Regular and chaotic recurrence in FPU cell-chains

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1. Introduction

This is an extended version of the conference paper [1] containing an extensive discussion of recurrence involving separation by manifolds and quasi-trapping in resonance zones, additional experiments and references.

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-neighbor interaction, see [2,3] and for a nice survey [4]. In the classical (symmetric) case all the masses \( m_i, i = 1, \ldots, n \) of the chain are equal. The original problem formulation was intended to show equipartition of energy between the modes of the FPU chain but, surprisingly the numerics showed strong recurrence. Much later, in 2001, it was shown by Rink [5] that in the classical FPU chain the dynamics is near-integrable producing KAM-tori and recurrent behavior. However, as we will show, if the masses are not equal the dynamics can be very different. To apply the results of normal form analysis we have to determine the possible resonances in this (inhomogeneous) case.

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 [6] with emphasis on the case of four particles with mass distribution producing the 3: 2: 1 resonance. For any periodic inhomogeneous FPU \( \alpha \)-chain with four dof and masses \( m_i, i = 1, \ldots, 4 \) we have, putting \( q_i = 1/m_i \), the system:

\[
\begin{align*}
q_1 &= v_1, \\
v_1 &= [-2q_1 + q_2 + q_4 - \epsilon((q_1 - q_4)^2 - (q_2 - q_3)^2)]q_1, \\
q_2 &= v_2, \\
v_2 &= [-2q_2 + q_3 + q_1 - \epsilon((q_2 - q_1)^2 - (q_3 - q_4)^2)]q_2, \\
q_3 &= v_3, \\
v_3 &= [-2q_3 + q_4 + q_2 - \epsilon((q_3 - q_2)^2 - (q_4 - q_1)^2)]q_3, \\
q_4 &= v_4, \\
v_4 &= [-2q_4 + q_1 + q_3 - \epsilon((q_4 - q_3)^2 - (q_1 - q_2)^2)]q_4.
\end{align*}
\]

The \( q_i \) indicate the positions of the particles, the \( v_i \) their velocity, \( \epsilon \) 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 [7], that in the classical periodic FPU problem with four identical particles the normal form of the system is integrable, see also [5]. The implication is that for ε small, the measure of chaos is in this classical case O(ε).

We assume that the Hamiltonian can be expanded in homogeneous polynomials as \( H = H_2 + εH_3 + ε^2 \cdots \) 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):

\[
m_1v_1 + m_2v_2 + m_3v_3 + m_4v_4 = \text{constant}.
\]  
(2)

The expression for the quadratic part of the Hamiltonian \( H_2 \) is:

\[
H_2 = \frac{1}{2} \sum_{l=1}^{4} \frac{v_l^2}{\alpha_l} + \frac{1}{2} [(q_2 - q_1)^2 + (q_3 - q_2)^2 + (q_4 - q_3)^2 + (q_1 - q_4)^2].
\]  
(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: \( \hat{H}(p, q) = H_2(p, q) + εH_3(p, q) \), we obtain an O(ε) approximation of the (exact) \( H_2(p(t), q(t)) \) valid for all time; for a proof see [8] Chapter 10 and [14].

The Poincaré recurrence theorem [9] states that a bounded conservative system always shows recurrent dynamics. This posed a serious problem in the early stages of development of the theory of statistical mechanics; for an introduction to both historical and modern aspects of Hamiltonian dynamics, see [10]. In this respect it is important to realize that the dynamics of a Hamiltonian system will show very different dynamical behavior in the case of an integrable system, a near-integrable one or a chaotic system. One of the aims of this paper is to illustrate these differences for FPU cell-chains. We start with the transformation to normal modes (quasi-harmonic form) after which we study recurrence and corresponding energy exchanges in a few chains.

In [6] the emphasis is on normal form analysis of the 3: 2 : 1 resonance. We extend that analysis to introduce cell-chains analyzed by normal forms and with numerics carried out by MATLAB ode78 under MATLAB. The results were checked by increasing the (high-)precision of the calculations until the resulting picture did not change anymore.

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 [6] that the \( ω_1 : ω_2 : ω_3 = 3 : 2 : 1 \) resonance arises in a one-parameter family of Hamiltonians; many other resonances can be found. Without loss of generality we choose:

\[
\omega_1^2 = \frac{9}{14}, \quad \omega_2^2 = \frac{4}{14}, \quad \omega_3^2 = \frac{1}{14}.
\]  
(4)

The one-parameter family of 3: 2: 1 resonances can be generated by the real parameter \( u ∈ [0, u_1) \) with \( u_1 = 0.887732 \). In an application later on we will choose a particular value of \( u \), called case 1 in [6]. To put system (1) in the standard form of quasi-harmonic equations we have to apply a suitable symplectic transformation \( L(u)^{-1} : p, q → y, x \) 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 \( H_2 + εH_3 \):

\[
H_2 = \frac{1}{2} \left( \dot{x}_1^2 + \frac{9}{14} \dot{x}_1^2 + \dot{x}_2^2 + \frac{4}{14} \dot{x}_2^2 + \dot{x}_3^2 + \frac{1}{14} \dot{x}_3^2 \right).
\]

and \( H_3 \) a cubic expression containing 10 terms, see for details [6]. Because of the 3: 2: 1 resonance, only two terms will be active in the normalized \( H_3 \); an intermediate normal form will be:

\[
\begin{align*}
\dot{x}_1 + 9x_1 &= -ε(14dx_1x_2x_3), \\
\dot{x}_2 + 4x_2 &= -ε(14(dx_1x_1 + dx_2x_1)), \\
\dot{x}_3 + x_3 &= -ε(14(dx_1x_2 + 2dx_2x_3)).
\end{align*}
\]  
(5)

The analysis of system [5] was carried out by normal form methods (see [8]) and can be found in [6].

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 [11] that a Shilnikov-Devaney bifurcation [12] 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). It is remarkable that in the classical case of equal masses, the normal form of the Hamiltonian equations is integrable. In this case the interpretation is that close to stable equilibrium the measure of chaos is exponentially small. In contrast to this, the 3: 2: 1 resonance (induced by unequal masses) has a normal form displaying two independent integrals, \( H_2 \) and \( H \), but it is chaotic. As we shall see this affects the dynamics of the corresponding cell-chains strongly.

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.
3. Energy exchange and recurrence in FPU cells

We will use particular values for the masses, in \([6]\) denoted by "case 1". We choose:

\[
\begin{align*}
q_1 &= 0.00510292, & q_2 &= 0.117265, & q_3 &= 0.0854008, & q_4 &= 0.292231,
\end{align*}
\]

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

\[
\begin{align*}
d_6 &= -0.0306229, & d_9 &= -0.0089438.
\end{align*}
\]

The analysis in \([6]\) for case 1 shows that the \(q_2\) 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 \(q_2, q_6, q_{10}, \ldots\) 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:

\[
\begin{align*}
H_2 = \frac{1}{2} \sum_{i=1}^{2} \frac{\dot{q}_i^2}{q_i} + \frac{1}{2} [ (q_2 - q_1)^2 + (q_3 - q_2)^2 + (q_4 - q_3)^2 + (q_1 - q_4)^2] + \frac{1}{2} \epsilon \mu(q_2 - q_6)^2
\end{align*}
\]

and \(q_i = a_i, i = 1, \ldots, 4; \epsilon\) scales the nonlinearities, \(\epsilon \mu\) scales the detuning. The equations of motion produce a 16-dimensional phase-space and become:

\[
\begin{align*}
\dot{q}_1 &= \dot{v}_1 = [-2q_1 + q_2 + q_4 - \epsilon ((q_1 - q_3)^2 - (q_2 - q_4)^2)]v_1, \\
\dot{q}_2 &= \dot{v}_2 = [-2q_2 + q_1 + q_3 - \epsilon ((q_2 - q_3)^2 - (q_2 - q_4)^2)]v_2, \\
\dot{q}_3 &= \dot{v}_3 = [-2q_3 + q_4 + q_2 - \epsilon ((q_3 - q_2)^2 - (q_4 - q_3)^2)]v_3, \\
\dot{q}_4 &= \dot{v}_4 = [-2q_4 + q_1 + q_3 - \epsilon ((q_4 - q_3)^2 - (q_1 - q_4)^2)]v_4, \\
\dot{q}_5 &= \dot{v}_5 = [-2q_5 + q_6 + q_8 - \epsilon ((q_5 - q_8)^2 - (q_6 - q_5)^2)]v_5, \\
\dot{q}_6 &= \dot{v}_6 = [-2q_6 + q_7 + q_3 - \epsilon \mu (q_2 - q_3) - \epsilon ((q_6 - q_5)^2 - (q_7 - q_6)^2)]v_6, \\
\dot{q}_7 &= \dot{v}_7 = [-2q_7 + q_8 + q_6 - \epsilon ((q_7 - q_6)^2 - (q_7 - q_8)^2)]v_7, \\
\dot{q}_8 &= \dot{v}_8 = [-2q_8 + q_5 + q_7 - \epsilon ((q_8 - q_7)^2 - (q_5 - q_8)^2)]v_8.
\end{align*}
\]

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 \([9]\) 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. In \([13]\) it is shown that in the case of a Hamiltonian system with 3 dof near stable equilibrium we have an upper bound \(L\) for the recurrence time, \(L = O(1/d^3),\) for two cells \(L = O(1/d^{15}),\) for three cells \(L = O(1/d^{21}).\) Here, \(E_p\) is the energy of the system, \(d\) is the Euclidean distance to the initial condition in phase-space. These estimates are valid without any additional knowledge about the dynamics of the FPU cells, in the near-integrable cases like the classical FPU chain the estimates are far too crude.
Table 1
The eigenmodes $e$ of the system in $x$ variables transformed to $q$ 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 $L(q)$ from [6] discussed in Section 2 gives us the relation between the normal modes of the system in quasi-harmonic coordinates $(x, x)$ and the initial conditions is the variables $(q, v)$ of system (7). This means that a given position vector $(q_1, q_2, q_3, q_4) = q$ is obtained from the $x$ normal modes by putting $q = L(q)$. 

<table>
<thead>
<tr>
<th>Initial values case 1</th>
<th>Classical FPU</th>
<th>Initial values classical FPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l(u)e_1$</td>
<td>$(-0.5)$</td>
<td>$(-0.45)$</td>
</tr>
<tr>
<td>0.09432273</td>
<td>0.5</td>
<td>0.45</td>
</tr>
<tr>
<td>0.029085</td>
<td>0.5</td>
<td>0.42</td>
</tr>
<tr>
<td>$l(u)e_3$</td>
<td>$(-0.2)$</td>
<td>$(-0.4)$</td>
</tr>
<tr>
<td>0.09695564</td>
<td>0.5</td>
<td>0.4</td>
</tr>
<tr>
<td>0.00817839</td>
<td>0.5</td>
<td>0.12</td>
</tr>
<tr>
<td>$l(u)e_6$</td>
<td>$(-0.1)$</td>
<td>$(-0.65)$</td>
</tr>
<tr>
<td>0.297538</td>
<td>1/$\sqrt{2}$</td>
<td>0.6</td>
</tr>
<tr>
<td>0.126704</td>
<td>0.3</td>
<td>0.1</td>
</tr>
<tr>
<td>$l(u)e_8$</td>
<td>$(-0.1)$</td>
<td>$(-0.65)$</td>
</tr>
<tr>
<td>0.2282669</td>
<td>1/$\sqrt{2}$</td>
<td>0.6</td>
</tr>
<tr>
<td>0.126704</td>
<td>0.3</td>
<td>0.1</td>
</tr>
<tr>
<td>$l(u)e_9$</td>
<td>$(-0.1)$</td>
<td>$(-0.65)$</td>
</tr>
<tr>
<td>0.2282669</td>
<td>1/$\sqrt{2}$</td>
<td>0.6</td>
</tr>
<tr>
<td>0.312061</td>
<td>0.05</td>
<td>0.02</td>
</tr>
<tr>
<td>$l(u)e_{10}$</td>
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<td>$(-0.65)$</td>
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<tr>
<td>0.2674725</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.0674775</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$l(u)e_{11}$</td>
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<td>$(-0.65)$</td>
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<td>0.2674725</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.0674775</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

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 behavior is relatively simple near a stable periodic solution. In nearly-integrable two dof systems a similar result can be obtained using the RKM 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 use the Euclidean norm:

$$d = \left[ \sum_{t=1}^{4} (q_t(t) - q_0(t))^2 + \sum_{t=1}^{4} v_t^2 + c \sum_{i=2}^{8} (q_i(t)^2 + v_i(t)^2) \right]^{1/2}.$$  

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 neighborhood of the normal modes indicated in the second and fourth column of Table 1. As the phase-flow is chaotic, see [11], 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 usually a [0, 5000] time interval with small relative tolerance and absolute tolerance.

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 $H_{1t}$ stored in cell 1 we have:

$$H_{1t} = \frac{1}{2} \sum_{i=1}^{5} E + \frac{1}{2} \left[ (q_2 - q_1)^2 + (q_3 - q_2)^2 + (q_4 - q_3)^2 + (q_5 - q_4)^2 \right]$$

$$+ \frac{1}{2} \left[ (q_2 - q_1)^3 + (q_3 - q_2)^3 + (q_4 - q_3)^3 + (q_5 - q_4)^3 \right].$$  

The energy of cell 2 is obtained from $H_{1t}$ 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 behavior 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 instance there exists the family of periodic solutions defined by:

\[ q_2(t) = q_4(t) = 0, \quad q_1(t) = -q_3(t), \quad \dot{q}_1 + 2q_1 = 0, \quad \dot{q}_3 + 2q_1 = 0. \]

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.

In the Figs. 3–5 on the left we have energy transfer starting near an unstable solution 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 a solution

We will explore recurrence phenomena for our systems of one cell (ε = 0, 8-dimensional) and two FPU cells (ε = 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 x2 normal mode, see Fig. 6 (left) and for two cells (right). In the classical FPU system we have rather regular recurrence near the x2 normal mode, see Fig. 7.

4. Discussion

Cell-chains of oscillators have many degrees of freedom which makes the analysis of dynamics complicated. In this paper we have studied a number of basic aspects, but of course many more details and phenomena are waiting to be discovered. We have stressed integrability and recurrence characteristics.

As indicated in Section 1, recurrence in conservative systems is well-known but not easy to characterize in a general way. The recurrence depends on the number of dof, the initial conditions and the particular dynamics of the system under consideration. The results of the last decades on normal form approximation theory and chaos theory enable us to understand more about recurrence.

In this paper we have compared cell-chains built from classical, near-integrable cells and chains built from chaotic cells. Both from theory and from our experiments it is clear that in the near-integrable case (the classical FPU cell) the recurrence times are expected to be smaller than the upper bound L given in Section 3. On the other hand, in the case of chaotic cells the recurrence will take much longer time intervals. We discuss some aspects.

4.1. Separation by invarian: manifolds

The delay in recurrence in the case of three or more dof can be qualitatively explained as follows. The stable solutions in one FPU cell with 4 particles and so 3 dof after reduction, are surrounded by 3-tori (dimension 3). The energy manifold is 5-dimensional (S^5) which means that the 3-tori do not separate S^5 in phase-space. The implication is that the solutions between the tori can move off into phase-space, they are only to some extent restricted by invariant manifolds. An increase
Fig. 8. Starting near the $x_2$ spectral normal mode of Table 1 in the first cell, mode 5 and 7 in the second cell are near to 1:1 resonance which is typical for the classical case. The $q_1 - q_1$ diagram left took 250 time steps, right 5000. The 1:1 resonance is very slowly destroyed, the recurrence in the system of two cells takes clearly more than 5000 time steps. Parameter values $m = 0.1$, $e = 0.2$, $\mu = 0.1$.

Fig. 9. Time series (0, 5000)) of $q_2(t)$ and $q_3(t)$ starting with zero initial conditions. The parameter values are as in Figs. 7 and 8.

of dimension by connecting two cells strengthens this effect. For two cells we have 8 particles and after reduction 7 dof or phase-space dimension 14. The energy manifold is $S^{13}$ with at most tori of dimension 7, there is no separation at all.

If the normal form of the system is integrable as is the case for the classical FPU cell in Fig. 7, this helps as approximate integral manifolds are present reducing the recurrence time. In the case of the chaotic 3:2:1 resonance which contains horseshoe dynamics and an infinite number of close unstable periodic solutions on the energy manifold, longer recurrence times can be expected.

4.2. Quasi-trapping resonance zones

Quasi-trapping is qualitatively discussed in [10]. Near stable equilibrium there exist periodic solutions with many different periods; the stable ones are associated with invariant tori that exist in resonance zones. The solutions starting outside such a zone cannot be trapped in such a zone but its passage can take long intervals of time; we call this quasi-trapping. This phenomenon explains to some extent the much longer recurrence times obtained for the systems displayed in Figs. 6 and 7. We illustrate this for the case of classical FPU cells of Fig. 7 in Fig. 8 where detailed numerics shows $q_1$ and $q_2$ to be in near 1:1 resonance. The 250 time steps in the left part of Fig. 8 show the resonance and running the system for 5000 time steps (right part of the figure) shows very slow drifting off the 1:1 resonance.

After a long time the solutions will return near their initial conditions in the first cell. Until then there is large transfer of energy to the second cell. This is shown in Fig. 9 where the positions $q_2(t)$ and $q_3(t)$ are shown for 5000 time steps. On this interval of time these modes in the second cell range between -0.3 and 0.3; energy transfer to the second cell has taken place.

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References