RECENT RESULTS ON THE FERMI-PASTA–ULAM PROBLEM

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Abstract. We revisit the celebrated model of Fermi, Pasta and Ulam with the aim of investigating the thresholds to equipartition in the thermodynamic limit. Starting with a particular class of initial conditions, i.e., with all the energy on the first mode, we observe that in a short time the system splits in two separate subsystems. We conjecture the existence of a function $\varepsilon_c(\omega)$, independent on the number N of particles in the chain, such that if the initial energy E satisfies $E/N < \varepsilon_c(\omega)$ then only the packet of modes with frequency not exceeding ω shares most of the energy.

1. Introduction

In a celebrated report of 1955 Fermi, Pasta and Ulam made the first numerical investigation on the dynamics of a chain of particles with a non linear coupling.[1] The model was intended to represent a discrete approximation of a non–linear string. According to the authors, *"The ergodic behaviour of such systems was studied with the primary aim of establishing, experimentally, the rate of approach to the equipartition of energy among the various degrees of freedom of the system"*. But the conclusion did not actually answer their initial question: *"Let us say here that the results of our computations show features which were, from the beginning, surprising to us. Instead of a gradual, continuous flow of energy from the first mode to higher modes, all of the problems show an entirely different behaviour. (...) Instead of a gradual increase of all the higher modes, the energy is exchanged, essentially, among only a certain few. It is, therefore, very hard to observe the rate of 'thermalization' or mixing in our problem, and this was the initial purpose of the calculation"*.

The aim of this paper is to revisit the phenomenon of "freezing of energy" on the low frequency modes that has been illustrated in the original report of Fermi, Pasta and Ulam. In particular, we investigate the possible existence of states that seem to be stable for very long times, if not forever. Such states are characterised by a concentration of energy on the low frequency modes, and appear to be of interest even in the thermodynamic limit, i.e., when the number N of particles in the chain is allowed to become very large.

The paper is organised as follows. In sect. 2 we recall the model and a few basic facts concerning the FPU phenomenon. In sect. 3 we give a very short account of some previous results, with particular emphasis on some facts that are at the basis of our approach. In sect. 4 we illustrate our results. The conclusions follow.

2. Recalling the model problem

The model is a one–dimensional chain of $N + 2$ particles with fixed ends, as described by the Hamiltonian

$$H(x, y) = H_2(x, y) + H_3(x) + H_4(x) \ , \tag{1}$$

with

$$H_2 = \frac{1}{2}\sum_{j=1}^{N} y_j^2 + \frac{1}{2}\sum_{j=0}^{N}\bigl(x_{j+1} - x_j\bigr)^2 \ ,$$

$$H_3 = \frac{\alpha}{3}\sum_{j=0}^{N}\bigl(x_{j+1} - x_j\bigr)^3 \ , \qquad H_4 = \frac{\beta}{4}\sum_{j=0}^{N}\bigl(x_{j+1} - x_j\bigr)^4 \ .$$

Here, $x_1, \ldots, x_N$ are the displacements with respect to the equilibrium position (that obviously exists), and $x_0 = x_{N+1} = 0$ are the fixed ends.

The normal modes are introduced via the canonical transformation

$$x_j = \sqrt{\frac{2}{N+1}}\sum_{k=1}^{N} q_k \sin\frac{jk\pi}{N+1} \ , \quad y_j = \sqrt{\frac{2}{N+1}}\sum_{k=1}^{N} p_k \sin\frac{jk\pi}{N+1} \ ,$$

(q_k, p_k) being the new coordinates and momenta. The quadratic part of the Hamiltonian in the normal coordinates is given the form

$$H_2 = \sum_{j=1}^{N} E_j \ , \quad E_j = \frac{1}{2}\bigl(p_j^2 + \omega_j^2 q_j^2\bigr) \ , \tag{2}$$

with harmonic frequencies

$$\omega_j = 2\sin\frac{j\pi}{2(N+1)} \ . \tag{3}$$

The problem, as first stated in the paper of Fermi, Pasta and Ulam, is concerned with the dynamical evolution of the harmonic energies E_j, as defined in (2). According to Classical Statistical Mechanics the time average of each of the harmonic energies should be the same (equipartition), at least in the harmonic approximation, i.e.,

$$\overline{E_j} = \lim_{t \to +\infty} \frac{1}{T} \int_0^T E_j(t)\mathrm{d}t = \frac{E}{N} \ ,$$

where E is the total energy. The goal of the numerical experiment was indeed to observe how the energy, initially given to the first mode only, flows towards other modes until equipartition is possibly reached.

3. A few historical remarks

Several years after the publication of the FPU report, Izrailev and Chirikov[2] first made an attempt to explain the lack of equipartition observed in the FPU system in the light of the KAM theorem.[3][4][5] According to these authors the existence of many KAM tori in the phase space could account for the lack of ergodicity in the system. More precisely, there might exist a *threshold to stochasticity* in the sense that if the energy of the system is below a critical energy, E_C say, then the system fails to relax to equipartition, while equipartition is reached if the energy exceeds E_C. Such a threshold could be in some sense related to the fact that invariant KAM tori are assured to exist only for small perturbations, i.e, small energies in the case of the FPU system. Thus, Izrailev and Chirikov raised the question whether the lack of ergodicity could persist in the thermodynamic limit. With some heuristic considerations they argue that the threshold should vanish for large N, i.e., that $E_C \to 0$ for $N \to \infty$, at least for an initial excitation of the high frequency modes. In a recent paper by Shepelyansky[6], using an improvement of their argument, it is suggested that the threshold should vanish also for excitation of low frequency modes.

On the opposite side, Bocchieri, Scotti Bearzi and Loinger performed a series of calculations on a nonlinear chain of particles interacting via a Lennard–Jones potential.[7] On the basis of the numerical simulations they conjectured the existence of a threshold in *specific energy* for the transition to stochasticity. More precisely, equipartition of energy would not occur if $\frac{E}{N} < \varepsilon_*$, where E is the total energy of the system and ε_* is independent of N (for large N).

The conjectures of Izrailev–Chirikov and Shepelyansky on the one hand, and that of Bocchieri–Scotti–Bearzi–Loinger on the other hand clearly lead to well different and opposite conclusions concerning the relevance of the FPU phenomenon for Statistical Mechanics. The question has been investigated by several authors during the last 30 years (see, e.g., [8]–[20]). However, it seems appropriate to say that no definite conclusion has been reached till now.

Let us first briefly discuss the applicability of KAM theory to the FPU system in the thermodynamic limit. KAM theory would lead to the expectation that for small energy most (in measure theoretic sense) of the invariant tori of the unperturbed system survive for all times, being only slightly deformed. However, the persistence of invariant tori requires quite strong irrationality hypotheses on the unperturbed frequencies, that are likely to be violated in view of the closeness to resonance of the lowest ad the highest frequencies in the spectrum (3). Thus, the applicability of KAM theory in the thermodynamic limit seems to be unlikely.

Nekhoroshev's theory assures that the harmonic actions of the system remain close to their initial value up to a time $\exp\bigl(E^{1/N})\bigr)$ (see for instance [21]). The bad dependence on N makes the estimate unsignificant if N grows too large. Moreover, both the KAM theorem and the theorem of Nekhoroshev apply only if the perturbation is *small enough*, i.e., if the energy E satisfies a condition $E < E^*$, where E^* depends on the parameters of the system, including the number N of particles, and the available analytical estimates give $E^* \to 0$ for $N \to \infty$.

The heuristic arguments of Izrailev and Chirikov, including the recent improvements due to Shepelyansky, essentially affirm that KAM theory does not extend to the thermodynamic limit. Concerning Nekhoroshev theory, a thorough comparison of the analytical estimates with the numerical results has been performed in [22], leading to the conclusion that the bad dependence of the analytical estimates on N is essentially optimal.

The above considerations seem to lead to the conclusion that the conjecture of Bocchieri et al. must be definitely rejected. But this would be a naive conclusion. For, the non applicability of KAM and Nekhoroshev's theory does not imply that the system is ergodic in the sense of Statistical Mechanics. Indeed, the quasi–invariance of *all* the harmonic actions assured by both KAM and Nekhoroshev theory is a very strong property, that needs not occur. Ergodicity is destroyed by the existence of only *one* quasi–invariant quantity. Thus, the question is whether or not such a quasi–invariant quantity may exists.

Identifying such a quantity is not difficult if one considers a modified FPU system with alternating heavy and light masses. The relevant fact is that the frequency spectrum of the normal modes splits into two well separated components, that are usually called the *acoustic* branch and the *optical* branch of the spectrum. In this case the whole system splits into two separate subsystems, and one can prove that the flow of energy from the acoustic subsystem to the optical one takes a time that grows exponentially with the ratio $\lambda = \omega^+/\omega-$, where ω^- and ω^+ are the typical acoustic and optical frequency, respectively[23][24]. A numerical confirmation of this phenomenon has been given in [22].

Now, splitting the FPU system in two separate components in the sense above seems to be impossible. For, the frequency spectrum exhibits no separation in different branches, and moreover the frequencies tend to become strongly resonant when N is increased, as we have already pointed out. As a matter of fact, most heuristic considerations in favour of the spreading of energy among the modes depend precisely on the latter property of the spectrum.

Now, it happened to us to realize that a spontaneous splitting of the system actually

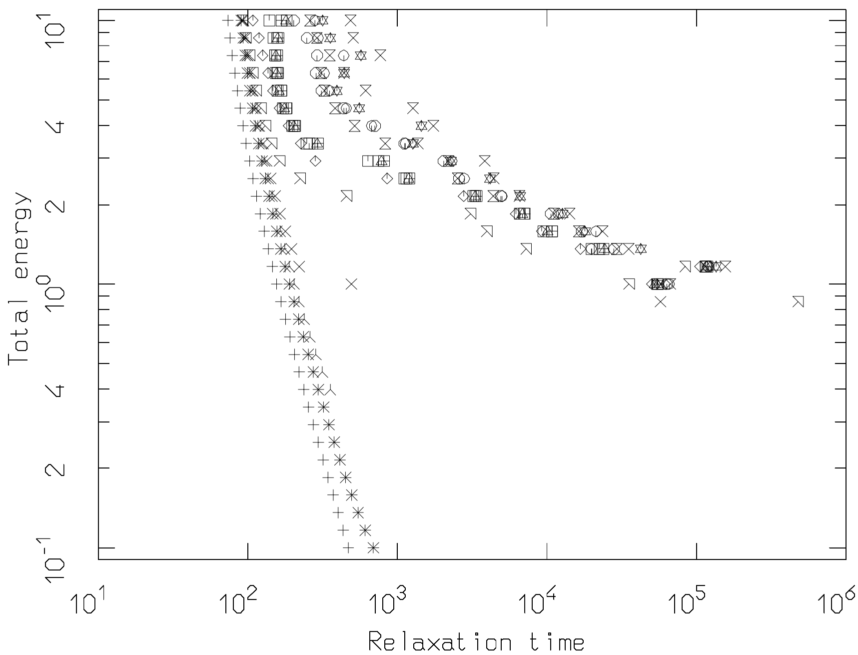

Figure 1. Relaxation time t_s^R for varying energy and number of modes in a packet. Moving horizontally, i.e., at a fixed energy, the packet of the first s modes loses 20% if its initial energy at time t_s^R. At a given energy, only a small packet of modes takes part on the sharing on energy in a short time. Different symbols correspond to different values of $s = 1, 2, \ldots$, from left to right. This figure is drawn for $N = 16$.

occurs, at least if one considers a particular class of initial conditions: we should simply ask the system itself how it likes to split. This is the spirit of a numerical experiment that we are going to discuss.

4. The numerical experiment

In the spirit of the first numerical experiment of Fermi, Pasta an Ulam we investigate how the energy, initially given only to the first harmonic mode, spreads towards higher and higher modes. Our main remark is that the system exhibits two different time scales, as illustrated in fig. 1. For $s = 1, \ldots, n$ we consider the time average of the total harmonic energy of the packet formed by the first s modes, namely of the quantities

$$(4) \qquad \mathcal{E}_1 = E_1 \ , \quad \mathcal{E}_2 = E_1 + E_2 \ , \ \ldots \ , \quad \mathcal{E}_s = E_1 + \ldots + E_s \ , \ \ldots$$

Since the initial energy is initially given to the first mode, we have $\mathcal{E}_s(0) = E$, the total energy. On the other hand, if the system evolves towards equipartition we expect $\overline{\mathcal{E}}_s(t) \to sE/N$ when time increases to infinity (overline denotes the time average), i.e., its energy has decreased by $(N - s)E/N$. We define the critical time t_s^R as the first

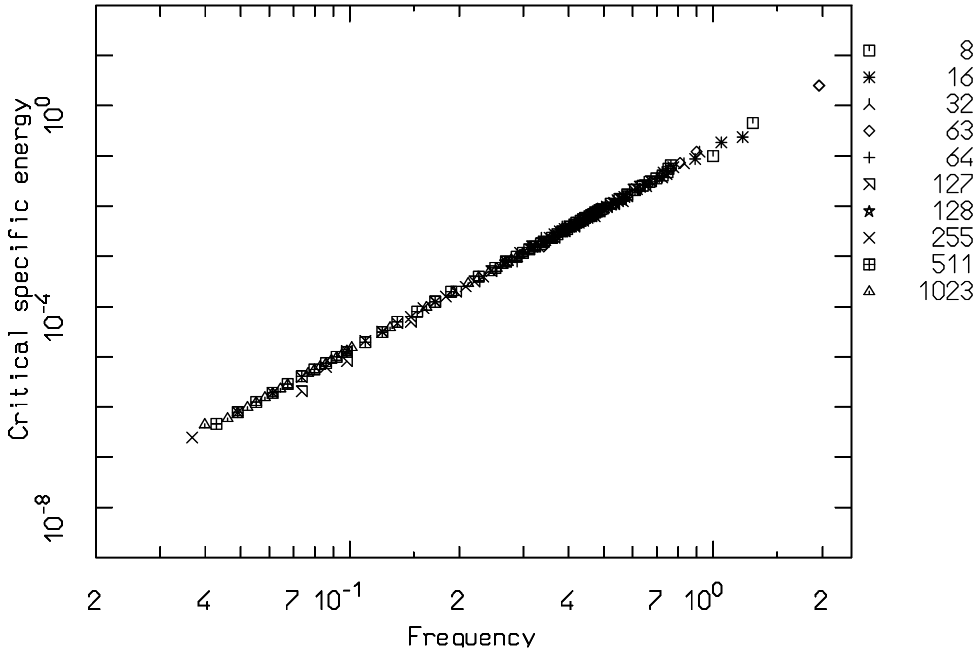

Figure 2. Plot of the numerically calculated values of $E^R(N,\omega)$ vs. ω, for different values of N as identified by the different symbols but with the specific energy $\varepsilon = E/N$ in ordinates. All the data look well aligned on the same curve (possibly a straight line). This defines the function $\varepsilon_c(\omega)$, as stated in the text.

instant at which $\overline{\mathcal{E}}_s(t)$ has lost 20 percent of the latter quantity. The numerical data for (t_s^R, E) are plotted in fig. 1. For a constant value of the initial energy, i.e., moving on a horizontal line, the points corresponding to increasing values of s are aligned from left to right and represented by different symbols.

The relevant information here is that the energy flows quite rapidly from the first packet to the second, third &c, but for some value of s the flow stops, and a much longer time is needed for the quantity $\overline{\mathcal{E}_s}(t)$ to lose 20% of $(N-s)E/N$. In this case we say that the first s modes form a natural packet that persists for a long time. The figure also shows that if we let the value of the energy decrease, then the length of the natural packet decreases, too, and the time needed for the energy to flow to higher modes significantly increases. The point of separation of the s–th curve defines a threshold energy $E^R(N,\omega)$ in the following sense: for initial energy less than $E^R(N,\omega)$ the natural packet contains only modes with frequency less than ω_s, the frequency of the s–th mode. This remark provides a quantitative description of the phenomenon of the formation of natural packets.

The most interesting fact is concerned with the dependence of the threshold energy $E^R(N,\omega)$ on the number N of particles. This is illustrated in fig. 2. By simply replacing the total energy E with the specific energy $\varepsilon = E/N$ all the data points turn out to be aligned on one and the same straight line, independent of N. This leads us to formulate the following conjecture: *there exists a specific energy threshold, namely a function $\varepsilon_c(\omega)$ with the following meaning: the natural packet includes the mode of frequency ω only if the initial specific energy ε is greater than $\varepsilon_c(\omega)$.*

5. Conclusions and open questions

The result of our numerical experiments strongly supports the conjecture of Bocchieri, Scotti, Bearzi and Loinger about the existence of a threshold to ergodicity which depends only on the specific energy of the system. For, recalling that the specturm of the FPU system has an upper limit $\omega_{\max} = 2$ the critical value $\varepsilon_* = \varepsilon_c(2)$ represents the limit above which all modes belong to the natural packet. For lower energies one is confronted with the existence of a second and much longer relaxation time, which still depends on the specific energy, ang grows very fast when the energy is decreased. The problem of the dependence of the latter relaxation time on the energy remains unsettled, although we have some preliminary indication that it might grow as fast as $\exp(1/\sqrt{\varepsilon})$.

Concerning the conjecture of Izrailev, Chirikov and Shepelyansky, we remark that the outcome of our numerical experiment is not in full contrast with their results. Indeed, the internal dynamics of the natural packet may well be chaotic – e.g., some of the Lyapounov exponents may be positive, as we have checked with calculations not reported here. This is precisely due to the existence of resonances, which constitutes the basis of the argument of those authors. However, the existence of a chaotic behaviour does not imply that the system is ergodic in the sense of classical Statistical Mechanics, because energy is not equally shared among all modes, at least for very long times. As a matter of fact, chaos seems to be confined inside the natural packet.

The results discussed here may have a certain impact on the foundations of Statistical Mechanics, and in particular on its relations with Quantum Mechanics. For, the long time persistence of the natural packet might result in a state of meta–equilibrium that in a physical experiment would appear as an actual equilibrium. Such a state would be characterized by a *freezing* of the high frequency modes that is known to be the main characteristic of the quantum behaviour. For a further discussion of this point we refer to [25].

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