Dynamics of a chain with four particles and nearest-neighbor interaction

Roelof Bruggeman and Ferdinand Verhulst
Mathematisch Instituut, PO Box 80.010
3508TA Utrecht, Netherlands

September 6, 2016

Abstract

We formulate the periodic FPU problem with four alternating masses which is the simplest nontrivial version. The analysis involves normal form calculations to second order producing integrable normal forms with three timescales. In the case of large alternating mass the system is an example of dynamics with widely separated frequencies and three timescales. The presence of approximate integrals and the stability characteristics of the periodic solutions lead to weak interaction of the modes of the system.

1 Introduction

For the mono-atomic case of the original periodic FPU-problem (Fermi-Pasta-Ulam problem) with all masses (or particles) equal it was shown in [4] for up to six degrees-of-freedom (dof) and for an arbitrary number of dof in [5], that the corresponding normal forms are governed by $1 : 1$ resonances and that these Hamiltonian normal forms are integrable. This explains the recurrence phenomena near stable equilibrium for long intervals of time.

In [1] we have studied the inhomogeneous FPU-problem which contains many different resonance cases. In [9] and [10] recurrence and near-integrability aspects of FPU cells were studied. The alternating case was studied in [2] for a FPU chain with fixed end-points using analytic and numerical tools to obtain insight in the equipartition of energy, in particular between the low (acoustic) frequency and the high (optical) frequency part. A preliminary but important conclusion in [2] is that for the masses considered and on long timescales no equipartition takes place; the evidence is numerical. Inspired by [2] we will study the periodic FPU-problem in the case of alternating masses. The simplest nontrivial form of this problem is for four particles, it is necessary to understand this problem first. In a subsequent paper we will study the more general problem with an even number of particles. The emphasis will be on periodic solutions, integrability of the normal forms (near-integrability of the original system), invariant manifolds and recurrence phenomena; for recurrence see also [9].

In a periodic chain, for (even) n particles with arbitrary masses $m_j > 0$, position q_j and momentum $p_j = m_j\dot{q}_j, j = 1 \ldots n$, the Hamiltonian (see [1]) is of the form:

$$H(p,q) = \sum_{j=1}^{n}\left(\frac{1}{2m_j}p_j^2 + V(q_{j+1} - q_j)\right) \text{ with } V(z) = \frac{1}{2}z^2 + \frac{\alpha}{3}z^3 + \frac{\beta}{4}z^4. \quad (1)$$

If $\alpha = 1, \beta = 0$ we will call this an α-chain, if $\alpha = 0, \beta = 1$ a β-chain. The quadratic part of the Hamiltonian is not in diagonal form; for $n = 4$ the linearized equations of motion can be written as:

$$\begin{cases} m_1\ddot{q}_1 + 2q_1 - q_2 - q_4 & = 0, \\ m_2\ddot{q}_2 + 2q_2 - q_3 - q_1 & = 0, \\ m_3\ddot{q}_3 + 2q_3 - q_4 - q_2 & = 0, \\ m_4\ddot{q}_4 + 2q_4 - q_1 - q_3 & = 0. \end{cases} \tag{2}$$

In system (2) the 4 alternating masses are $1, m, 1, m$, with $m > 1$. Although this number of particles is small, the problem of the dynamics of such a periodic chain is by no means trivial. Moreover we will indicate that the dynamics of a small number of particles in the chain is in a certain sense typical for much larger systems.

The mass ratio $m : 1$ is the important parameter, we put $a = 1/m, 0 < a < 1$.
The eigenvalues of system (2) will be indicated by λ_i, $i = 1, \ldots, 4$, the corresponding frequencies of the linear normal modes are $\omega_i = \sqrt{\lambda_i}$. The numerical value of H_2 for given initial conditions is indicated by E_0. We will use symplectic transformation to put the linear part of the equations of motion in quasi-harmonic form. The solutions in the eigendirections of the equations of motion linearized near the origin are called the linear normal modes of the system, they can be continued for the nonlinear system. The transformation to quasi-harmonic form is natural but introduces an interpretation problem. Intuitively we expect the masses 1 to be more excitable than the masses m. However, after symplectic transformation we have in the resulting equations of motion a mix of both sets of particles and at the same time a splitting of the spectrum in $O(1)$ frequencies with modes that we will call 'optical' and $O(\sqrt{a})$ frequencies called 'acoustical'. The behaviour of the solutions within the two sets of particles can not in a simple way be identified with the normal mode (quasi-harmonic) equations corresponding with the optical and acoustical part of the spectrum.

In the following sections the analysis by averaging-normal forms is a basic tool. For the general theory and results in the case of Hamiltonian systems see [6]. Resonances in the frequency-spectrum of the linearized equations of motion, generated by the quadratic part of the Hamiltonian H_2, play a fundamental part in the analysis. The cubic part H_3 and if necessary the quartic part H_4 will be normalized to $\bar{H}_3, \bar{H}_4$.

In [1] we have discussed a number of technical normal form aspects of averaging for Hamiltonian systems. In a system of n perturbed harmonic equations we will often transform to polar coordinates. If the frequencies are ω_j, $1 \leq j \leq n$ we introduce

$$x_j \;=\; r_j \cos(\omega_j t + \varphi_j)\,, \quad y_j \;=\; -r_j\,\omega_j \sin(\omega_j t + \varphi_j) \qquad (1 \leq j \leq 7) \tag{3}$$

to produce an equivalent first-order system in the variables

$$X \;=\; (r_1, r_2, \ldots, r_n, \varphi_1, \ldots, \varphi_n)\,.$$

This system is equivalent with the n dof system of perturbed harmonic equations outside the normal mode planes.

The numerical experiments were carried out by MATCONT under MATLAB with ode solver 78. The precision was increased until the picture did not change anymore with typical relative error e^{-15}, absolute error e^{-17}. A number of algebraic manipulations were carried out using MATHEMATICA.

It will turn out that for the α- and β-chain especially the analysis for large mass is interesting. The normal form systems are in this case examples of integrable systems with widely separated frequencies. The dynamics involves periodic solutions, among which three normal modes; their stability can be established from the equations and the integrals. The normal form analysis has to be carried out to second order and uses three timescales. Using these results we can sketch a global picture of the phase-flow with a number of characteristic examples of recurrence phenomena. In the discussion we will mention the relevance of our results for FPU-systems with many more particles.

2 Periodic FPU chains with 4 alternating masses

We find from the equations of motion, both for an α- and for a β-chain, the momentum integral:

$$\dot{q}_1 + m\dot{q}_2 + \dot{q}_3 + m\dot{q}_4 = \text{constant.} \tag{4}$$

For the linear system (2) we find the 4 eigenvalues:

$$\lambda_i = 2(a+1),\ 2,\ 2a,\ 0.$$

with frequencies $\omega_i^2 = \lambda_i, i = 1, \ldots, 4$. We perform a symplectic transformation to eigenmodes of the form $q = L_a x$, $p = K_a y$, with the matrices

$$L_a = \begin{pmatrix} -\frac{1}{\sqrt{2a+2}} & -\frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{a}{2\,a+2}} \\ \frac{a}{\sqrt{2a+2}} & 0 & -\frac{\sqrt{a}}{\sqrt{2}} & \sqrt{\frac{a}{2a+2}} \\ -\frac{1}{\sqrt{2a+2}} & \frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{a}{2\,a+2}} \\ \frac{a}{\sqrt{2a+2}} & 0 & \frac{\sqrt{a}}{\sqrt{2}} & \sqrt{\frac{a}{2a+2}} \end{pmatrix}, \tag{5}$$

$$K_a = \begin{pmatrix} -\frac{1}{\sqrt{2a+2}} & -\frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{a}{2\,a+2}} \\ \frac{1}{\sqrt{2a+2}} & 0 & -\frac{1}{\sqrt{2}\sqrt{a}} & \frac{1}{\sqrt{a}\sqrt{2a+2}} \\ -\frac{1}{\sqrt{2a+2}} & \frac{1}{\sqrt{2}} & 0 & \sqrt{\frac{a}{2\,a+2}} \\ \frac{1}{\sqrt{2a+2}} & 0 & \frac{1}{\sqrt{2}\sqrt{a}} & \frac{1}{\sqrt{a}\sqrt{2a+2}} \end{pmatrix}. \tag{6}$$

The coordinates (x_4, y_4) correspond to the momentum integral (4). We proceed with the reduced system (x_j, y_j), $1 \leq j \leq 3$, in which the components of the Hamiltonian take the following form:

$$\begin{cases} H_2 = & (1+a)x_1^2 + x_2^2 + ax_3^2 + \frac{1}{2}(y_1^2 + y_2^2 + y_3^2), \\ H_3 = & -2\sqrt{2a(1+a)}x_1x_2x_3, \\ H_4 = & \frac{1}{4}((1+a)^2x_1^4 + x_2^4 + 6ax_2^2x_3^2 + a^2x_3^4 + 6(1+a)x_1^2(x_2^2 + ax_3^2)). \end{cases} \tag{7}$$

The usual procedure for normalization as an approximation procedure is to rescale in a neighborhood of equilibrium, in this case $x_i \to \varepsilon x_i$, $y_i \to \varepsilon y_i$, $i = 1, 2, 3$ with ε a small positive parameter. This procedure yields, after dividing by ε^2 in the Hamiltonian a system with a small parameter which is a measure for the distance to equilibrium. The procedure will be implicit in our statements in the case that a is not a small parameter. If $0 < a \ll 1$ (large mass

m) we will also leave out the scaling with ε as a will be a natural small parameter. Still, also in this case, we will assume for the solutions to be in a neighborhood of equilibrium; when starting closer to equilibrium (small energy) the normal form results will improve.

3 The α-chain

The equations of motion are for the α-chain with $\gamma = 2\sqrt{2a(1+a)}$:

$$\begin{cases} \ddot{x}_1 + 2(1+a)x_1 & = \gamma x_2 x_3, \\ \ddot{x}_2 + 2x_2 & = \gamma x_1 x_3, \\ \ddot{x}_3 + 2a x_3 & = \gamma x_1 x_2. \end{cases} \tag{8}$$

Special solutions are the normal modes associated with the eigenvalues $2(1+a)$, 2 and $2a$. These exact solutions are harmonic for an α-chain. The equilibria of system (8) are the origin in phase-space and the points with coordinates:

$$(x_1, x_2, x_3, y_1, y_2, y_3) = (\frac{\delta_1}{\sqrt{2(1+a)}}, \frac{\delta_2}{\sqrt{2}}, \frac{\delta_3}{\sqrt{2a}}, 0, 0, 0)\,,$$

with $\delta_i = \pm 1, i = 1, 2, 3$ with $\delta_1\delta_2\delta_3 = 1$. The energy value of the four equilibria outside the origin is in all cases 0.5. The energy manifold bifurcates geometrically in the critical points of the energy manifold, the corresponding equilibria of the equations of motion are unstable. For values of the energy between 0 and 0.5, the energy manifold is compact.

The first order resonances in a three dof system like (8) are $1:2:1$, $1:2:2$, $1:2:3$ and $1:2:4$. Considering the spectrum of the linearized system (8) we find no three dof first order resonances in a cell with four particles.
Two dof first order resonances occur if $a = \frac{1}{4}, \frac{1}{3}$. Second order resonances arise if $a = \frac{1}{8}, \frac{1}{9}$ and if $0 < a \ll 1$. It was shown in [6] section 10.4, that the normal form of a two dof Hamiltonian system is integrable. Adding a third dof with non-commensurable third frequency as is the case here keeps to high order these normal forms integrable as the added terms remain separated from the resonant two dof.

We conclude that for $0 < a < 1$ a periodic FPU α-chain with four alternating masses is in normal form near-integrable. The dynamics (periodic solutions and stability) of the two dof cases can be found in the literature (for references see [6]) but is in this case fairly degenerate. The case of values of a very close to zero have to be considered separately.

3.1 The α-chain for large mass m

For large values of the mass we have a in a neighborhood of zero. Two of the frequencies will be near $\sqrt{2}$, one will be $\sqrt{2a}$, the associated modes will be called the optical group (x_1, x_2) and the acoustical group (x_3). System (8) is an example of a system with widely separated frequencies, see [7] and further references there. Following the analysis in [7] we apply normalization considering x_3 as slowly varying. The slow dynamics of x_3 becomes more transparent when rescaling the Hamiltonian to a related standard form by

$$x_3 \to (2a)^{-\frac{1}{4}} x_3,\; y_3 \to (2a)^{+\frac{1}{4}} y_3. \tag{9}$$

This results in:

$$H_2 = (1+a)x_1^2 + x_2^2 + \frac{1}{2}(y_1^2 + y_2^2) + \frac{1}{2}\sqrt{2a}(x_3^2 + y_3^2)$$

and

$$H_3 = -\bar{\gamma}x_1x_2x_3,\ \bar{\gamma} = 2^{\frac{5}{4}}\sqrt{1+a}\,a^{\frac{1}{4}}.$$

In the equations of motion we rescale $x_i \to a^{\frac{1}{8}}x_i, i = 1,2$; this choice is optimal for keeping as many interactive terms in the approximations as possible. In [8] this is called a significant degeneration of the differential operator. System (8) becomes with the rescalings:

$$\begin{cases} \ddot{x}_1 + 2x_1 = \bar{\gamma}x_2x_3 - 2ax_1, \\ \ddot{x}_2 + 2x_2 = \bar{\gamma}x_1x_3, \\ \dot{x}_3 = \sqrt{2a}y_3,\ \dot{y}_3 = \bar{\gamma}a^{\frac{1}{4}}x_1x_2 - \sqrt{2a}x_3. \end{cases} \tag{10}$$

The terms with small parameter $\bar{\gamma} = O(a^{\frac{1}{4}})$ dominate. Introducing polar coordinates

$$x_1 = r_1\cos(\sqrt{2}t + \phi_1), \dot{x}_1 = -\sqrt{2}r_1\sin(\sqrt{2}t + \phi_1),$$

$$x_2 = r_2\cos(\sqrt{2}t + \phi_2), \dot{x}_2 = -\sqrt{2}r_2\sin(\sqrt{2}t + \phi_2),$$

we find after transformation and normalization to $O(\bar{\gamma})$:

$$\begin{cases} \dot{r}_1 = -\frac{\bar{\gamma}}{2\sqrt{2}}r_2\sin(\phi_1 - \phi_2)x_3,\ \dot{\phi}_1 = -\frac{\bar{\gamma}}{2\sqrt{2}}\frac{r_2}{r_1}\cos(\phi_1 - \phi_2)x_3, \\ \dot{r}_2 = +\frac{\bar{\gamma}}{2\sqrt{2}}r_1\sin(\phi_1 - \phi_2)x_3,\ \dot{\phi}_2 = -\frac{\bar{\gamma}}{2\sqrt{2}}\frac{r_1}{r_2}\cos(\phi_1 - \phi_2)x_3, \\ \dot{x}_3 = 0,\ \dot{y}_3 = 0. \end{cases} \tag{11}$$

For the third mode we find with $y_3(0) = 0$:

$$x_3 = x_3(0),\ y_3 = 0.$$

We put $\chi = \phi_1 - \phi_2$. The solutions of the normal form have error $O(a^{\frac{1}{4}})$ on the timescale $a^{-\frac{1}{4}}$, see the appendix.

Integrals of the normalization. System (11) has the integral of motion $E_3 = \frac{1}{2}\sqrt{2a}(x_3^2 + y_3^2)$ and the second integral

$$\frac{1}{2}(r_1^2 + r_2^2) = E_1 \tag{12}$$

with E_1 a positive constant. This integral is valid with error $O(a^{\frac{1}{4}})$. The choice of polar coordinates means that we have to exclude normal modes, but we know already that the original system (8) has three normal mode solutions. We have

$$\frac{d}{dt}\chi = -\frac{\bar{\gamma}}{2\sqrt{2}}\left(\frac{r_2}{r_1} - \frac{r_1}{r_2}\right)x_3\cos\chi.$$

From the equations for r_1 in system (11) and the equation for χ we find

$$\frac{dr_1}{d\chi} = r_2\frac{\sin\chi}{\left(\frac{r_2}{r_1} - \frac{r_1}{r_2}\right)\cos\chi}.$$

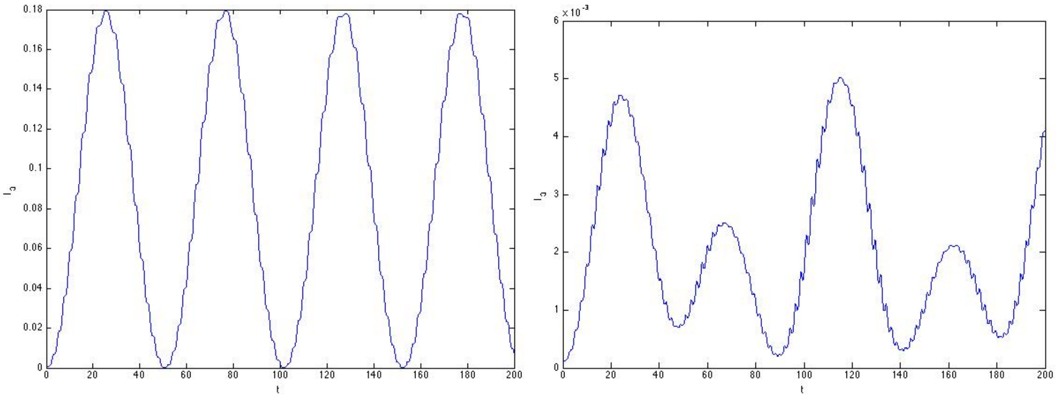

Figure 1: Interactions with the x_3 mode for $a = 0.01$ in system (8). Left the action $I_3 = \frac{1}{2}(\dot{x}_3^2 + 2ax_3^2)$ with initial conditions $x_1(0) = x_2(0) = 0.5, x_3(0) = 0.1$ and initial velocities zero so $I_1(0) = I_2(0) = 0.25, I_3(0) = 10^{-4}$ resulting in $0 < I_3 < 0.18$. Right I_3 if $x_1(0) = 0.1, x_2(0) = 0.5, x_3(0) = 0.1$ so $I_1(0) = 0.01, I_2(0) = 0.25, I_3(0) = 10^{-4}$ resulting in (much smaller) $0 < I_3 < 0.005$.

Eliminating r_2 with integral (12) the equation becomes separable. We find:

$$r_1 r_2 \cos\chi = C, \tag{13}$$

which is a third integral of motion of system (11); C is a constant determined by the initial conditions. We conclude that to first order of approximation we have no interaction between the first two modes (the optical part) and the third mode (the acoustical part). However, a numerical experiment suggests that the x_3 mode is interacting with the other modes, see fig. 1, so to show this analytically we will compute a second order approximation later on.

Periodic solutions. At first order a special solution arises if

$$\chi = 0, \pi.$$

This is possible if

$$\frac{d}{dt}\chi = -\frac{\bar{\gamma}}{2\sqrt{2}}\left(\frac{r_2}{r_1} - \frac{r_1}{r_2}\right) x_3 \cos\chi = 0. \tag{14}$$

We conclude for this special solution $r_1 = r_2$ with solutions for x_1, x_2 given by:

$$x_1(t) = \sqrt{E_1}\cos(\sqrt{2}t + \phi_0),\ x_1(t) = \pm x_2(t), \tag{15}$$

an approximation valid on the timescale $a^{-1/4}$. Choosing $x_3(0), y_3(0)$, solutions (15) are determined uniquely. These solutions $(x_i, y_i, i = 1, 2, 3)$ form manifold M_1 embedded in the energy manifold defined by the quadratic integrals E_3 and E_1 of system (11).

Another special solution of (14) arises if

$$\chi = \frac{\pi}{2}, 3\frac{\pi}{2}.$$

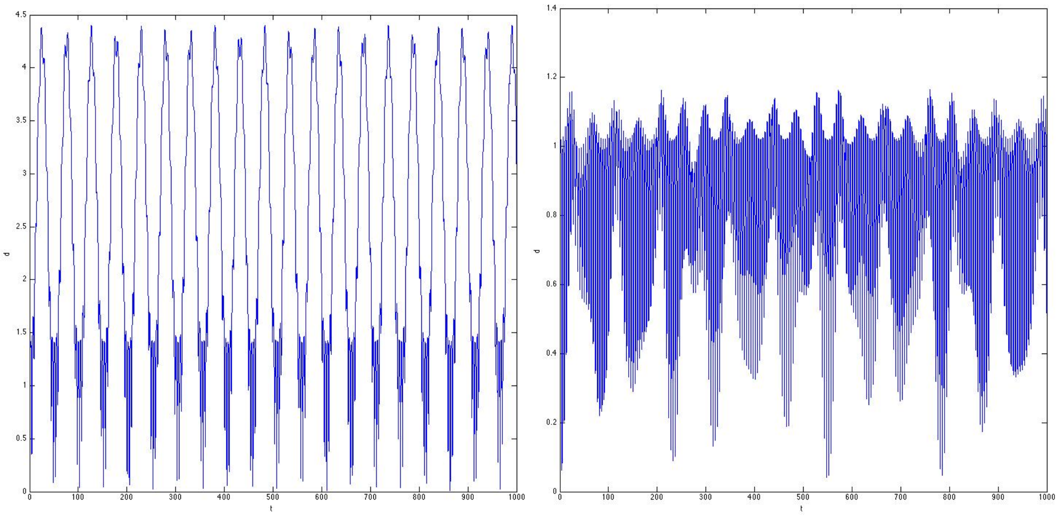

Figure 2: Recurrence indicated by the Euclidean distance d with respect to the initial values as a function of time in the α-chain with the conditions as in fig. 1. If $x_1(0) \neq x_2(0)$ (right) the recurrence takes longer.

In this case the solutions of system (11) are determined by:

$$\begin{cases} r_1(t) &= A\cos(\frac{\bar{\gamma}}{2\sqrt{2}}x_3(0)t) + B\sin(\frac{\bar{\gamma}}{2\sqrt{2}}x_3(0)t), \\ r_2(t) &= \mp A\frac{\bar{\gamma}}{2\sqrt{2}}x_3(0)\sin(\frac{\bar{\gamma}}{2\sqrt{2}}x_3(0)t) \pm B\frac{\bar{\gamma}}{2\sqrt{2}}x_3(0)\cos(\frac{\bar{\gamma}}{2\sqrt{2}}x_3(0)t), \end{cases} \tag{16}$$

with $x_3(t) = x_3(0), \phi_1(0) - \phi_2(0) = \pi/2, 3\pi/2$ and constants A, B; analogously to the case of M_1, the solutions $x_i, y_i, i = 1, 2, 3$ form manifold M_2 embedded in the energy manifold.

Both for special solution (15) and (16) we have families of periodic solutions on the energy manifold. This may signal a degeneration of the normal form at first order in the sense of Poincaré [3] vol. 1. This gives another reason to compute a second order approximation.

Integrability and recurrence. The normal form (11) of the α-chain for large mass is clearly integrable. The three normal form integrals can be written as quadratic expressions:

$$\frac{1}{2}\sqrt{2a}(x_3^2 + y_3^2) = E_3,\ \dot{x}_1^2 + 2x_1^2 + \dot{x}_2^2 + 2x_2^2 = 2E_1,\ 2x_1x_2 + \dot{x}_1\dot{x}_2 = 2C. \tag{17}$$

The three integrals are exact integrals of the normal form equations (11) and approximate integrals of the original equations (10). Remarkably enough the recurrence properties of the phase flow are different in the two cases of fig. 1. In the case where $x_1(0) = x_2(0) = 0.5$, we have rather strong recurrence, see fig. 2 left, in the case $x_1(0) = 0.1, x_2(0) = 0.5$ the recurrence times are longer; see fig. 2. The two special solutions obtained above suggest an explanation. Starting at the first special solution we have to first approximation periodicity with period $\sqrt{2}\pi$, for the second special solution we find a modulation of the period $O(\bar{\gamma}x_3(0))$.
We conclude that even if we have a system with integrable normal form, its recurrence properties depend strongly on the initial conditions. We will return to this in section 6.

3.2 Second order approximation for the α-chain

A second order approximation according to [6] can be computed using MATHEMATICA. As before we do not change the notation for the variables r_1, ϕ_1 etc. to avoid too many new symbols. We find with $\bar{\gamma} = O(a^{\frac{1}{4}})$ (and a mix of variables):

$$\begin{cases} \dot{r}_1 = -\frac{\bar{\gamma}}{2\sqrt{2}} r_2 x_3 \sin\chi,\ \dot{\phi}_1 = -\frac{\bar{\gamma}}{2\sqrt{2}} \frac{r_2}{r_1} x_3 \cos\chi - \frac{1}{4} a^{\frac{1}{2}} x_3^2, \\ \dot{r}_2 = +\frac{\bar{\gamma}}{2\sqrt{2}} r_1 x_3 \sin\chi,\ \dot{\phi}_2 = -\frac{\bar{\gamma}}{2\sqrt{2}} \frac{r_1}{r_2} x_3 \cos\chi - \frac{1}{4} a^{\frac{1}{2}} x_3^2, \\ \dot{x}_3 = (2a)^{\frac{1}{2}} y_3,\ \dot{y}_3 = -(2a)^{\frac{1}{2}} x_3 + (2)^{\frac{1}{4}} (a)^{\frac{1}{2}} r_1 r_2 \cos\chi. \end{cases} \tag{18}$$

We deduce from system (18) that the quadratic integral (12) persists; $d\chi/dt$ does not change at second order, so also the quadratic integral (13) persists. The two special solutions (15) and (16) are slightly modified but correspond at second order still with manifolds of special solutions. For x_3, y_3 we can write

$$\ddot{x}_3 + 2ax_3 = 2ar_1r_2\cos\chi.$$

Using integral (13) we have with $y_3(0) = 0$ as second order approximation:

$$x_3(t) = (x_3(0) - C)\cos(\sqrt{2a}\,t) + C \tag{19}$$

with $C = r_1(0)r_2(0)\cos\chi(0)$.This establishes the interaction with the x_3 normal mode as for initial values of x_1, x_2 producing an $O(1)$ value of C, the amplitude of x_3 will grow even if $x_3(0)$ is small.
From system (8), so before rescaling, we can find the equivalent integral equation for $x_3(t)$ which also holds for the rescaled quantities:

$$x_3(t) = x_3(0)\cos\sqrt{2a}t + 2\sqrt{1+a}\int_0^t x_1(\tau)x_2(\tau)\sin(\sqrt{2a}(t-\tau))d\tau, \tag{20}$$

where we have chosen $\dot{x}_3(0) = 0$. The oscillating integral can be evaluated using approximations for $x_1(t), x_2(t)$ for instance the special solutions (15) (interaction timescales t and $a^{1/2}t$) and (16) (interaction timescales $t, a^{1/4}t$ and $a^{1/2}t$).
Note that inspection of system (10) shows that neglecting terms $O(a)$, we have $x_1(t) = \pm x_2(t)$ exactly. This means that in this particular case $x_1(t)x_2(t)$ will be sign definite in the integral of (20) at this level of approximation.

4 The β-chain for large mass m

The Hamiltonian given by (7) is positive definite outside the origin, so the origin is the only equilibrium. The energy manifolds are compact. The remarks on the possible resonances of the α-chain apply also to the β-chain. So we restrict ourselves to the case of large mass m. The equations of motion are more complicated and are without scaling of the coordinates:

$$\begin{cases} \ddot{x}_1 + 2(1+a)x_1 &= -(1+a)^2x_1^3 - 3(1+a)x_1(x_2^2 + ax_3^2), \\ \ddot{x}_2 + 2x_2 &= -x_2^3 - 3ax_2x_3^2 - 3(1+a)x_1^2x_2, \\ \ddot{x}_3 + 2ax_3 &= -3ax_2^2x_3 - a^2x_3^3 - 3a(1+a)x_1^2x_3. \end{cases} \tag{21}$$

The three normal modes are exact solutions (elliptic functions) of the system. To apply normalization we will assume that a is small and will rescale with respect to equilibrium:

$$(x_i, y_i) \to a^{\frac{1}{4}}(x_i, y_i) i = 1, 2, x_3 \to (2a)^{-\frac{1}{4}} x_3,\ y_3 \to (2a)^{+\frac{1}{4}} y_3.$$

This scaling keeps as many interaction terms as possible. We find after scaling:

$$\begin{cases} \ddot{x}_1 + 2x_1 & = -2ax_1 - \sqrt{a}(1+a)^2 x_1^3 - 3\sqrt{a}(1+a)x_1(x_2^2 + \frac{1}{2}\sqrt{2}x_3^2)), \\ \ddot{x}_2 + 2x_2 & = -\sqrt{a}x_2^3 - \frac{3}{2}\sqrt{2a}x_2 x_3^2 - 3\sqrt{a}(1+a)x_1^2 x_2, \\ \dot{x}_3 = \sqrt{2a}y_3,\ \dot{y}_3 & = -\sqrt{2a}x_3 - a(\frac{3}{2}\sqrt{2}x_2^2 x_3 + \frac{1}{2}x_3^3 + \frac{3}{2}\sqrt{2}(1+a)x_1^2 x_3). \end{cases} \tag{22}$$

Neglecting terms $O(a)$ we find with $\chi = \phi_1 - \phi_2$ the normal form:

$$\begin{cases} \dot{r}_1 & = +\frac{3\sqrt{a}}{8\sqrt{2}} r_1 r_2^2 \sin 2\chi,\ \dot{\phi}_1 = \frac{\sqrt{a}}{16}\left(3\sqrt{2}(r_2^2\cos 2\chi + 2r_2^2 + r_1^2) + 12x_3^2\right), \\ \dot{r}_2 & = -\frac{3\sqrt{a}}{8\sqrt{2}} r_1^2 r_2 \sin 2\chi,\ \dot{\phi}_2 = \frac{\sqrt{a}}{16}\left(3\sqrt{2}(r_1^2\cos 2\chi + 2r_1^2 + r_2^2) + 12x_3^2\right), \\ \dot{x}_3 & = \sqrt{2a}y_3, \dot{y}_3 = -\sqrt{2a}x_3. \end{cases} \tag{23}$$

We find again the integral $E_3 = \frac{1}{2}\sqrt{2a}(x_3^2 + y_3^2)$ and the second normal form integral (12). The equation for χ becomes

$$\frac{d}{dt}\chi = -\frac{3\sqrt{2}}{8}\sqrt{a}(r_1^2 - r_2^2)\cos^2\chi.$$

From system (23) we find also the third integral (13):

$$r_1 r_2 \cos\chi = C,$$

with C determined by the initial conditions.
A special solution with constant amplitudes r_1 and r_2 may arise if

$$\chi = \varphi_1 - \phi_2 = 0, \pi/2, \pi, 3\pi/2.$$

From the equation for $\chi = \phi_1 - \phi_2$ we find the requirement $r_1 = r_2$ corresponding with four periodic solutions of the first order normal form. The initial values $x_3(0), y_3(0)$ are still free, the solutions $x_i, y_i, i = 1, 2, 3$ produce manifold M_1 embedded in the energy manifold.
Analogous to the case of the α-chain we find solutions from the equation for $d\chi/dt$ with constant phase difference. These are found if

$$r_1 \neq r_2,\ \chi = \frac{\pi}{2}, 3\frac{\pi}{2}.$$

For $r_1(t), r_2(t)$ we find in this case goniometric functions of $\sqrt{a}t$ and, as for the α-chain, a manifold M_2 of special solutions $x_i, y_i, i = 1, 2, 3$ embedded in the energy manifold.

At this level of approximation we find no interaction between the optical and the acoustical group. This motivates us to compute the second order normal form.

4.1 Second order approximation for the β-chain

A second order approximation according to [6] can be computed using again MATHEMATICA. We do not change the notation for the variables r_1, ϕ_1 etc. to avoid too many new symbols. We find for the $O(a)$-terms to be added to the derivatives $\dot{r}_1, \dot{\phi}_1, \dot{r}_2, \dot{\phi}_2, \dot{x}_3, \dot{y}_3$ in the normal form of system (23):

$$\begin{cases} -\frac{3}{512} r_1 r_2^2 \sin(2\chi)\left(17\sqrt{2}\left(r_1^2+r_2^2\right)+48x_3^2\right) \\ \frac{-288x_3^2\left(r_2^2(\cos(2\chi)+2)+r_1^2\right)-51\sqrt{2}\left(2r_2^2r_1^2(2\cos(2\chi)+3)+r_2^4(2\cos(2\chi)+3)+r_1^4\right)-144\sqrt{2}x_3^4}{1024}+\frac{1}{\sqrt{2}} \\ \frac{3}{512} r_1^2 r_2 \sin(2\chi)\left(17\sqrt{2}\left(r_1^2+r_2^2\right)+48x_3^2\right) \\ \frac{-288\, x_3^2\left(r_1^2(\cos(2\chi)+2)+r_2^2\right)-51\sqrt{2}\left(r_1^4(2\cos(2\chi)+3)+2r_2^2r_1^2(2\cos(2\chi)+3)+r_2^4\right)-144\sqrt{2}x_3^4}{1024} \\ 0 \\ -\frac{1}{4}x_3\left(3\sqrt{2}\left(r_1^2+r_2^2\right)+2x_3^2\right) \end{cases} \tag{24}$$

Integral (12) is conserved again to second order. The condition for constant amplitudes r_1 and r_2 is again

$$\chi = \varphi_1 - \phi_2 = 0, \pi/2, \pi, 3\pi/2.$$

The requirement $d\chi/dt = 0$ is satisfied for $r_1 = r_2 + O(\sqrt{a})$, producing four periodic solutions.
For the third mode we find with integral (12) the equation:

$$\ddot{x}_3 + (2a + 3a^{\frac{3}{2}} E_1)x_3 = -\frac{1}{2}\sqrt{2}a^{\frac{3}{2}} x_3^3. \tag{25}$$

The only critical point (equilibrium) is $(0,0)$ which is stable. This means that starting near the origin, the solution will not move away. The results show for the β-chain weak interaction between acoustical and optical group and dependence on the initial conditions. In general the solutions for the β-chain depend on the timescales t, $\sqrt{a}t$, at.

5 Stability of the periodic solutions for large mass m

The first and second order normal form analysis enables us to establish the stability of the periodic solutions. Note however that for three and more dof instability in Hamiltonian systems from a perturbation (normal form) analysis is conclusive, stability is not. Purely imaginary eigenvalues guarantee 'stability on a certain timescale'.

- The x_1 and x_2 normal modes.
  If either $x_1(0)$ or $x_2(0)$ is small, we conclude with integral (13) that C is small. For the α- and the β-chain this implies with eqs. (19) and (25) that if $x_3(0)$ is small, $x_3(t)$ remains small.
  Consider now a neighborhood of the x_1 normal mode for the α-chain.
  Choose $x_3(0) > 0, \chi(0) = 0$ and $\varepsilon > 0$ such that if $r_2(0) = \varepsilon$ we have $C = x_3(0)/2$. From integral (13) we have that $\cos\chi(t)$ can not vanish so that $\chi(t)$ has to oscillate between $-\pi/2$ and $+\pi/2$. As $x_3(t)$ may only change sign on the timescale $1/\sqrt{a}$, we

have that $d\chi/dt$ is sign definite unless $r_2(t)$ grows. We conclude to instability of the x_1 normal mode.
The same reasoning applies to the x_2 normal mode of the α-chain.

For the β-chain the reasoning is similar but simpler as the equation for χ does not depend on x_3. With $\chi(0) = 0$ we have that $\chi(t)$ has to oscillate between $-\pi/2$ and $+\pi/2$. The second order normal form for $d\chi/dt$ can only change sign if $r_1^2 - r_2^2 + O(\sqrt{a})$ changes sign. Both normal modes are unstable for the β-chain.

- The x_3 normal mode.
  If both x_1 and x_2 are small we conclude with integral (12) that these modes remain small. The normal mode x_3 is stable both for the α- and the β-chain.

- The solution manifold M_1 for $r_1 = r_2, \chi = 0, \pi$.
  We will use the first order approximations as using the second order does not change the results qualitatively. We can consider the stability behavior with respect to the x_1, x_2 modes and the x_3 mode in the first order approximations separately.

  The α-chain. Regarding the behaviour with respect to the x_1, x_2 modes we eliminate r_2 with integral (12) after which we linearize the normal form equations of motion (11) and (23) in a neighborhood of $r_1 = r_2, \chi = 0, \pi$. For the α-chain we have the system:

$$\dot{r}_1 = -\frac{\bar{\gamma}}{2\sqrt{2}} x_3 \sqrt{2E_1 - r_1^2} \sin \chi), \; \dot{\chi} = \frac{\bar{\gamma}}{2\sqrt{2}} x_3 \left(\frac{\sqrt{2E_1 - r_1^2}}{r_1} - \frac{r_1}{\sqrt{2E_1 - r_1^2}} \right) \cos \chi. \quad (26)$$

  The Jacobian matrix yields if $r_1 = r_2 = \sqrt{E_1}, \chi = 0, \pi$ the eigenvalue equation:

$$\lambda^2 - 4\frac{\bar{\gamma}^2}{2} x_3^2 = 0.$$

  This produces eigenvalues with opposite signs, we have instability.
  From integral (12) we find $C = \pm E_1$. The approximation for x_3 of the α-chain (19) shows that also x_3 will grow in size.

  The β-chain. Repeating the analysis for the β-chain we find for the x_1, x_2 modes the corresponding equations:

$$\dot{r}_1 = +\frac{3\sqrt{a}}{8\sqrt{2}} r_1 (2E_1 - r_1^2) \sin 2\chi, \; \dot{\chi} = -\frac{3\sqrt{2}}{4} \sqrt{a} (r_1^2 - E_1) \cos^2 \chi.$$

  The Jacobian matrix yields if $r_1 = r_2 = \sqrt{E_1}, \chi = 0, \pi$ the eigenvalue equation:

$$\lambda^2 + \frac{9}{8} a E_1^2 = 0$$

  and purely imaginary eigenvalues; the second order does not change this.
  The second order approximation of x_3 for the β-chain described by eq. (25) does not grow in size; we have stability of M_1 for the β-chain.

- The solution manifold M_2 for $\chi = \pi/2, 3\pi/2$.
  In this case there is no restriction on r_1, r_2. We can expand the normal form equation for χ near $\chi = \pi/2, 3\pi/2$. We find from the equations obtained above for $d\chi/dt$ that if $r_1 \neq r_2$, χ will change. The case $r_1 = r_2$ produces eigenvalues zero and is left as a degenerate case. Both for the α-chain and the β-chain we find instability if $r_1 \neq r_2$.

6 The global picture for large mass

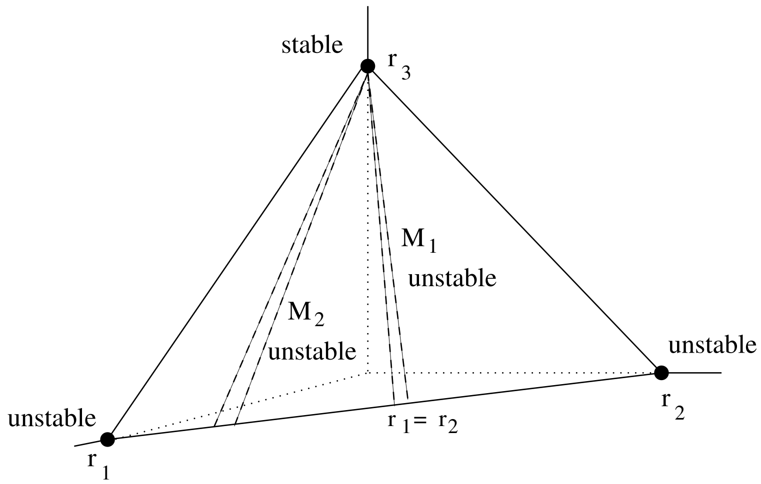

Figure 3: The amplitude-symplex for the α-chain that is a projection omitting the phases (or angles). The front triangle corresponds with $H_2 =$ constant. The dots at the vertices indicate normal mode periodic solutions. The manifolds M_1 ($r_1 = r_2$) corresponds with tori that are unstable in the case of the α-chain, stable for the β-chain. M_2 is unstable if $r_1 \neq r_2$ with $r_1 = r_2$ undecided.

We consider compact energy manifolds for the α-chain (energy between 0 and 0.5) and the β-chain not too far from the origin of phase-space. The energy manifolds and of course the manifold corresponding with $H_2 = E_0$ (constant), are topologically the sphere S^5. Both for the α- and the β-chain, we have that the x_1 and x_2 modes for fixed E_1 are restricted to the ellipsoid M_{12} which is S^3 described by integral (12) and is embedded in the energy manifold with in general $0 < E_1 < E_0$.
A transversal of the flow on S^5 will be 4-dimensional. Consider the transversal D determined by $y_3 = 0$ with x_3 eliminated using the integral $H_2 = E_0$. The coordinate plane x_1, y_1 is located in D containing as boundary the x_1 normal mode which is S^1. Perpendicular to this plane is the coordinate plane x_2, y_2 in D with as a boundary the normal mode x_2; the boundary does not belong to the transversal. As for the x_2 normal mode we have $x_1 = y_1 = 0$, the x_2 normal mode will go through this point in the centre of the x_1, y_1 coordinate plane. This means that the x_1 and x_2 normal modes are linked. We can repeat this reasoning for a transversal containing the x_3 normal mode. We conclude that the three normal modes are linked on S^5. The stable normal modes are surrounded by invariant tori embedded in the energy manifold.
The x_3 mode plays a special part. The dynamics on M_{12} is still determined by the third mode

through the phases (or angles in action-angle representation). The integral (13) restricts the dynamics on manifold M_{12}. The solutions around the x_3 normal mode move on tori on the 5-dimensional energy manifold that extend to the normal modes x_1 and x_2 and of which the size depends on the initial conditions of all variables.

The special solution (15) produces a torus M_1 on the energy manifold with $r_1 = r_2$ and shrinking diameter as $x_3(t)$ becomes more prominent. For the α-chain, the torus is unstable, for the β-chain we have stability if $x_3(0)$ is small enough.

The special solution (16) of the normal form produces a torus M_2 for which in general $r_1 \neq r_2$. It is unstable and may not persist under higher order perturbations. For the α-chain the instability poses a problem when connecting the stable normal mode x_3 with the unstable tori. Note however that the instability of M_1 arises only if C of integral (13) is not small which it is near the x_3 normal mode. As a further illustration consider the linearization of the normal form equations (26). If $r_1, r_2 = O(a^{\frac{1}{4}})$ and $r_1 \neq r_2$ we have near the x_3 normal mode that $\dot{r}_1 = O(\sqrt{a}), \dot{\chi} = O(a^{\frac{1}{4}})$ which is an obstruction to the validity of linearization. For an illustration of the stability results by an amplitude-simplex see fig. 3.

Consequences for recurrence

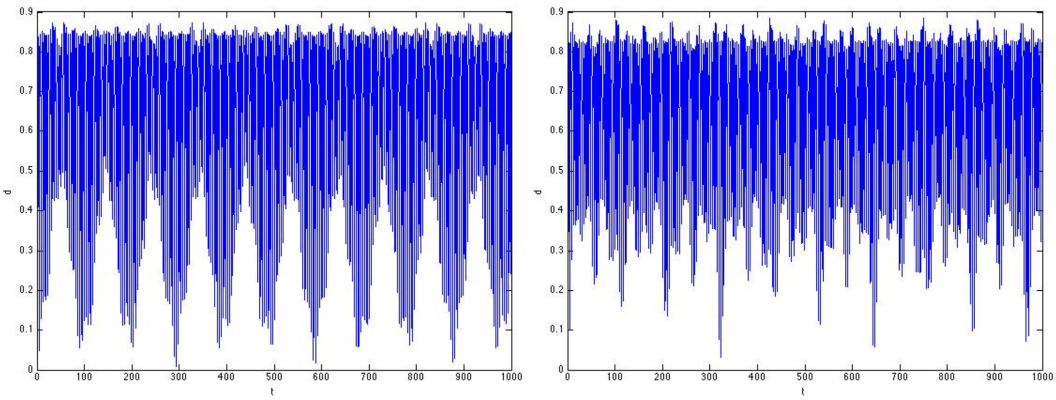

Figure 4: Recurrence for 1000 timesteps indicated by the Euclidean distance d with respect to the initial values as a function of time in the α-chain with $a = 0.04$, energy 0.1762. Left the conditions $x_1(0) = 0.05, x_2(0) = 0.4168, x_3(0) = 0.01$ near the x_2 normal mode; we have recurrence with $0 \leq d \leq 0.9$. Right the case where $x_3(0)$ is also small but more removed from the normal modes with $x_1(0) = 0.4, x_2(0) = 0.1, x_3(0) = 0.01$; the instability weakens the recurrence ($0 \leq d \leq 0.9$).

Recurrence of the flow as guaranteed by the Poincaré recurrence theorem, provides us with additional information about the dynamics in phase-space. We will consider some aspects for the α-chain as this chain has most instability. In fig. 4 we start near the stable x_2 normal mode which results in relatively strong recurrent motion, as expected. The result is rather different when starting away from the normal modes with $x_1(0) \neq x_2(0)$; the recurrence is weakened by the instability of M_2 although the normal form is integrable.

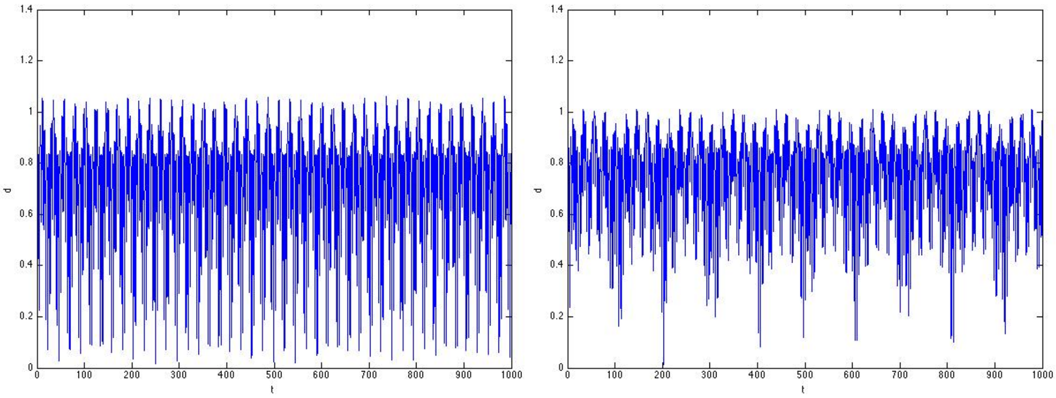

Figure 5: Recurrence for 1000 timesteps indicated by the Euclidean distance d with respect to the initial values as a function of time in the α-chain with $a = 0.04$, energy 0.1762. Left the conditions $x_1(0) = 0.2943, x_2(0) = 0.2943, x_3(0) = 0.01$; starting near M_1 we have fairly good recurrence with $0 \leq d \leq 1.1$. Right the case where $x_1(0) = 0.37, x_2(0) = 0.2167$ and $x_3(0) = 0.5$, away from the normal modes; the motion along the tori weakens the recurrence ($0 \leq d \leq 1.1$). Extending the picture to 5000 time steps does not improve the recurrence.

In fig. 5 we start near manifold M_1 to observe good short-time recurrence. Right we move to more general position on the energy manifold with $x_1(0) \neq x_2(0)$; this produces rather bad recurrence.

7 Conclusions and discussion

1. The periodic FPU-problem with 4 particles and alternating masses can be reduced to a three dof Hamiltonian problem. The normal modes are exact periodic solutions of the reduced system both for the α- and the β-chain.

2. Normal form calculations lead to an integrable system with three normal form integrals and additional periodic solutions.

3. A second order normal form calculation is necessary to characterize the phase-flow. This involves three timescales with the conclusion that we have weak interaction between the acoustical and the optical part of the system.

4. The integrability of the normal form, corresponding with approximate integrability of the original system, keeps the system recurrent with fairly short intervals of time.

5. We will show in a subsequent paper the important fact that the dynamics of the four particles problem is in a certain sense typical for periodic FPU problems with alternating masses and many more particles.

8 Appendix

In the error estimates of the normal form analysis integral inequalities can be useful. We will use the *specific Gronwall lemma* formulated in [6], lemma 1.3.3.

Lemma 8.1
Let ϕ be a real-valued continuous (or piecewise continuous) functions on a real t interval $I : t_0 \leq t \leq T$. Assume $\phi(t) > 0$ on I and $\delta_1(\varepsilon), \delta_2(\varepsilon)$ positive order functions (ε a small, positive parameter). If the inequality

$$\phi(t) \leq \delta_2(\varepsilon)(t - t_0) + \delta_1(\varepsilon) \int_{t_0}^{t} \phi(s) ds,$$

holds on I, then

$$\phi(t) \leq \frac{\delta_2(\varepsilon)}{\delta_1(\varepsilon)} e^{\delta_1(\varepsilon)(t-t_0)}.$$

We apply the *specific Gronwall lemma* to obtain:

Lemma 8.2
Consider the perturbation problem:

$$\dot{x} = \delta_1(\varepsilon) f(t, x) + \delta_2(\varepsilon) R(t, x), x(t_0) = x_0,$$

for $I : t_0 \leq t \leq T, x \in D \subset \mathbb{R}^n$, $\delta_1, \delta_2, \delta_3(\varepsilon)$ order functions with $\delta_2(\varepsilon) = o(\delta_1(\varepsilon))$ as $\varepsilon \to 0$ and continuous differentiability of the vector fields f, R on $I \times D$; in particular we have $||R(t, x)|| \leq M, M > 0$ for $t \geq 0$. We neglect small terms to consider the solution of

$$\dot{y} = \delta_1(\varepsilon) f(t, y), y(t_0) = x_0$$

and we approximate $y(t)$ by a procedure (averaging) for which we know that $||y(t) - \bar{y}(t)|| = O(\delta_3(\varepsilon))$ on the timescale $1/\delta_1(\varepsilon)$. Then we have on the timescale $1/\delta_1(\varepsilon)$ the estimate

$$x(t) - y(t) = O(\frac{\delta_2(\varepsilon)}{\delta_1(\varepsilon)} + \delta_3(\varepsilon)) \text{ on the timescale } 1/\delta_1(\varepsilon).$$

Proof We formulate the equivalent integral equations for $x(t), y(t)$:

$$x(t) = x_0 + \delta_1(\varepsilon) \int_{t_0}^{t} f(x(s), s) ds + \delta_2(\varepsilon) \int_{t_0}^{t} R(x(s), s) ds,\ y(t) = x_0 + \delta_1(\varepsilon) \int_{t_0}^{t} f(y(s), s) ds.$$

Subtracting the two equations we have:

$$x(t) - y(t) = \delta_1(\varepsilon) \int_{0}^{t} (f(x(s), s) - f(y(s), s)) ds + \delta_2(\varepsilon) \int_{0}^{t} R(x(s), s) ds.$$

Using the Lipschitz continuity of f (Lipschitz constant L) and the estimate for R we have:

$$||x(t) - y(t)|| \leq \delta_1(\varepsilon) L \int_{t_0}^{t} ||x(s) - y(s)|| ds + \delta_2(\varepsilon) M t,$$

and with lemma 8.1:

$$||x(t) - y(t)|| \leq \delta_1(\varepsilon) \frac{M}{L} e^{\delta_1(\varepsilon) L t} - \frac{\delta_2(\varepsilon)}{\delta_1(\varepsilon)} \frac{M}{L}.$$

We conclude that $y(t)$ approximates $x(t)$ with error $O(\frac{\delta_2(\varepsilon)}{\delta_1(\varepsilon)})$ on the timescale $1/\delta_1(\varepsilon)$. We conclude with the triangle inequality that

$$||x(t) - \bar{y}(t)|| = ||x(t) - y(t) + y(t) - \bar{y}(t)|| \leq ||x(t) - y(t)|| + ||y(t) - \bar{y}(t)||,$$

or

$$||x(t) - \bar{y}(t)|| \leq O(\frac{\delta_2(\varepsilon)}{\delta_1(\varepsilon)}) + O(\delta_3(\varepsilon))$$

on the timescale $1/\delta_1(\varepsilon)$. $\square$

References

[1] Roelof Bruggeman and Ferdinand Verhulst, *The inhomogenous Fermi-Pasta-Ulam chain*, submitted (2015), arXiv:1510.00560 [math.DS].

[2] L. Galgani, A. Giorgilli, A. Martinoli and S. Vanzini, On the problem of energy partition for large systems of the Fermi-Pasta-Ulam type: analytical and numerical estimates, Physica D 59, pp. 334-348 (1992).

[3] Henri Poincaré, *Les Méthodes Nouvelles de la Mécanique Célèste*, 3 vols. Gauthier-Villars, Paris, 1892, 1893, 1899.

[4] Bob Rink and Ferdinand Verhulst, *Near-integrability of periodic FPU-chains*, Physica A 285, pp. 467-482 (2000).

[5] B. Rink, *Symmetry and resonance in periodic FPU-chains*, Comm. Math. Phys. 218, pp. 665-685 (2001).

[6] J.A. Sanders, F. Verhulst, and J. Murdock, *Averaging methods in nonlinear dynamical systems*, Applied Mathematical Sciences vol. 59, 2d ed., Springer (2007).

[7] J.M. Tuwankotta and F. Verhulst, *Hamiltonian systems with widely separated frequencies*, Nonlinearity 16, pp. 689-706 (2003).

[8] Ferdinand Verhulst, *Methods and applications of singular perturbations*, Springer (2005).

[9] Ferdinand Verhulst, *A chain of FPU cells*, 13th International Conference Dynamical Systems - Theory and Applications, Proc. vol. Control and Stability (eds. J.Awrejcewicz, M.Kazmierczak, J.Mrozowski, P.Oleinik) pp. 603-612, Lodz, December 7-10 (2015). Extended version *Regular and chaotic recurrence in FPU cell-chains* publ. in Appl. Math. Modelling (2016).

[10] Ferdinand Verhulst, *Near-ntegrability and recurrence in FPU cells*, Submitted (2016).