A chain of FPU cells

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Abstract: In contrast to the classical Fermi-Pasta-Ulam (FPU) chain, the inhomogeneous FPU chain shows nearly all the principal resonances. Using this fact, we can construct a periodic FPU chain of low dimension, for instance a FPU cell of four degrees-of-freedom, that can be used as a building block for a chain of FPU cells. Differences between chains in nearest-neighbour interaction and those in overall interaction are caused by symmetry. We will also show some results on the dynamics of a particular chain of FPU cells where different kinds of chaos play a part.

1. Introduction

The Fermi-Pasta-Ulam (FPU) chain or lattice is an n degrees-of-freedom (dof) Hamiltonian system that models a chain of oscillators with nearest-neighbour interaction, see [3] and [4]. In the classical (symmetric) case all the masses $m_i, i = 1, \ldots, n$ of the chain are equal. To find prominent resonances in the inhomogeneous case poses an inverse problem for the spectrum of the linearized equations of motion. Inhomogeneous nonlinear FPU chains were studied in [1] with emphasis on the case of four particles with mass distribution producing the $3:2:1$ resonance. For any periodic inhomogeneous FPU α-chain (quadratic nonlinearities) with four dof and masses m_i, $i = 1, \ldots, 4$ we have, putting $a_i = 1/m_i$, the system:

$$\begin{cases} \dot{q}_1 &= v_1,\, \dot{v}_1 = [-2q_1 + q_2 + q_4 - \varepsilon((q_1 - q_4)^2 - (q_2 - q_1)^2)]a_1, \\ \dot{q}_2 &= v_2,\, \dot{v}_2 = [-2q_2 + q_3 + q_1 - \varepsilon((q_2 - q_1)^2 - (q_3 - q_2)^2)]a_2, \\ \dot{q}_3 &= v_3,\, \dot{v}_3 = [-2q_3 + q_4 + q_2 - \varepsilon((q_3 - q_2)^2 - (q_4 - q_3)^2)]a_3, \\ \dot{q}_4 &= v_4,\, \dot{v}_4 = [-2q_4 + q_1 + q_3 - \varepsilon((q_4 - q_3)^2 - (q_1 - q_4)^2)]a_4. \end{cases} \tag{1}$$

The q_i indicate the positions of the particles, the v_i their velocity, ε is a small parameter; sometimes it is convenient to use momentum-position variables p, q. We call the case with quartic terms in the Hamiltonian added (cubic terms in the equations of motion) a β-chain. It was shown in [8], that in the classical periodic FPU problem with four identical particles the normal form of the system is integrable, see also [9]. The implication is that for ε small, the measure of chaos is in this classical case $O(\varepsilon)$.

We assume that the Hamiltonian can be expanded in homogeneous polynomials as $H = H_2 + \varepsilon H_3 + \varepsilon^2 \dots$ with the index indicating the degree of the polynomial. Apart from the Hamiltonian H we have as a second (translational) momentum integral of system (1):

$$m_1 v_1 + m_2 v_2 + m_3 v_3 + m_4 v_4 = \text{constant}. \tag{2}$$

The expression for the quadratic part of the Hamiltonian H_2 is:

$$H_2 = \frac{1}{2}\sum_{i=1}^{4} a_i p_i^2 + \frac{1}{2}[(q_2 - q_1)^2 + (q_3 - q_2)^2 + (q_4 - q_3)^2 + (q_1 - q_4)^2]. \tag{3}$$

H_2 is a first integral of the linearized system (1), it is also a first integral of the normal form of the full system (1). This has the following implication: When using H_2 from the solutions of the truncated normal form indicated by: $\bar{H}(p,q) = H_2(p,q) + \varepsilon \bar{H}_3(p,q)$, we obtain an $O(\varepsilon)$ approximation of the (exact) $H_2(p(t), q(t))$ valid for all time; for a proof see [10] chapter 10.

2. Transformation to a quasi-harmonic form

The presence of the momentum integral enables us to reduce system (1) to a three dof system. It has been shown in [1] that the $\omega_1 : \omega_2 : \omega_3 = 3 : 2 : 1$ resonance arises in a one-parameter family of Hamiltonians; many other resonances can be found. Without loss of generality we choose

$$\omega_1^2 = \frac{9}{14}, \omega_2^2 = \frac{4}{14}, \omega_3^2 = \frac{1}{14}. \tag{4}$$

The one-parameter family of $3 : 2 : 1$ resonances can be generated by the real parameter $u \in [0, u_1)$ with $u_1 = 0.887732$. In an application later on we will choose a particular value of u, called case 1 in [1]. To put system (1) in the standard form of quasi-harmonic equations we have to apply a suitable symplectic transformation $L(u)^{-1} : p, q \to y, x$ with x the vector of the new position variables that is three-dimensional because of the reduction by the momentum integral (2). This leads to a transformed Hamiltonian $H_2 + \varepsilon H_3$:

$$H_2 = \frac{1}{2}(\dot{x}_1^2 + \frac{9}{14}x_1^2 + \dot{x}_2^2 + \frac{4}{14}x_2^2 + \dot{x}_3^2 + \frac{1}{14}x_3^2)$$

and H_3 a cubic expression containing 10 terms, see for details [1]. Because of the $3 : 2 : 1$ resonance, only two terms will be active in the normalized H_3; an intermediate normal form will be:

$$\begin{cases} \ddot{x}_1 + 9x_1 &= -\varepsilon 14 d_6 x_2 x_3, \\ \ddot{x}_2 + 4x_2 &= -\varepsilon 14(d_6 x_1 x_3 + d_9 x_3^2), \\ \ddot{x}_3 + x_3 &= -\varepsilon 14(d_6 x_1 x_2 + 2d_9 x_2 x_3), \end{cases} \tag{5}$$

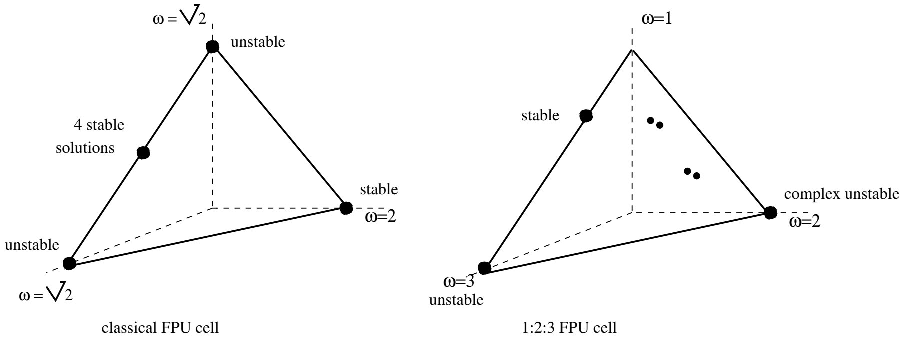

Figure 1. Action simplices. A dot indicates one or more periodic solutions, at the vertices one finds the normal modes if these exist. Left the actions of the classical FPU chain with four particles, the $\sqrt{2} : \sqrt{2} : 2$ resonance has two unstable normal modes. Right the case of the FPU chain with four particles in $1 : 2 : 3$ resonance. The normal modes corresponding with $\omega = 3$ and 2 exist but are unstable, in the second case with complex eigenvalues.

It was shown in this case that for nearly all parameter values, one of the short-periodic solutions is complex unstable. This is highly relevant for the characterization of the chaotic dynamics of the system as it was shown in [5] that a Shilnikov-Devaney bifurcation [2] can take place in the $3 : 2 : 1$ resonance. For a summary of the results in the parameter case $0 < u < u_1$ see the action simplex in fig. 1 (right).

In the sequel we will treat such a FPU chain with 4 particles as a FPU cell, and we will construct a chain of FPU cells. Such a chain is depicted in fig. 2.

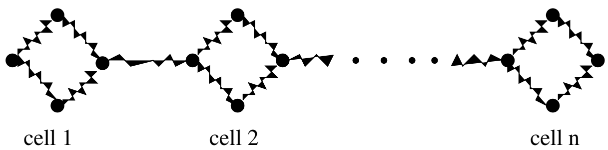

Figure 2. A chain of FPU cells, each consisting of four particles.

3. Energy exchange and recurrence in PFU cells

We will use particular values for the masses, in [1] denoted by “case 1”. We choose:

$$a_1 = 0.00510292, a_2 = 0.117265, a_3 = 0.0854008, a_4 = 0.292231,$$

leading to the frequencies (4). With these mass ($a_i = 1/m_i$) values the symplectic transformation of the four-particles system produces :

$d_6 = -0.0306229$, $d_9 = -0.0089438$.

The analysis in [1] for case 1 shows that the x_2 normal mode of an isolated cell is complex unstable. We will study a chain of FPU cells with this choice of masses; the cells interact weakly by the mass points $q_2, q_6, \ldots$ etc. so that the $3:2:1$ resonances of the cells experience only a slight detuning. Consider as an illustration the case of two cells with:

$$\begin{cases} H_2 = & \frac{1}{2}\sum_{i=1}^{8}\frac{v_i^2}{a_i} + \frac{1}{2}[(q_2-q_1)^2+(q_3-q_2)^2+(q_4-q_3)^2+(q_1-q_4)^2] + \frac{1}{2}\varepsilon\mu(q_2-q_6)^2 \\ & +\frac{1}{2}[(q_6-q_5)^2+(q_7-q_6)^2+(q_8-q_7)^2+(q_5-q_8)^2], \end{cases} \tag{6}$$

and $a_i = a_{i+4}$, $i = 1, \ldots, 4$; ε scales the nonlinearities, $\varepsilon\mu$ scales the detuning. The equations of motion produce a 16-dimensional phase-space and become:

$$\begin{cases} \dot{q}_1 &= v_1,\ \dot{v}_1 = [-2q_1+q_2+q_4-\varepsilon((q_1-q_4)^2-(q_2-q_1)^2)]a_1, \\ \dot{q}_2 &= v_2,\ \dot{v}_2 = [-2q_2+q_3+q_1-\varepsilon\mu(q_2-q_6)-\varepsilon((q_2-q_1)^2-(q_3-q_2)^2)]a_2, \\ \dot{q}_3 &= v_3,\ \dot{v}_3 = [-2q_3+q_4+q_2-\varepsilon((q_3-q_2)^2-(q_4-q_3)^2)]a_3, \\ \dot{q}_4 &= v_4,\ \dot{v}_4 = [-2q_4+q_1+q_3-\varepsilon((q_4-q_3)^2-(q_1-q_4)^2)]a_4, \\ \dot{q}_5 &= v_5,\ \dot{v}_5 = [-2q_5+q_6+q_8-\varepsilon((q_5-q_8)^2-(q_6-q_5)^2)]a_1, \\ \dot{q}_6 &= v_6,\ \dot{v}_6 = [-2q_6+q_7+q_5+\varepsilon\mu(q_2-q_6)-\varepsilon((q_6-q_5)^2-(q_7-q_6)^2)]a_2, \\ \dot{q}_7 &= v_7,\ \dot{v}_7 = [-2q_7+q_8+q_6-\varepsilon((q_7-q_6)^2-(q_8-q_7)^2)]a_3, \\ \dot{q}_8 &= v_8,\ \dot{v}_8 = [-2q_8+q_5+q_7-\varepsilon((q_8-q_7)^2-(q_5-q_8)^2)]a_4. \end{cases} \tag{7}$$

The recurrence theorem for volume-preserving maps was formulated by Poincaré in 1890 in his prize essay for Oscar II; it can also be found in [7] vol. 3. It implies, loosely formulated, that for Hamiltonian systems on a compact energy manifold, nearly all solutions return after a finite time arbitrarily close to their original position in phase-space. Analysis of recurrence adds to our understanding of the dynamics.

For a one dof system on a compact domain recurrence is trivial as under these conditions nearly all solutions are periodic. For two dof systems that are integrable, recurrence behaviour is relatively simple near a stable periodic solution. In nearly-integrable two dof systems a similar result can be obtained using the KAM theorem, but in general this is already not so easy for chaotic two dof systems.

To measure recurrence for a system of two FPU cells we will start with zero energy in the second cell and consider energy exchange between the FPU cells. To study recurrence we will also use the Euclidean norm:

$$d = \left[\sum_{i=1}^{4} (q_i(t) - q_i(0))^2 + \sum_{i=1}^{4} v_i^2 + c \sum_{i=5}^{8} (q_i(t)^2 + v_i(t)^2) \right]^{1/2} . \tag{8}$$

In the case of one cell, $c = 0$, for two cells $c = 1$. It would be natural to apply weights, based on the masses, to the displacements but this does not change the picture qualitatively.

3.1. Set-up of the experiments

We will start with initial values in cell 1 and will be interested in the energy transfer to cell 2. The initial values of the velocities were chosen to be zero. As the chain is Hamiltonian, the flow will be recurrent, but we expect differences between the classical case of equal masses and the case of the $3:2:1$ resonance where the flow is chaotic. We restrict ourselves to initial values in a neighbourhood of the normal modes indicated in the second and fourth column of table 1. As the phase-flow is chaotic, see [5], we expect the transfer of energy between the cells and the recurrence to be different from the case of a nearly integrable cell system like the classical FPU chain with all masses equal. The numerics involves a $[0, 5000]$ time interval with relative tolerance e^{-7}, absolute tolerance e^{-10}.

The $3:2:1$ resonance will be detuned by the interaction between the cells. Keeping the interaction small by choosing $\varepsilon = 0.2, \mu = 0.1$, the detuning does not disturb the qualitative picture of the resonance. With the mass distribution of case 1 we have for the frequencies of the linearized system $\omega_1 = 0.8019\,(0.8018), \omega_2 = 0.5487\,(0.5345), \omega_3 = 0.2742\,(0.2673)$ with between brackets the frequencies of isolated cells ($\varepsilon = \mu = 0$).

For the instantaneous energy E_{c1} stored in cell 1 we have:

$$\begin{cases} E_{c1} = & \frac{1}{2}\sum_{i=1}^{4} \frac{v_i^2}{a_i} + \frac{1}{2}[(q_2-q_1)^2 + (q_3-q_2)^2 + (q_4-q_3)^2 + (q_1-q_4)^2] \\ & + \frac{\varepsilon}{3}[(q_2-q_1)^3 + (q_3-q_2)^3 + (q_4-q_3)^3 + (q_1-q_4)^3]. \end{cases} \tag{9}$$

The energy of cell 2 is obtained from E_{c1} by adding 4 to all the indices.

3.2. Energy transfer between two cells

We compare the energy transfer to cell 2 between the $1:2:3$ resonance of case 1 with the behaviour of the classical FPU chain with four equal particles. In this classical case the frequencies of the linearized system are $\sqrt{2}, \sqrt{2}, 2, 0$. For reasons of comparison we choose for the masses in the classical case $m = 0.1$. The symmetry induced by the equal masses means that we have to choose the initial conditions in the classical FPU case with care. For

Table 1. The eigenmodes $\mathbf{e}$ of the system in $\mathbf{x}$ variables transformed to $\mathbf{q}$ variables for the $1:2:3$ resonance (case 1, 2nd column) and the classical FPU case (4th column). Because of the presence of the momentum integral (2), the reduction to three dof makes the values produced for the 4th eigenvector redundant. The initial values of the positions for the numerical integrations have been chosen near the eigenmodes; the initial velocities are zero. The symplectic transformation $L(u)$ from [1] discussed in section 2 gives us the relation between the normal modes of the system in quasi-harmonic coordinates $(x, \dot{x})$ and the initial conditions in the variables (q, v) of system (7). This means that a given position vector $(q_1, q_2, q_3, q_4) = \mathbf{q}$ is obtained from the $\mathbf{x}$ normal modes by putting $\mathbf{q} = L(u)\mathbf{x}$.

	Case 1	Initial values case 1	Classical FPU	Initial values classical FPU
$L(u)\mathbf{e_1}$	$\begin{pmatrix} -0.00432273 \\ 0.0290855 \\ -0.0969556 \\ 0.506839 \end{pmatrix}$	$\begin{pmatrix} -0.1 \\ 0.1 \\ -0.2 \\ 0.3 \end{pmatrix}$	$\begin{pmatrix} -0.5 \\ 0.5 \\ -0.5 \\ 0.5 \end{pmatrix}$	$\begin{pmatrix} -0.4 \\ 0.45 \\ -0.4 \\ 0.42 \end{pmatrix}$
$L(u)\mathbf{e_2}$	$\begin{pmatrix} 0.00315777 \\ -0.297518 \\ 0.126704 \\ 0.127029 \end{pmatrix}$	$\begin{pmatrix} 0.1 \\ -0.2 \\ 0.3 \\ -0.1 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix}$	$\begin{pmatrix} 0.1 \\ 0.6 \\ -0.1 \\ -0.65 \end{pmatrix}$
$L(u)\mathbf{e_3}$	$\begin{pmatrix} -0.0228266 \\ 0.152804 \\ 0.235358 \\ 0.121061 \end{pmatrix}$	$\begin{pmatrix} -0.1 \\ 0.3 \\ 0.4 \\ 0.05 \end{pmatrix}$	$\begin{pmatrix} -1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \\ 0 \end{pmatrix}$	$\begin{pmatrix} -0.65 \\ 0.1 \\ 0.6 \\ -0.1 \end{pmatrix}$
$L(u)\mathbf{e_4}$	$\begin{pmatrix} 0.0674775 \\ 0.0674775 \\ 0.0674775 \\ 0.0674775 \end{pmatrix}$	$\begin{pmatrix} 0.0 \\ 0.0 \\ 0.0 \\ 0.0 \end{pmatrix}$	$\begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}$	$\begin{pmatrix} 0.0 \\ 0.0 \\ 0.0 \\ 0.0 \end{pmatrix}$

instance there exists the family of periodic solutions defined by:

$$q_2(t) = q_4(t) = 0,\ q_1(t) = -q_3(t),\ \ddot{q}_1 + 2q_1 = 0,\ \ddot{q}_3 + 2q_1 = 0.$$

As the link between the cells involves the second particle, this means that there is no energy transfer between the cells when starting with these solutions. It is easy to obtain a few exact solutions by generalizing this result for the classical FPU chain with $2n$ dof.

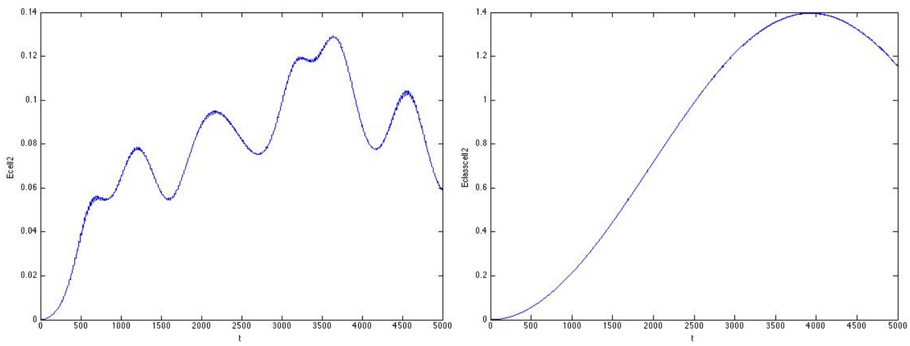

Figure 3. Time series ($[0, 5000]$) of the energy of the second cell, left the $1:2:3$ resonance (scale $[0, 0.14]$), right the classical case (scale $[0, 1.4]$). The link is linear and exists between q_2 and q_6; The initial conditions of the first cell start near the eigenmode x_1 and are given in table 1, the second cell starts with zero energy; $\varepsilon = 0.2, \mu = 0.1$.

In the figs 3 - 5 on the left we have energy transfer starting near respectively 3 unstable solutions in a chaotic dynamical system; the transfer is irregular but assumes at certain times a considerable part, more than 90 % of the energy of cell 1. On the right side of the figs 3 - 5 we have energy transfer starting in the classical FPU case showing a rather regular pattern. The (ir)regularity of the energy transfer is the main difference.

3.3. The recurrence of an solution

We will explore recurrence phenomena for our systems of one cell ($c = 0$, 8-dimensional) and two FPU cells ($c = 1$, 16-dimensional) using the Euclidean distance d, see eq. (8). Increasing the dimension will in general increase the recurrence times but other aspects of the dynamics play a part. We will use again the initial values given in table 1. We explore the recurrence in the first cell with the initial conditions near the complex unstable x_2 normal mode, see fig. 6 (left) and for two cells (right). In the classical FPU system we have rather regular recurrence near the x_2 normal mode, see fig. 7.

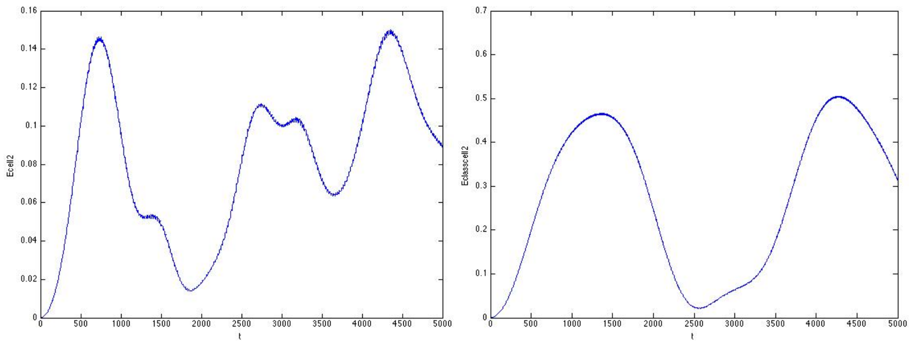

Figure 4. Time series ($[0, 5000]$) of the energy of the second cell, left the $1:2:3$ resonance (scale $[0, 0.16]$), right the classical case (scale $[0, 0.7]$). The link is linear and exists between q_2 and q_6; The initial conditions of the first cell start near the eigenmode x_2 and are given in table 1, the second cell starts without energy; $\varepsilon = 0.2, \mu = 0.1$.

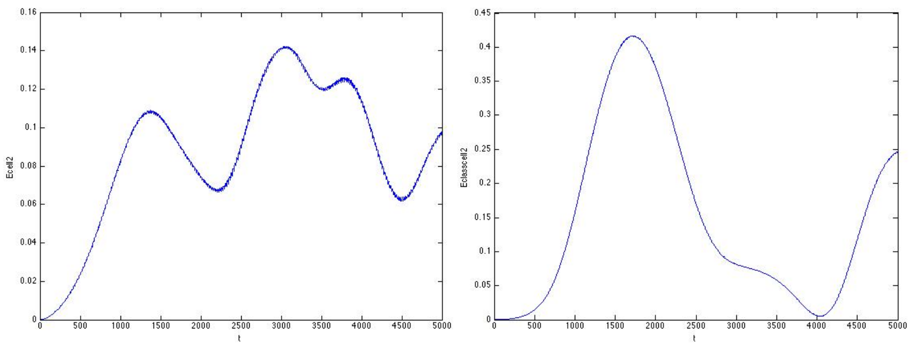

Figure 5. Time series ($[0, 5000]$) of the energy of the second cell, left the $1:2:3$ resonance (scale $[0, 0.16]$), right the classical case (scale $[0, 0.45]$). The link is linear and exists between q_2 and q_6; The initial conditions of the first cell start near the eigenmode x_3 and are given in table 1, the second cell starts without energy; $\varepsilon = 0.2, \mu = 0.1$.

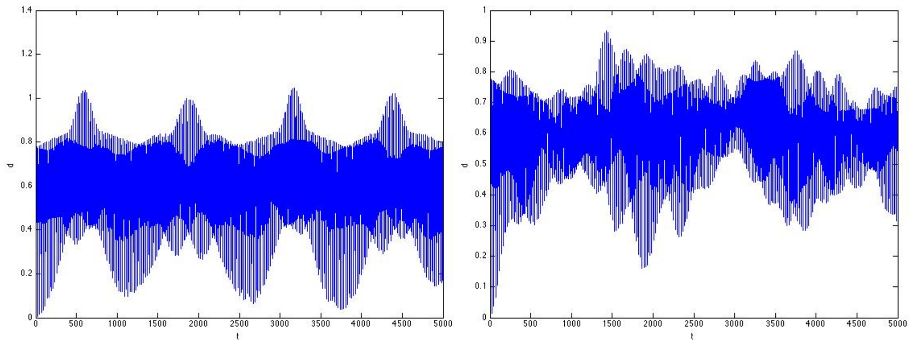

Figure 6. Time series ($[0, 5000]$) of the Euclidean distance d starting near the complex unstable normal mode x_2 in the first FPU cell in $1 : 2 : 3$ resonance (left, scale $[0, 1.4]$). The recurrence for 5000 time steps is delayed on the right (scale $[0, 1]$) where we started with the same initial conditions (table 1) for two cells.

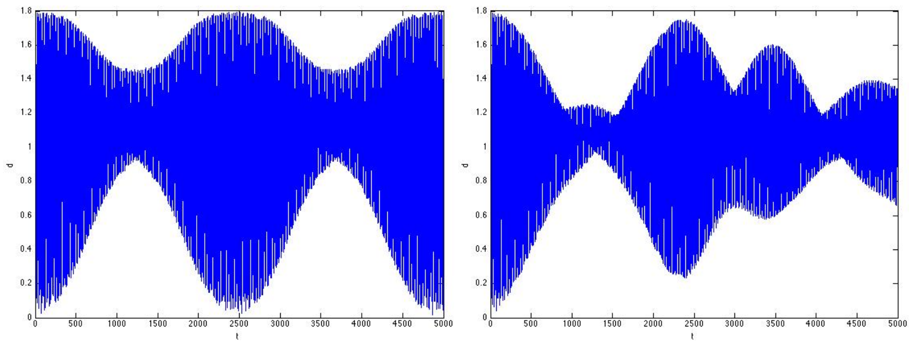

Figure 7. Time series ($[0, 5000]$) of the Euclidean distance d starting near the x_2 eigenmode in the first classical FPU cell (left, scale $[0, 1.8]$). For the initial conditions indicated in table 1 the recurrence is quite good. On the right (scale $[0, 1.8]$) the time series for two cells with the same initial conditions; the recurrence is delayed.

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