LOCALIZATION OF ENERGY IN FPU CHAINS

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Abstract. We revisit the celebrated model of Fermi, Pasta and Ulam with the aim of investigating, by numerical computations, the trend towards equipartition in the thermodynamic limit. We concentrate our attention on a particular class of initial conditions, namely, with all the energy on the first mode or the first few modes. We observe that the approach to equipartition occurs on two different time scales: in a short time the energy spreads up by forming a packet involving all low–frequency modes up to a cutoff frequency ω_c, while a much longer time is required in order to reach equipartition, if any. In this sense one has an energy localization with respect to frequency. The crucial point is that our numerical computations suggest that this phenomenon of a fast formation of a natural packet survives in the thermodynamic limit. More precisely we conjecture that the cutoff frequency ω_c is a function of the specific energy $\varepsilon = E/N$, where E and N are the total energy and the number of particles, respectively. Equivalently, there should exist a function $\varepsilon_c(\omega)$, representing the minimal specific energy at which the natural packet extends up to frequency ω. The time required for the fast formation of the natural packet is also investigated.

1. Introduction

In a celebrated report of the year 1955 Fermi, Pasta and Ulam performed 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"*. It is well known that

the authors actually found some unexpected result. In the very words of the authors: *"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 the present paper is to revisit the phenomenon of "freezing of energy" on the low frequency modes that was illustrated in the original report of Fermi, Pasta and Ulam. The problem amounts to establishing the existence of states that appear to be stable for very long times, if not forever, and are characterized by a concentration of energy on the low frequency modes, to which we give the name of natural packets. Our aim is to investigate whether the phenomenon of the existence of natural packets persists in the thermodynamic limit, i.e., when the number N of particles and the total energy E of the chain are allowed to become very large, keeping the specific energy $\varepsilon = E/N$ constant.

The paper is organized as follows. In sect. 2 we recall the model and the main problem. In sect. 3 we illustrate our numerical experiment, while the conclusions are drawn in sect. 4. A discussion concerning the time required for the fast formation of the natural packet, and the dependence of the results on the number of initially excited modes, is deferred to an appendix.

2. Recalling the model and the 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

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

$$H_3 = \frac{\alpha}{3}\sum_{j=0}^{N}\big(x_{j+1}-x_j\big)^3 \ ,$$

$$H_4 = \frac{\beta}{4}\sum_{j=0}^{N}\big(x_{j+1}-x_j\big)^4 \ .$$

Here, $x_1, \ldots, x_N$ are the displacements with respect to the equilibrium positions (that obviously exist), and $x_0 = x_{N+1} = 0$ are the fixed ends. The normal modes are intro-

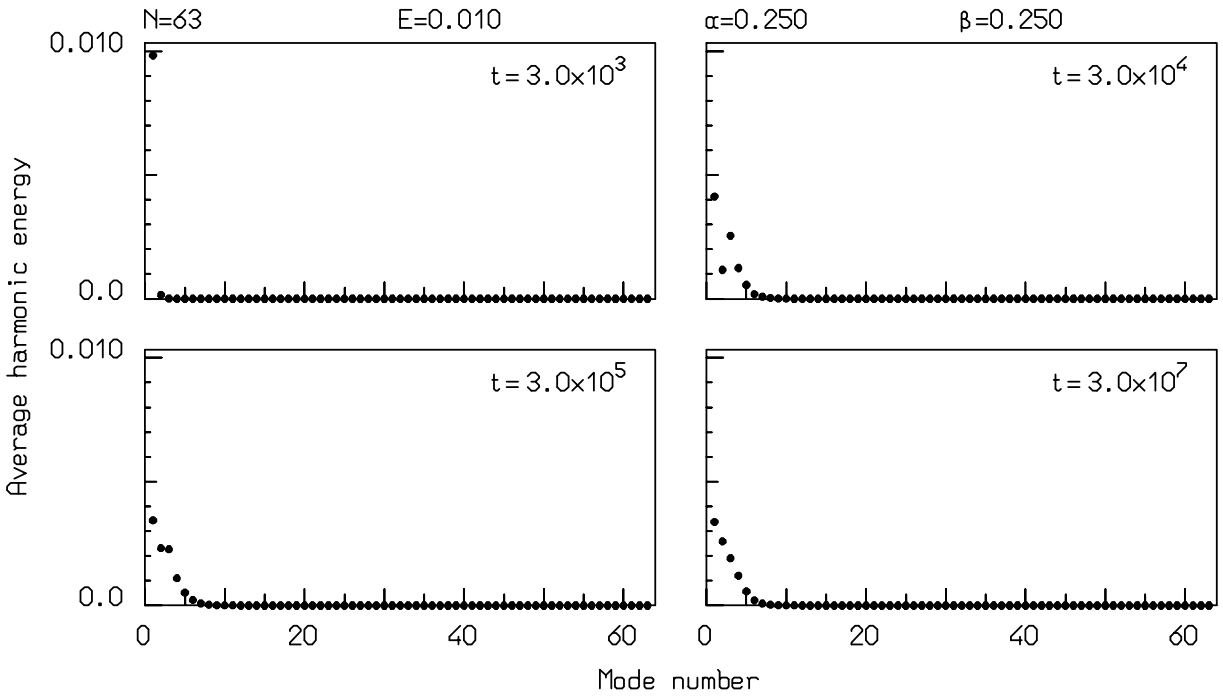

Figure 1. Distribution of energy (in time average) among the normal modes at different times for $N = 63$ and $E = 0.01$. Here and in the whole paper, $\alpha = \beta = 1/4$. As was pointed out in the FPU report, only a few modes do actually share the whole energy.

duced 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

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

with harmonic frequencies

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

Notice that the period of the fastest oscillator tends to π as $N \to \infty$, while the lowest frequency mode has period $\sim \frac{\pi}{N+1}$.

All of our numerical computations were performed with $\alpha = \beta = 1/4$, and with N ranging from 8 to 1023. The integration was performed using a leap–frog method, with typical time step 0.05.

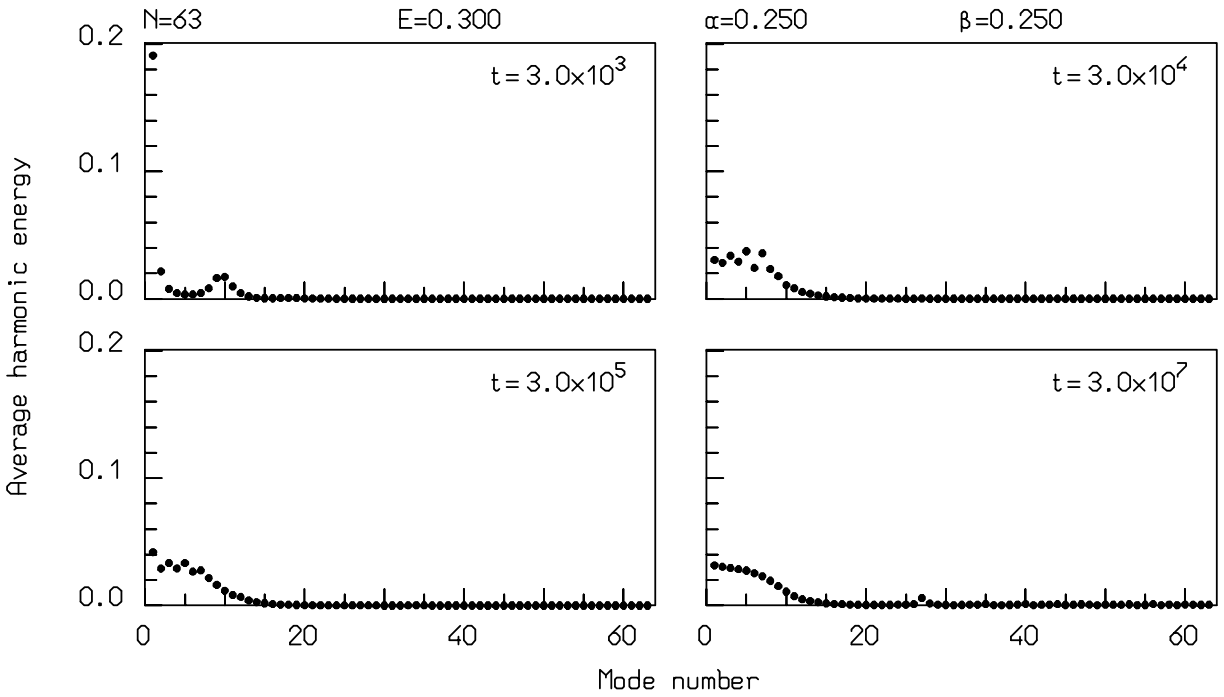

Figure 2. Same as fig. 1 with initial energy $E = 0.3$. The number of modes that take part in the sharing of energy is definitely larger than in the previous case. Note also that some of the first modes seem to have reached a sort of internal equipartition.

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 defined in (2). In Classical Statistical Mechanics, in the infinite time limit one expects that the time average $\overline{E_j}$ of each of the harmonic energies should be the same (equipartition), at least in the so–called harmonic approximation, i.e., one should have

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

where $\varepsilon = E/N$ is the specific energy. The goal of the numerical experiment was indeed to observe how the energy, initially given to the first mode only, flows towards the other modes until equipartition is possibly reached.

The phenomenon observed by Fermi, namely that the energy is exchanged essentially among only a certain few low–frequency modes, is illustrated in fig. 1, which refers to $N = 63$ and $E = 0.01$: in a short time ($t \sim 10^4$) a packet of low–frequency modes involved in the energy sharing is formed, and the distribution of energy does not essentially change up to time $t \sim 10^7$. The idea that such a phenomenon should disappear if the total energy E of the chain is raised was first put forward by Izrailev and Chirikov[2], who conjectured the existence of an energy threshold E_c above which the system would

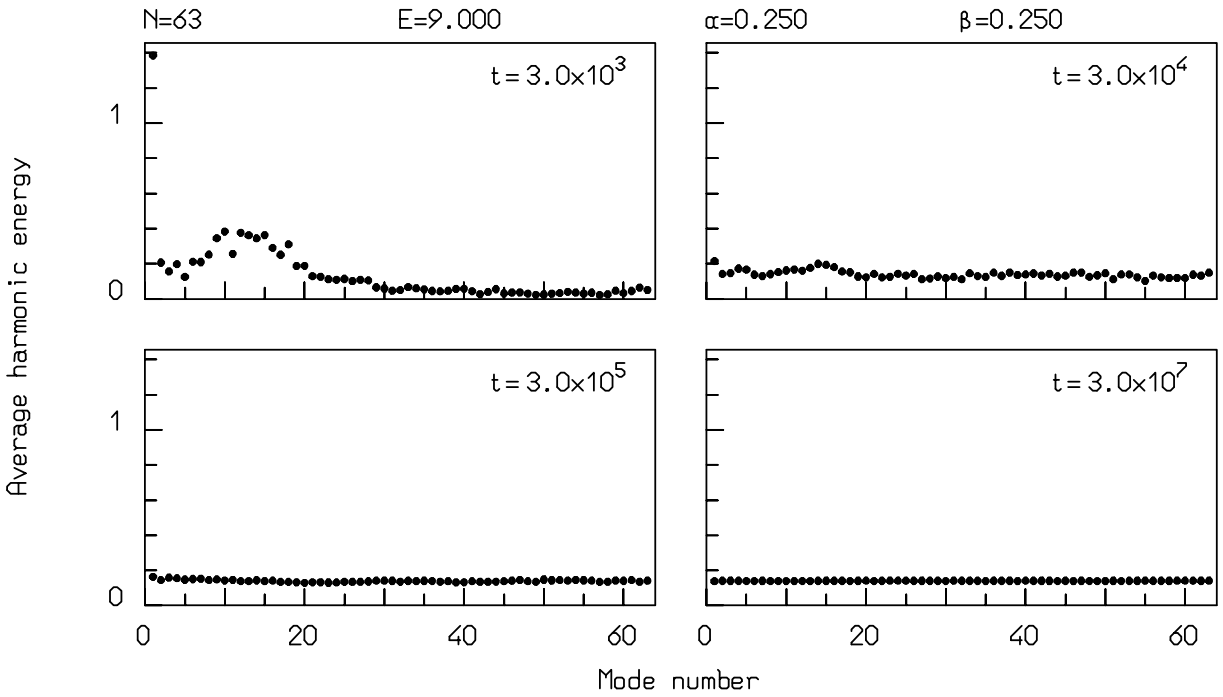

Figure 3. Same as fig. 1 with initial energy $E = 9$. A significant sharing of energy among the modes occurs. The final distribution of energy looks fully consistent with equipartition.

rapidly reach equipartition. In fact, this is exhibited in figs. 2 and 3. The number of particles is still $N = 63$, while the total energy is 0.3 and 9, respectively. Fig. 3 shows that at $E = 9$ equipartition is essentially reached in the short time $t \sim 10^4$, while an intermediate behaviour occurs in the case of fig. 2, at $E = 0.3$.

Concerning the dependence of the energy threshold on the number N of particles, Bocchieri, Scotti, Bearzi and Loinger[3] put forward the explicit conjecture that E_c should be proportional to N, i.e., that there should exist a critical specific energy ε_c such that equipartition would rapidly show up if $\varepsilon > \varepsilon_c$.

This question was widely discussed during the last 30 years ([4] and [11]–[19]). However, in our opinion, a definite conclusion is still lacking.

3. The numerical experiment

Our starting point is the spreading of energy among a few low–frequency modes that is observed in figs. 1 and 2. We emphasize that such a spreading occurs in a quite short time, while the subsequent flow of energy towards higher order modes seems to be very slow — if it occurs at all. Moreover, the number of modes that take part in the energy

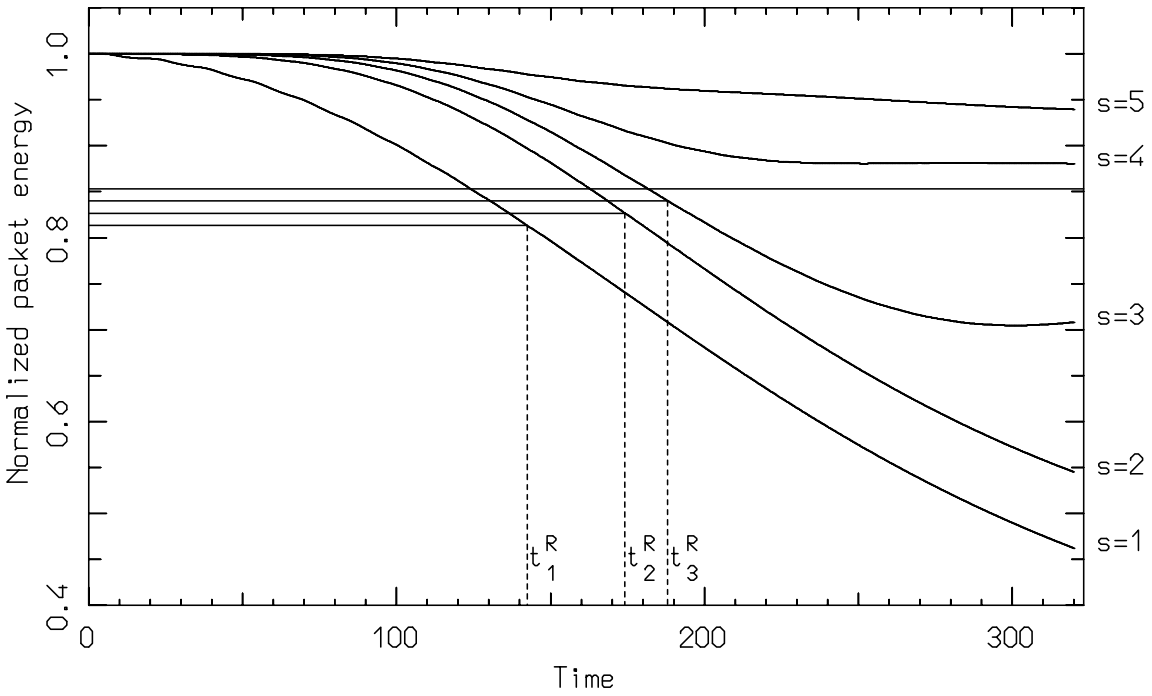

Figure 4. Illustrating how the relaxation time t_s^R is determined. The five curves represent as functions of time the quantities ϑ_s, as defined in (5), for the first five packets. The horizontal lines mark the thresholds for the first four packets, as described in the paper. In this figure, $N = 15$, and $E = 1$.

sharing seems to increase with the total energy. Hence we introduce the quantities

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

as good candidates to quasi–invariance. That is, we consider the total harmonic energy of a packet of modes — the first s modes, $s = 1, \ldots, n$. Correspondingly, we also introduce the normalized mean energies of such packets

$$\vartheta_s = \frac{\overline{\mathcal{E}}_s}{\sum_{j=1}^{N} \overline{\mathcal{E}}_j} \ . \tag{5}$$

We presently consider only initial data with all the energy on the first mode (as in Fermi's paper); later we will discuss how the results change if the energy is initially given to a number of low frequency modes proportional to N. Thus we have initially $\vartheta_s^0 = 1$ for $s = 1, \ldots, N$. The value expected according to equipartition is instead $\vartheta_s^{\rm eq} = s/N$.

Let us take a fixed value for N. If we plot $\vartheta_s(t)$ vs. t for different values of s we typically get the graph of fig. 4. Of course, we have $\vartheta_1 < \vartheta_2 < \ldots$, so that different curves correspond to increasing values of s, starting from the bottom curve $s = 1$. From the figure, which refers to $N = 16$, one has the clear impression that in a short time the

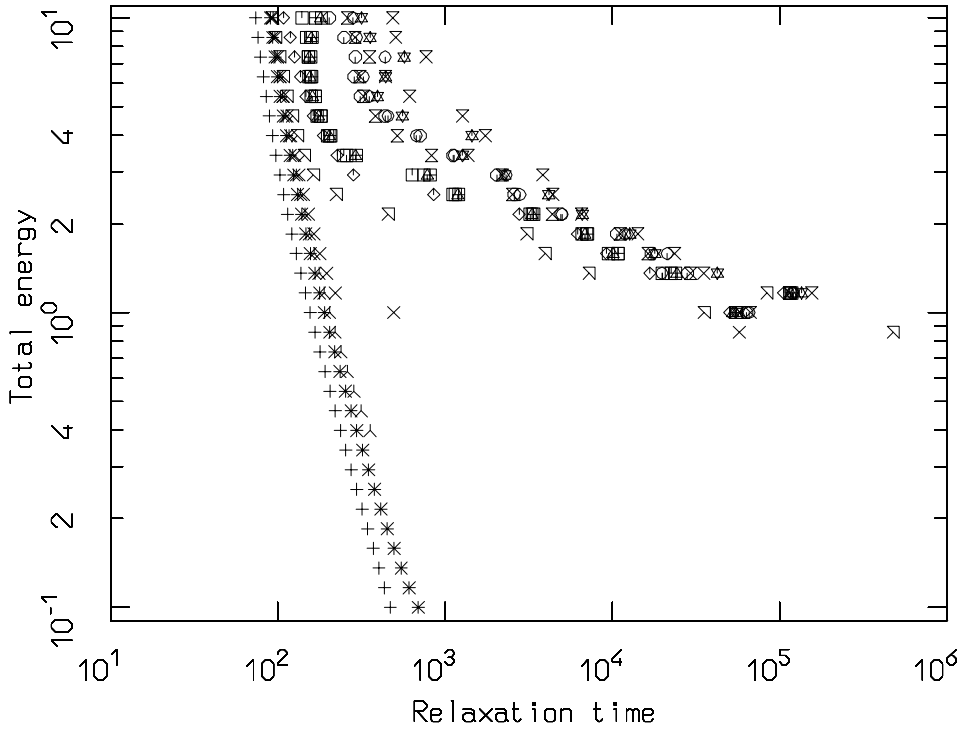

Figure 5. Relaxation time t_s^R for varying energy and number of modes in a packet. Different symbols correspond to different values of $s = 1, 2, \ldots$, from left to right. This figure is drawn for $N = 15$.

packet of the first three modes has lost a significant fraction of its initial energy, while the packet of the first four modes seems to keep most of its initial energy. We could say that the dynamics involves essentially the first four modes. We now attempt to give this information a quantitative form. To this end, we notice that the s–th packet reaches equipartition when it has lost enough energy, namely ϑ_s has decreased by a quantity $\Delta\vartheta_s = (N-s)/N$. Thus, we introduce the *relaxation time* t_s^R defined as the first instant at which ϑ_s has decreased by a fraction $\gamma\Delta\vartheta_s$ with a positive $\gamma < 1$. Equivalently, this is the first time for which one has $\vartheta_s = 1 - \gamma + \gamma s/N$. In our calculations we take $\gamma = 0.2$. Thus, letting the total energy E vary, we are given a set of pairs $\left(t_s^R, E\right)$ that we plot in fig. 5, which still refers to $N = 15$. For a constant value of the energy, i.e., moving on a horizontal line, the points corresponding to increasing values of s are aligned from left to right, in agreement with the qualitative behaviour of fig. 2.

The relevant information here is that, for a fixed E, the energy flows quite rapidly from the first packet to the second, third &c, but for some value of s the fast flow stops, and a much longer time is needed for the quantity $\vartheta_s(t)$ to fall below the wanted threshold. In this case we say that a good quasi–invariant quantity is the energy $\mathcal{E}_s$ of the packet of the first s modes, i.e., a fast formation of a natural packet of s low–frequency modes has occurred. If we let the energy decrease, then we see that the number s of

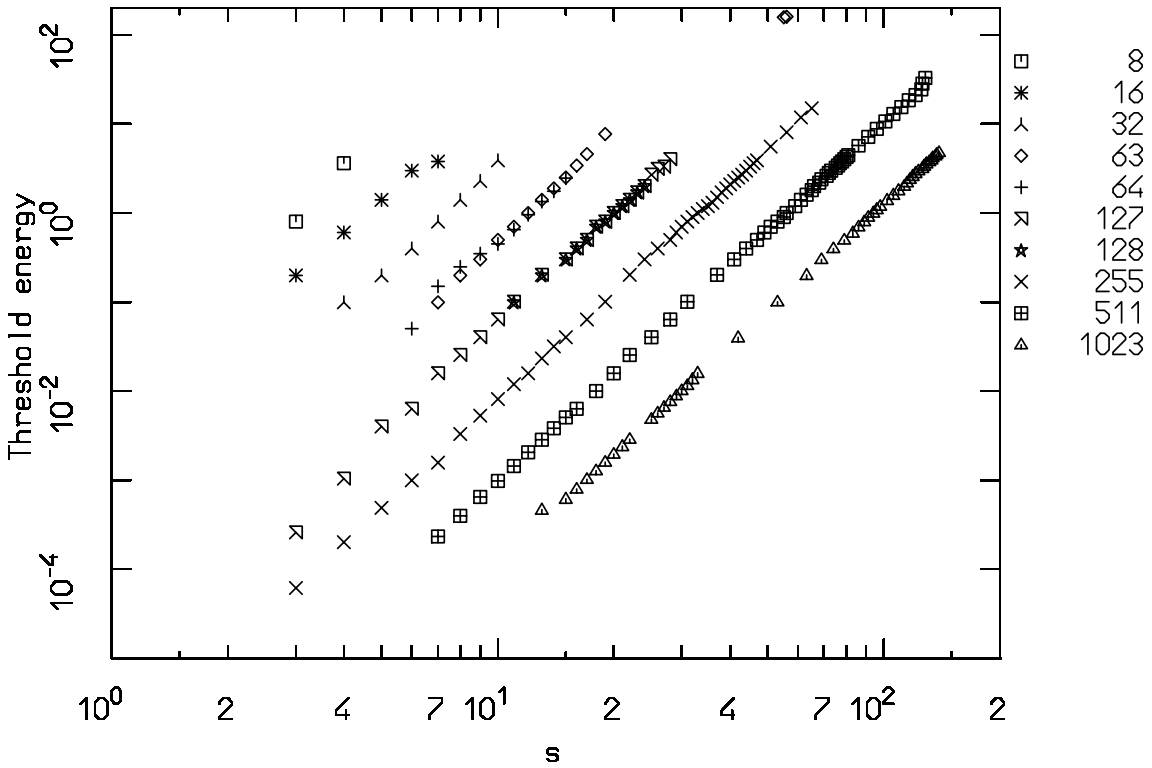

Figure 6. Plot of the numerically calculated values of $E^R(N,s)$ vs. s, for different values of N as identified by the different symbols.

modes forming the natural packet decreases, too. This is exhibited by the fact that for a fixed s the points $\left(t_s^R, E\right)$ look aligned on a straight line for high values of the energy, but suddenly separate from such a straight line going very rapidly towards the right. The slope of the straight line indicates a dependence $t_s^R \sim E^{-1/2}$.

The point of separation of the s–th curve defines a threshold energy $E^R(s)$ in the following sense: for initial energy less than $E^R(s)$ the natural packet contains at most s modes. Thus, recalling that we are working at a fixed value of N, we are given a threshold energy $E^R(N,s)$ as a function of N and s.

Let now N vary, and let us plot $E^R(N,s)$ vs. s for different values of N. We get the graph in fig. 6, where different symbols have been used for different values of N. The data look aligned on parallel lines, each line corresponding to a different N. The regular spacing among the lines strongly suggests that something proportional to N must be hidden inside these data. Thus, we replace the packet number s and the energy E by the fraction s/N of the total number of modes and by the specific energy ε, respectively. Moreover, recalling the form (3) of the frequency spectrum we remark that there is a one–to–one correspondence between s/N and ω. Therefore, in fig. 7 we plot the same data of fig. 6 on a different scale, using the frequency ω as abscissa and the specific energy ε as ordinate. It is immediately evident that all the points are well aligned on a

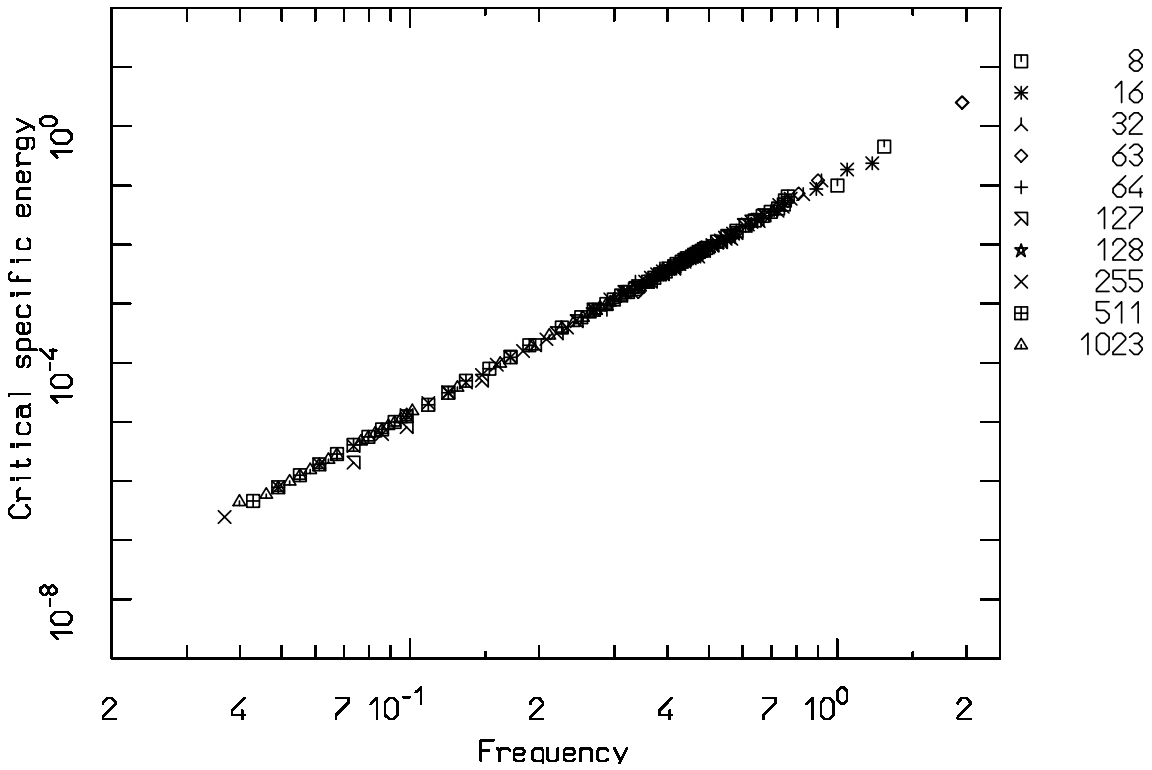

Figure 7. Same data as in fig. 6, but with the frequency ω in abscissas and the specific energy in ordinates. All points look well aligned on the same curve (possibly a straight line). This defines the function $\varepsilon_c(\omega)$, as defined in the text.

unique curve, very close to a straight line, which does not depend on N, at least in the range $8 \leq N \leq 1023$.

4. Conclusion

Our numerical investigations strongly suggest that there exist two separate time scales for the energy sharing among modes, when energy is initially given to the first mode. In a rather short time the energy spreads over a natural packet involving the modes up to a certain critical frequency ω_c. Further spreading of energy over all modes, possibly leading to equipartition, requires a much longer time scale, that we are presently unable to quantify.

Quantitative estimates are instead available for the fast spreading of energy inside the natural packet. Precisely from the graph of fig. 7 we conjecture that *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 $\varepsilon_c(\omega)$*. In particular, as $\omega = 2$ is the maximal frequency in the spectrum

of our model, the quantity $\varepsilon_c(2)$ defines a specific energy threshold above which the natural packet covers the whole available spectrum. This should somehow correspond to the specific energy threshold for fast equipartition observed by Bocchieri, Scotti, Bearzi and Loinger. Our result can be equivalently expressed by saying that *there exists a function $\omega_c(\varepsilon)$, the inverse of the function $\varepsilon_c(\omega)$, which gives the width of the natural packet, as a function of the specific energy ε.*

Actually, fig. 7 suggests a rather definite functional form for the functions introduced above, namely $\varepsilon_c(\omega) \sim \omega^4$, i.e., $\omega_c(\varepsilon) \sim \varepsilon^{1/4}$. Presently, no theoretical justification of this fact is available to us.

Our numerical calculations allowed us to estimate the time needed for the formation of the natural packet and to confirm the persistence of a separate and longer time scale to equipartition in case one takes initial conditions involving a number of low modes proportional to N. Obviously, the initial distribution of energy should still be localized around the first mode. E.g., the size of the initially excited packet should not exceed half the size of the natural packet. In such a case we observe that one still has a fast formation of a natural packet similar to that of the previous calculations. The main point is that with such a class of initial conditions the times needed for the fast formation of the natural packet exhibit a strong dependence on the initial distribution of energy, but the qualitative behaviour indicating that the natural packet survives for a long time before the system relaxes to equipartition appears to persist. This is discussed in the Appendix below.

Appendix

We address first of all the problem of the dependence of the relaxation time t_s^R (namely the time of formation of the natural packet as represented in fig. 5) on the number N of degrees of freedom, at a fixed specific energy; this turns out to strongly depend on the type of initial conditions. With all the energy initially on the lowest frequency mode we found that for the values of s that corresponds to modes belonging to the natural packet one has $t_s^R \sim N$. An example of this is illustrated in fig. 8, where the relaxation time t_1^R for the mode 1 is plotted vs. N, and represented by black dots. The figure refers to the case of initial specific energy $\varepsilon = 0.01$, and to values of N of the form $N = 2^r - 1$ with $r = 4, 5, \ldots, 17$, i.e., $N = 15, 31, 63, \ldots, 131\,071$. (Actually, for the case of one–mode excitation the points for $N > 32\,767$ are missing, because the calculation would require an exceedingly long time.)

Thus, the time of formation of the natural packet would seem to tend to infinity with N. However, this way of posing the problem is not relevant for the thermodynamic limit, being related to the very particular class of initial conditions considered till now, namely with all the energy given initially to the lowest frequency mode. By the way, the behaviour $t_1^R \sim N$ in such a case may be understood if one remarks that the period of the lowest frequency mode, according to formula (3), is $T_1 = 2\pi/\omega_1 \sim 1/N$. Since only

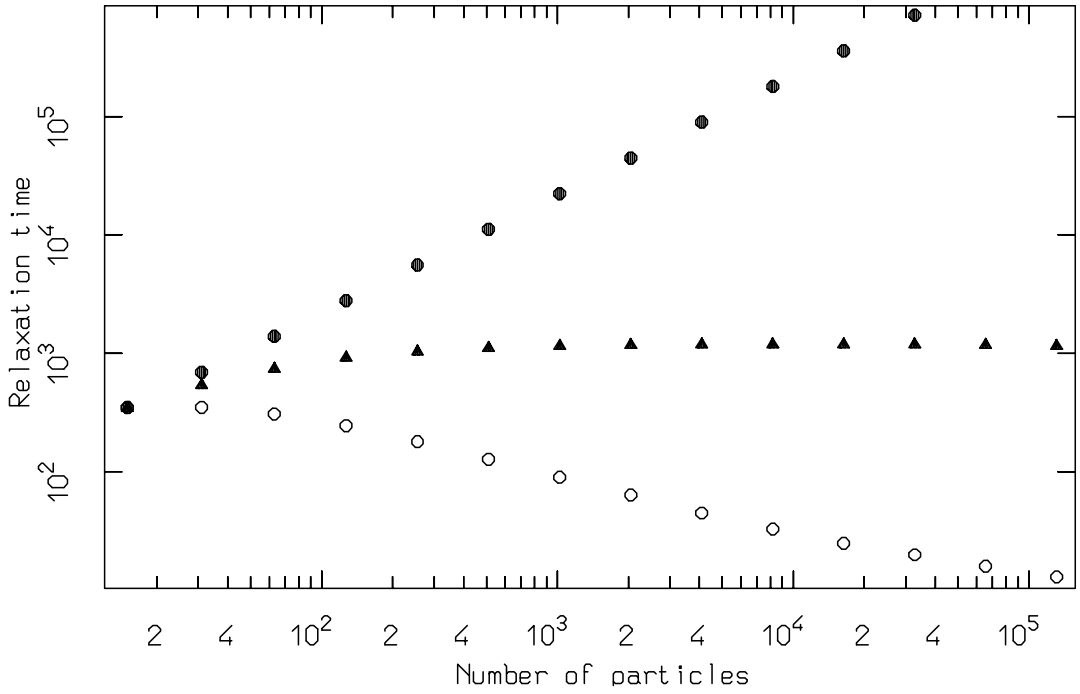

Figure 8. Dependence of the relaxation time t_s^R on N and on the initial distribution of energy among the low frequency modes. The dots represent the relaxation time t_1^R for $N = 15, 31, 63, 127, \ldots, 32\,767$, with all the energy initially on the lowest frequency mode. The triangles and the circles correspond to initial conditions with energy distributed among the first $s = (N+1)/16$ modes. Thus, for $N = 15, 31, \ldots, 131\,071$ the size of the initially excited packet of modes is $s = 1, 2, \ldots, 8\,192$, respectively. This means that the initial packet contains all modes of frequency not exceeding a fixed value $\hat{\omega}$ (which in our case can be identified with the lowest frequency for $N = 15$). The triangles correspond to the case of initial conditions with energy linearly decreasing from the first mode to the $(s+1)$–th mode, with zero energy on the mode $s+1$. The circles correspond to the case of initial conditions with energy equally distributed among the s modes of the initially excited packet. In both these cases we plot the relaxation time t_s^R for the initial packet. In all cases the specific energy is $\varepsilon = 0.01$.

the lowest frequency mode is actually excited, it seems reasonable to expect that the typical time scale of the dynamics during the first phase of the evolution is the period of the lowest frequency mode. This makes the linear dependence on N understandable.

In view of this argument, the dependence of the relaxation time on N might be expected to drastically change if the energy is initially shared by a packet of low frequency modes of length depending on N in some proper way. In order to check this fact let us consider initial conditions with the energy distributed among the modes with frequency not exceeding a fixed $\hat{\omega}$. This means that the size of the initial packet is proportional

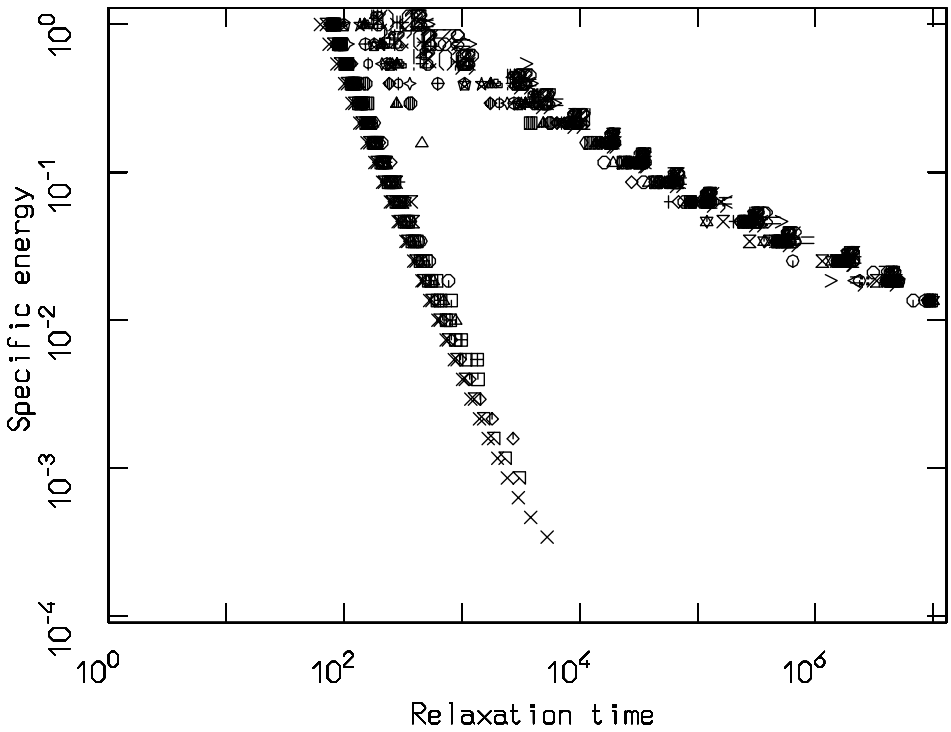

Figure 9. Relaxation times for $N = 63$, with energy initially distributed among the first 4 modes and specific energy 0.01. One clearly sees that the qualitative behavior is similar to that of fig. 5, thus showing the persistence of the phenomenon of existence of two well separated time scales. Here, the symbol $\times$ refers to the relaxation time for the packet of the first four modes.

to N. Of course, $\hat{\omega}$ should be chosen such that the size of the initial packet packet does not exceed the size of the natural packet. For instance, looking at fig. 5, which refers to $N = 15$, we see that for specific energy $\varepsilon = 0.01$, i.e., total energy $E = 0.15$, the natural packet contains two modes, i.e., $(N+1)/8$ modes. Thus, let us choose $\hat{\omega}$ as the smallest frequency for $N = 15$, so that the size of the initial packet is $(N+1)/16$, corresponding to half the size of the natural packet. That is, for $N = 31, 63, 127, \ldots$ we start with an initial packet of $s = 2, 4, 8, \ldots$ modes, respectively, and look for the relaxation time t_s^R, namely the time at which the initially excited packet has lost a significant fraction of its initial energy, in a sense analogous to the previously considered one.

We consider two different classes of initial conditions. In the first class we distribute the energy so that it decreases linearly from the first mode to the mode s, and the mode $s+1$ has initially zero energy. In the second class we start with the initial energy equally distributed among the first s modes. The result is illustrated in fig. 8, for initial specific energy $\varepsilon = 0.01$ and for the values of N as above. The data for the first case are reported by triangles, and the relaxation time appears to tend to a constant value. The data for the second case are plotted as circles, and the relaxation time appears to decrease with

N. Thus, it appears that the formation of the natural packet takes a time that dtrongly depends on the initial distribution of energy inside the packet. The divergence with N seems to be peculiar to a class of extremely localized excitations.

Let us finally turn to the problem of the existence of two well separated time scales in order to check whether it may be confirmed also for the latter class of initial conditions. In particular, it is interesting to check whether the long time persistence of the natural packet still occurs for the second class on initial conditions discussed above. The qualitative answer is given by fig. 9, where $N = 63$ and the energy is initially equally distributed among the 4 lowest frequency modes. By comparison with fig. 5 one observes the same qualitative behaviour, namely the formation of a natural packet that persists for longer and longer times when the specific energy is decreased.

Thus, the existence of two well separated time scales for the evolution appears to be confirmed for a significant class of initial conditions with energy concentrated on a packet of low frequency modes, and this is the most relevant conclusion of the present paper.

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