**

1. Our analysis is strongly dependent on the embedding **Theorem 1.1** and the identification of submanifolds in Section 4.3.
2. For  $\alpha$ -chains with alternating large mass we have shown interaction between optical and acoustic modes for chains with  $N = 4n, 6n, 10n$  particles ( $n$  an arbitrary natural number). This means that for the chains with number of particles ranging from 4 to 100 we have covered more than 70% of the cases. As the prime numbers are thinning out if  $N$  increases, the percentage will slowly increase with  $N$ .
3. The formulation of Section 4.3 for invariant manifolds contained in chains with  $2p$  particles where  $p$  is prime has the same symmetries and structure as in the special formulation for 6 and 10 particles. This is strong evidence for interaction between optical and acoustic modes in the cases  $p$  arbitrary. Consider for instance the  $\alpha$ -chains with alternating large mass and number of particles 32 (a 4-fold), 34 (2 times prime number 17) and 36 (a 4- and 6-fold). The dynamics in the 3 cases will be slightly different but according to the analysis started in Section 4 we expect in each case interaction between optical and acoustic modes. In a subsequent paper we will extend our results to  $\alpha$ -chains with  $N = 2pn$  particles where  $p \geq 7$  is prime.
4. The interaction question for  $\beta$ -chains is more difficult than for  $\alpha$ -chains. We conclude that even for  $\beta$  small enough or at low energy values we have at this stage no evidence for interaction between optical and acoustic groups in  $\beta$ -chains, but weak interaction might be expected.
5. High–low frequency interaction and localisation of modes play an important part in both conservative and engineering mechanics. For classical FPU-chains localisation has been studied in [4] and [19], it is tied in with the presence of bushes of invariant manifolds. For FPU-chains with alternating mass again special invariant manifolds can be identified that lead to localisation for appropriately chosen initial values. For dissipative systems an early paper is [20] where high–low frequency interaction is studied analytically and numerically for a cantilever beam subjected to base excitation and damping. Related problems for microresonator arrays are considered in [21]. Differences are that conservative systems involve recurrence and localisation in submanifolds whereas dissipative systems often contain a measure of focusing by excitation and damping.

**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.

**Acknowledgements**

There were useful discussions with Roelof Bruggeman who also provided system (21) and Table 1 by using MATHEMATICA. Wilberd van der Kallen kindly provided the quasi-harmonic system corresponding with system (34) by a MATHEMATICA calculation. Two anonymous referees provided references and stimulated additional discussion.

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

**Table 1**

Non-zero coefficients in the description of  $H_3$  in the eigencoordinates  $x_j$ .  $W = \sqrt{1 - a + a^2}$ .

$i,j,k$	$d_{i,j,k}$
{1,2,5}	$2\sqrt{a}\sqrt{a+1} = 2\sqrt{a+a^{3/2}} + O(a^2)$
{1,3,4}	$2\sqrt{a}\sqrt{a+1} = 2\sqrt{a+a^{3/2}} + O(a^2)$
{2,2,3}	$\frac{3a(W+1)}{4W^{3/2}\sqrt{-a+W+1}} = \frac{3a}{2\sqrt{2}} + O(a^2)$
{2,2,5}	$-\frac{\sqrt{a(a^2+a(W+2)-2(W+1))}}{4W^{3/2}} \sqrt{-a+W+1} = \frac{\sqrt{a}}{\sqrt{2}} + \frac{a^{3/2}}{8\sqrt{2}} + O(a^2)$
{2,3,4}	$\frac{\sqrt{a(a^2+a(W+2)-2(W+1))}}{2W^{3/2}\sqrt{-a+W+1}} = -\sqrt{2}\sqrt{a} - \frac{a^{3/2}}{4\sqrt{2}} + O(a^2)$
{2,4,5}	$-\frac{a(2a^2-2a(W+1)+W-1)}{2W^{3/2}\sqrt{-a+W+1}} = O(a^2)$
{3,3,3}	$-\frac{a(W+1)}{4W^{3/2}\sqrt{-a+W+1}} = -\frac{a}{2\sqrt{2}} + O(a^2)$
{3,3,5}	$\frac{\sqrt{a(a^2+a(W+2)-2(W+1))}}{4W^{3/2}\sqrt{-a+W+1}} = -\frac{\sqrt{a}}{\sqrt{2}} - \frac{a^{3/2}}{8\sqrt{2}} + O(a^2)$
{3,4,4}	$\frac{a(2a^2-2a(W+1)+W-1)}{4W^{3/2}\sqrt{-a+W+1}} = O(a^2)$
{3,5,5}	$-\frac{a(2a^2-2a(W+1)+W-1)}{4W^{3/2}\sqrt{-a+W+1}} = O(a^2)$
{4,4,5}	$\frac{3a^{3/2}(a-W)}{4W^{3/2}\sqrt{-a+W+1}} = -\frac{3a^{3/2}}{4\sqrt{2}} + O(a^2)$
{5,5,5}	$\frac{a^{3/2}(W-a)}{4W^{3/2}\sqrt{-a+W+1}} = \frac{a^{3/2}}{4\sqrt{2}} + O(a^2)$

**Appendix**

In the table we present the coefficients  $d_{ijk}$  used for the system with 6 dof in Section 3.

**References**

- [1] A.H. Nayfeh, D.T. Mook, *Nonlinear Oscillations*, John Wiley, Interscience publ., 1979.
- [2] A. Degasperis, S. Lombardo, M. Sommacal, *Integrability and linear stability of nonlinear waves*, *J. Nonlinear Sci.* 28 (2018) 1251–1291.
- [3] E. Fermi, J. Pasta, S. Ulam, Los Alamos Report LA-1940, in: E. Fermi, *Collected Papers*, vol. 2, 1955, pp. 977–988.
- [4] H. Christodoulidi, Ch. Efthymiopoulos, T. Bountis, *Energy localization on  $q$ -tori, long-term stability, and the interpretation of Fermi-Pasta-Ulam recurrences*, *Phys. Rev. E* 81 (2010) 6210.
- [5] T. Bountis, H. Skokos, *Complex Hamiltonian Dynamics*, Springer, 2012.
- [6] D.K. Campbell, P. Rosenau, G.M. Zaslavsky (Eds.), *The Fermi-Pasta-Ulam Problem. The First 50 Years*, in: *Chaos, Focus issue*, vol. 15, 2005.
- [7] G. Galavotti (Ed.), *The Fermi-Pasta-Ulam Problem: A Status Report*, in: *Lecture Notes in Physics*, Springer, 2008.
- [8] Ferdinand Verhulst, *Variations on the Fermi-Pasta-Ulam chain, a survey*, *Chaotic Model. Simul.* (2020) submitted for publication, arXiv:2003.09156.
- [9] L. Galgani, A. Giorgilli, A. Martinoli, S. Vanzini, *On the problem of energy partition for large systems of the Fermi-Pasta-Ulam type: analytical and numerical estimates*, *Physica D* 59 (1992) 334–348.
- [10] Roelof Bruggeman, Ferdinand Verhulst, *Near-integrability and recurrence in FPU chains with alternating masses*, *J. Nonlinear Sci.* 29 (2019) 183–206, <http://dx.doi.org/10.1007/s00332-018-9482-x>.
- [11] G.M. Czechin, D.S. Ryabov, K.G. Zhukov, *Stability of low-dimensional bushes of vibrational modes in the Fermi-Pasta-Ulam chains*, *Physica D* 203 (2005) 121–166.
- [12] P. Poggi, S. Ruffo, *Exact solutions in the FPU oscillator chain*, *Physica D* 103 (1997) 251–271.
- [13] R.W. Bruggeman, F. Verhulst, *Dynamics of a chain with four particles and nearest-neighbor interaction*, in: M. Belhaq (Ed.), *Recent Trends in Applied Nonlinear Mechanics and Physics*, CSNDD 2016, Springer, 2018, pp. 103–120, [http://dx.doi.org/10.1007/978-3-319-63937-6\\_6](http://dx.doi.org/10.1007/978-3-319-63937-6_6).
- [14] Roelof Bruggeman, Ferdinand Verhulst, *FPU-chains with large alternating masses (plus appendix)*, 2020, arXiv:2004.03876.
- [15] J.A. Sanders, F. Verhulst, J. Murdock, *Averaging Methods in Nonlinear Dynamical Systems*, second ed., in: *Appl. Math. Sciences*, vol. 59, Springer, 2007.
- [16] A. Weinstein, *Normal modes for nonlinear Hamiltonian systems*, *Invent. Math.* 20 (1973) 47–57.
- [17] A.P. Seyranian, A.A. Mailybaev, *Multiparameter Stability Theory with Mechanical Applications*, in: *Series A*, vol. 13, World Scientific, 2003.
- [18] J.J. Stoker, *Nonlinear Vibrations in Mechanical and Electrical Systems*, Wiley Classics Library Edition, 1992, ed. 1950, repr.
- [19] H. Christodoulidi, Ch. Efthymiopoulos, *Stages of dynamics in the Fermi-Pasta-Ulam system as probed by the first Toda integral*, *Math. Eng.* 1 (2) (2019) 359–377.



- [20] T.J. Anderson, A.H. Nayfeh, B. Balachandran, Coupling between high-frequency modes and a low-frequency mode: Theory and experiment, *Nonlinear Dynam.* 11 (1996) 17–36.
- [21] Andrew J. Dick, Balakumar Balachandran, C. Daniel Mote Jr., Localization in microresonator arrays: Influence of natural frequency tuning, *J. Comput. Nonlinear Dynam.* 5 (1) (2010) 011002, (11 pages), <http://dx.doi.org/10.1115/1.4000314>.