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Recurrence and diffusion in FPU chains with alternating masses

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1 Introduction

This summary is based on joint work with Roelof Bruggeman to be published in [3]. In [1] we have studied the inhomogeneous Fermi-Pasta-Ulam (FPU) problem which contains many different resonance cases. In [8] and [9] recurrence and near-integrability aspects of FPU cells were studied. Inspired by [6] we will discuss the inhomogeneous periodic FPU-problem in the case of alternating masses $1, m, 1, m, \ldots,\ m \geq 1, a = 1/m$, see [2] and [3]. In a periodic chain, for (even) n particles with arbitrary masses $m_j > 0$, position q_j and momentum $p_j = m_j \dot{q}_j, j = 1 \ldots n$, $\varepsilon \geq 0$ a small parameter, 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 $\alpha \neq 0, \beta = 0$ we will call this an α-chain, if $\alpha = 0, \beta \neq 0$ a β-chain. The momentum integral:

$$m_1\dot{q}_1 + m_2\dot{q}_2 + \ldots + m_n\dot{q}_n = P_0 \quad (2)$$

can be used to reduce the system to $n-1$ degrees-of-freedom (dof). Our analysis is for a large part based on averaging normal form theory, the numerical illustrations on MATCONT under MATLAB with ode78.

2 Invariant manifolds

Studying the alternating FPU-chain with 8 particles we observed an invariant manifold equivalent to the system with 4 particles. This phenomenon turns out to be much more general, as will become clear in Theorem 1 below. It can be considered as an illustration of the theory of Chechin and Sakhenko in [4],

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see also [5].
We consider the system $\mathrm{FPU}_{2n}(a;\alpha,\beta)$ of second order differential equations

$$\begin{aligned} m_j\ddot{q}_j = &+(q_{j+1}-q_j)+\alpha(q_{j+1}-q_j)^2+\beta(q_{j+1}-q_j)^3 \\ &-(q_j-q_{j-1})-\alpha(q_j-q_{j-1})^2-\beta(q_j-q_{j-1})^3 \end{aligned} \tag{3}$$

for $1 \le j \le 2n$, with indices taken modulo $2n$. The masses are $m_{2j-1}=1$ and $m_{2j}=a^{-1}$ with $a>0$. If $m_{2j}=1$ we have the classical periodic FPU chain. The parameters $\alpha,\beta \in \mathbb{R}$ regulate the non-linearity of the system. If $\alpha=\beta=0$ the system is linear, with associated matrix $-A_{2n}C_{2n}$, where A_{2n} is a $2n \times 2n$ diagonal matrix with diagonal $(1,a,1,a,\ldots)$, and C_{2n} has the form

$$\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ -1 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}. \tag{4}$$

The system of differential equations (3) has the same structure if we allow α and β to be complex, and $a \in \mathbb{C} \setminus \{0\}$. In this complex context we have the following result:

Theorem 1. *Let $n \ge 2$ and let k be a multiple of n. There is a $2n$-dimensional subspace $M_{k,n} \subset \mathbb{C}^{2k}$ such that the restriction of the system $\mathrm{FPU}_{2k}(a;\alpha,\beta)$ to $M_{k,n}$ is equivalent to the system $\mathrm{FPU}_{2n}(a;\alpha,\beta)$.*

By equivalence we mean that there is a bijective map $\Phi : \mathbb{C}^{2n} \to M_{k,n}$ such that the image $t \mapsto \Phi q(t)$ of the solution $t \mapsto q(t)$ with initial values $(q(0),q'(0)) \in \mathbb{C}^{2n}$ is the solution in $\mathbb{C}^{2k}$ with initial values $\big(\Phi q(0), \Phi q'(0)\big)$.
An implication is that a system of 4 particles in an FPU chain with alternating masses can be found in the dynamics of submanifolds in systems with $8, 12, 16, \ldots$ etc. particles. Likewise a FPU chain with 8 particles can be found in in the dynamics of submanifolds in systems with $16, 24, 32, \ldots$ etc. particles.

3 The FPU chain with 8 particles

The case of 4 particles has been extensively discussed in [2]. As an illustrative example we consider the case of an FPU α-chain with 8 alternating masses. The eigenvalues $\lambda_i = \omega_i^2$ are

$$\lambda_i = 2(1+a),\ 1+a+\sqrt{1+a^2}\,(\text{twice}),\ 2,\ 2a,\ 1+a-\sqrt{1+a^2}\,(\text{twice}),\ 0.$$

The momentum integral (2) enables us to reduce the equations of motion to 7 dof.

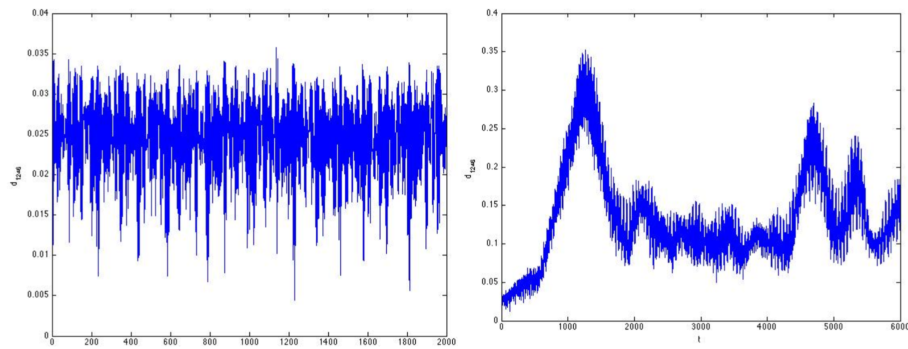

Fig. 1. Timeseries for α-chains based on the FPU-like system with 8 particles near M_{357}, 2000 timesteps, $\varepsilon = 0.5$ (the figure contains parameter values different from figs. in [3]). Vertical the Euclidean distance d_{1246} to the initial values of the modes $1, 2, 4, 6$ with initial values 0.01 and $x_3(0) = x_5(0) = x_7(0) = 0.2$. Left the quasi-stable case $a = 0.5$ ($0 \leq d_{1246} < 0.04$), right the unstable case $a = 0.75$ ($0 \leq d_{1246} < 0.35$) extended to 6000 timesteps. Note that the picture does not display the recurrence theorem as we only show the modes starting outside but near M_{357}.

3.1 The α-chain for $a = 0.5$ and $a = 0.75$

First order averaging-normalization produces already non-trivial results for $a = 0.5$ and $a = 0.75$. From the normal form we find three invariant manifolds with three dof each, so 6-dimensional. Numbering the eigenvalues from largest to smallest we have the invariant manifolds from the modes $1, 4, 5$: M_{145}, modes $2, 5, 6$: M_{256}, modes $3, 5, 7$: M_{357}; the fifth mode plays a pivotal role. For M_{357} we demonstrate stability if $a = 0.5$, instability for $a = 0.75$ in fig. 1. In the case $a = 0.75$ the normal form has seven integrals and is integrable, in the case $a = 0.5$ we found six independent integrals. Using the recurrence theorem as a tool has been neglected in the literature, probably because for statistical mechanics the theorem does not give much information. *For finite-dimensional Hamiltonian systems the recurrence theorem can produce valuable insight in the dynamics of the phase-flow.* Hamiltonian systems will contain many resonance zones associated with stable and unstable periodic solutions. Using the recurrence theorem as a tool we can identify in this problem some of the prominent zones where $2 : 1 : 1$ resonances are present.

3.2 The α-chain for large m (a small)

The assumption of m large induces strong resonances. In the case of 8 particles we have for the reduced 7 dof system the frequencies $\sqrt{2} + O(a)$ for the first four modes, the so-called optical group and the frequencies $\sqrt{2a}, a, a$ for the modes $5, 6, 7$, the acoustical group. The normal form changes accordingly and we find again invariant manifolds. Using recurrence, quasi-trapping in resonance zones near the optical and the acoustical group can be identified with $1 : 1$ resonances.

Conclusions

- Many of our considerations hold also for the classical periodic FPU chain. We have shown in [1] and [2] that in the case of four particles the presence of two equal masses produces a symmetry in the dynamical system that makes the system structurally unstable (a small perturbation of the parameters produces qualitatively different dynamics). This means that the classical periodic FPU chain with all masses equal is also structurally unstable and that it is misleading as a model.
- The averaging-normal form technique we have used is valid for an arbitrary number of particles as long as the total energy of the chain is finite and small. This enables us to extend the analysis to chains with many particles as was shown in [7].
- The dynamics on the energy manifold is structured by approximate invariant manifolds, some of them valid for all time, some with finite but long validity ($1/\varepsilon^m$ intervals for some positive m). At the same time the Poincaré recurrence theorem produces relatively short recurrence times, see [9]. Altogether this suggests that the classical periodic FPU chain for low energy values does not lead to equipartition of energy and is not a good model for statistical mechanics.

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