Numerical studies on boundary effects on the FPU paradox

D. Bambusi, D. Muraro and T. Penati*
Università degli Studi di Milano,
Dipartimento di Matematica "F. Enriques",
Via Saldini 50, 20133 Milano, Italy

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Abstract

We study numerically the dynamics of a chain of particles subjected to an on site restoring nonlinear force and a first neighbour harmonic coupling. We excite the first linear mode and investigate the distribution of the average harmonic energies, in the spirit of Fermi Pasta Ulam experiment. The limit distribution turns out to strongly depend on the boundary conditions. A heuristic explaination is also given.

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KEYWORDS: FPU model, Metastability, Boundary effects

1 Introduction

In their celebrated paper ([5]) Fermi Pasta and Ulam (FPU) studied the problem of thermalization in a weakly nonlinear chain of oscillators. Precisely they observed an approximatively recurrent behaviour of the system and showed that the time average $\langle E_k \rangle$ of the energies E_k of the normal modes of the system quickly relax to a distribution which is different from equipartition. This is what we call FPU paradox.

Since the paper of FPU, many numerical computations have been done and in particular it has been put into evidence the fact that the limit distribution is exponential. In particular Berchialla Galgani and Giorgilli [3] have shown that it behaves as $\exp\left(-\sigma k/\epsilon^{1/4}\right)$ where ϵ is the energy density of the system. Such a behaviour has been partially justified rigorously in [1].

The motivation of the present work has to be found in the comparison of the result by Benettin [2] and that by Carati [4]. Indeed Benettin studied numerically the behaviour of a 2-dimensional FPU lattice with Dirichlet boundary condition on a domain having the size of a hexagon, with the particles situated at the corners of equilateral triangles and interacting through nonlinear springs situated along the sides of the triangles. He found that in such a lattice the FPU phenomenon essentially disappears in the sense that for large enough number of particles the so called spectral entropy quickly relaxes to the equipartition value. Subsequently Carati studied a related model where the particles are again at the vertexes of an equilateral triangle, but the total domain form a rhomboid. Moreover he imposed periodic boundary conditions to the system. His numerical studies (unpublished) showed that in his model the average of the harmonic energies immediately relaxes to a distribution exponentially decreasing and then the situation seems to stabilize. Thus Carati's computation seems to indicate that the FPU paradox could persist in his model. Recently Benettin and Gradenigo [BG07] performed a systematic numerical investigation of the triangular lattice with different boundary conditions. They confirmed that a difference between

**corresponding author*: penati@mat.unimi.it, Ph.Num: 0039.02.50316131, FAX 0039.02.50316090

the periodic and the Dirichlet case occurs and that the periodic case is more stable.

So it is quite natural to try to understand the role of the boundary conditions in order to separate between boundary and dimensional effects. To this end we start by investigating a one dimensional model where we show that the dynamical behaviour crucially depends on the boundary conditions.

We consider the chain of particles described by the Hamiltonian

$$\begin{aligned} H(q,p) &= \sum_n \frac{p_n^2+q_n^2}{2} + a\frac{(q_n-q_{n-1})^2}{2} + \\ &+ \sum_n \alpha\frac{q_n^3}{3} + \beta\frac{q_n^4}{4}, \end{aligned} \tag{1}$$

where n runs from 0 to N in the case of Dirichlet boundary conditions (DBC), namely $q_0 = q_{N+1} = 0$, while it runs from $-(N+1)$ to N in the case of periodic boundary conditions (PBC), i.e. $q_{-N-1} = q_{N+1}$. With this choice the two system have the same frequencies (see (4) below). Moreover, *in the case* $\alpha = 0$ the system with DBC can be considered as a subsystem of the system with PBC, as it is seen by extending a sequence with DBC on $[0, N]$ to a skew symmetric periodic sequence on $[-(N+1), N]$.

To understand heuristically the behaviour of the system and the influence of boundary conditions, consider long wavelength initial data and an interpolating function u for the lattice, namely a function such that $u(\mu j) = q_j$, with $\mu \sim \frac{1}{N}$ being the discretization parameter. At first order, the equation for the interpolating function takes the form

$$u_{tt} = -u + a\mu^2 u_{xx} - \alpha u^2 \ . \tag{2}$$

Such an equation has a completely different behaviour in the case of periodic or Dirichlet boundary conditions. Indeed, in the first case its dynamics is well posed in spaces of smooth functions, and thus one has a fast decay of the Fourier coefficients. On the contrary, in the second case the solution has only a finite smoothness. Correspondingly, in the case of DBC, the energy quickly flows to high frequency modes. We remark that in the case of the β model no such phenomenon appears.

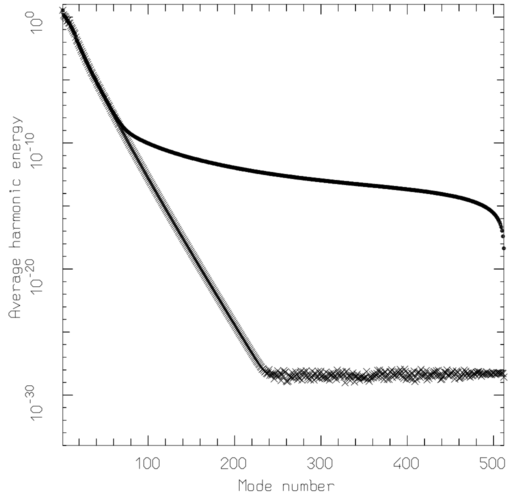

Figure 1: Averaged harmonic energies distribution. DBC (dots) and PBC (crosses) with $N = 511$, $a = .5$, $\alpha = \beta = 0.25$, $\epsilon = 0.01$, $T = 10^5$.

We will show that in the model (1) the limit distribution decreases exponentially in the case of periodic boundary conditions. In the case of the α model with Dirichlet boundary conditions, the limit distribution presents a first part which is still exponential with a slope dependent on the energy density ϵ, and a second part whose decay is close to $|k|^{-6}$ and thus with slope independent of ϵ.

2 The results

Introducing the variables of the normal modes the Hamiltonian takes the form

$$H(\hat{q},\hat{p}) := \sum_k \frac{\hat{p}_k^2 + \omega_k^2\hat{q}_k^2}{2} + \alpha H_3(\hat{q}) + \beta H_4(\hat{q}) \tag{3}$$

where k runs from 1 to N in the DBC case, and again from $-(N+1)$ to N in the PBC case. The frequencies ω_k have the same law for both the boundary conditions, indeed

$$\omega_k^2 = 1 + 4a\sin^2\left(\frac{k\pi}{2N+2}\right). \tag{4}$$

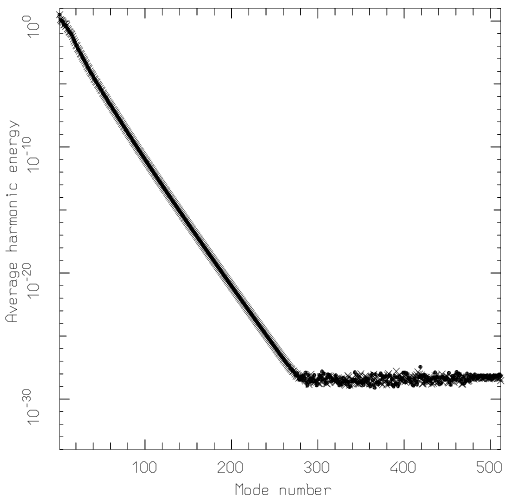

Figure 2: Averaged harmonic energies distribution. DBC (dots) and PBC (crosses) with $N = 511$, $a = .5$, $\beta = 0.25$, $\epsilon = 0.01$, $T = 10^5$.

In both cases define the energy of the normal mode by

$$E_k(t) := \frac{\hat{p}_k^2 + \omega_k^2 \hat{q}_k^2}{2},$$

and its time average by

$$\langle E_k \rangle(t) = \frac{1}{t} \int_0^t E_k(s) ds \ .$$

In the case of PBC the oscillators of index k and $-k$ are in resonance, so the relevant quantity to be observed is the average $\overline{\langle E_k \rangle} = \frac{1}{2}(\langle E_k \rangle + \langle E_{-k} \rangle)$.

We take an initial data with small specific energy concentrated only on the first Fourier mode. As we will show in the appendix the corresponding dynamics involves only modes with odd index. For this reason in the figures we plot only odd modes[1]. After a short transient the quantities $\langle E_k \rangle(t)$ relax to a well defined distribution that persists for long times as in the Fermi Pasta Ulam experiment.

In figures 1 and 2 we plot in a semilog scale the time average of the energy at time $T = 10^5$ as a function of the index of the mode for the α and β models. In each figure the dots refer to the DBC case while the crosses pertains the PBC one.

While in figure 2 one clearly observes a perfect overlapping of the exponential part of the decays, in figure 1 a sharp difference arises. Indeed, while the PBC solution is once more characterised by an exponential distribution, in the case of DBC one sees a reacher behaviour: at an energy approximatively equal to 10^{-8} there is crossover and a new regime presenting what we will show to be a power low decay appears[2]. Nevertheless, a striking similarity among the exponential part of the two dynamics is evident; the explanation of such a fact can probably be obtained by the methods of [1], but at present we do not have definitive results.

To describe more carefully the regime of the high frequency modes in the case of Dirichlet BC we plot in figures 3 and 4 four different distributions of the quantities $\langle \mathcal{E}_k \rangle = \frac{\langle E_k \rangle}{\sqrt{N+1}}$, respectively in a semilog and in a log-log scale. They corresponds to different values of the energy density. In the first one we plot the first part of the distribution: we notice that by decreasing the energy density, the slope of the exponential decay of the low frequencies increases. In the second figure, instead, we focus our attention on the second part of the distribution: we see that the corresponding curves are parallel. Except for the last part (due to discreteness effects) the curves are very well interpolated by a straight line giving a power decay with an exponent close to -6, therefore of the form k^{-6}.

To understand the behaviour k^{-6} consider equation (2). First remark that in the continuum limit the normal modes are given by the sins, and in particular the first Fourier mode is $\sin x$. Now, put such a normal mode in the r.h.s. of (2), i.e. compute $\sin^2 x$ and expand again on the basis of the Fourier modes *i.e. the functions* $\sin(kx)$. A direct computation shows that such Fourier coefficients decay as k^{-3} showing that the $k-$th Fourier mode, in the case of

[1]If one excites two modes then the dynamics involves all the Fourier modes, but the figures turn out to be less clean. In the appendix we will briefly discuss the corresponding figures

[2]If one increases the value of a also a resonant peak as in [6] appears. Since we are not interested in this kind of phenomenon we decided to use $a = 1/2$. Indeed, the theory of [6] easily predicts that the peak cannot appear for such value of a.

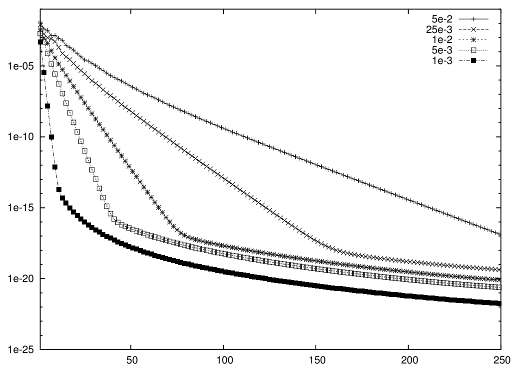

Figure 3: Averaged harmonic energies distribution in semilog scale. DBC with parameters: $N = 511, a = 0.5, \alpha = 0.1, T = 10^5$. Energies: $\epsilon = 0.05, 0.025, 0.01, 0.005, 0.001$.

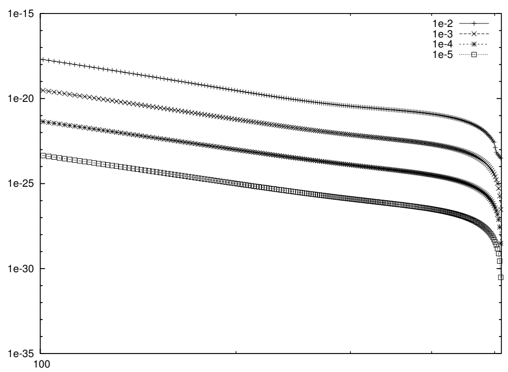

Figure 4: Averaged harmonic energies distribution in log-log scale. DBC with parameters: $N = 511, a = 0.5, \alpha = 0.1, T = 10^5$. Energies: $\epsilon = 0.01, 0.001, 0.0001, 0.00001$.

Dirichlet BC is forced in a way proportional to k^{-3}. This is the heuristic explanation of the k^{-6} behaviour of the energies.

3 Conclusion

In this letter we have shown that in a one dimensional lattice of coupled particles the boundary conditions can have a strong effect on the so called FPU paradox. In particular we have shown that in our model the energy flows to high frequencies in a completely different way according to the boundary conditions. We gave a partial heuristic description of this phenomenon through the finite regularity of solutions of an approximating PDE. However, we gave no explanation of the fact that also in the case of Dirichlet BC there is a first part of the spectrum which is exponential decreasing. Work is in progress.

A final consideration pertains the relation of this work with the investigation of the FPU phenomenon in a 2D lattice. First we remark that our results are in agreement with the previous ones, according to which the case of DBC is more unstable than the case of PBC. Furthermore, we think that in higher dimensions the mechanism that we found responsible for the quick flow of energy to high frequency modes should be much more general than in one dimension. The main reason is that what prevents such a mechanism to be active in the original 1-d FPU model is the fact that such a model naturally embeds into a longer lattice with periodic boundary conditions. This is clearly exceptional in higher dimensional domains with arbitrary geometry.

Moreover, we think that the way the boundary affects the solution's regularity could lead to dramatic effects in higher dimension. This is due to the fact that in PDEs, there is a minimal smoothness required in order to ensure existence and uniqueness of solutions, and such smoothness, which depends on the space dimension could be distroyed by the boundary effects. A possible consequence is that the FPU paradox may disappear in sufficiently high dimension *when some kind of boundary conditions are imposed*. We would like also to emphasise that the phenomenon we put into evidence here is *a boundary effect*, so that it is not clear whether it is relevant or not for the study of the thermalization problem. In particular we think that our results clearly shows that a good choice of the boundary conditions is very important for the study of the thermalization problem.

4 Appendix A. The invariant manifold of odd modes.

Consider the continuous limit equation (2) with DBC: split $u = p + d$, where p can have only Fourier coefficients on $\sin(2kx)$ while d has only Fourier coefficients on $\sin((2k+1)x)$. Correspondingly equation (2) is equivalent to the system

$$\begin{cases} p_{tt} = -p + a\mu^2 p_{xx} - \alpha 2pd, \\ d_{tt} = -d + a\mu^2 d_{xx} - \alpha(p^2 + d^2), \end{cases} \tag{5}$$

from which one sees that if $p = 0$ at $t = 0$ then one has $p(t) = 0$ for all t's. The contrary is not true. So, if instead of what we did in the main body of the paper one considers initial data in which the first two Fourier modes are excited, then the corresponding solution involves all Fourier modes. In fig. 5 we show the typical result of a computation obtained exciting the second mode only, in order to emphasise the effect. One sees in particular that even and odd modes relax to qualitatively identical distributions which however are quantitatively slightly separated. Due to this the figures one obtains by exciting two Fourier modes are less clean than those obtained by exciting only the first one. For this reason, and since our main interest is to put into evidence boundary effects, we decided to plot only odds modes.

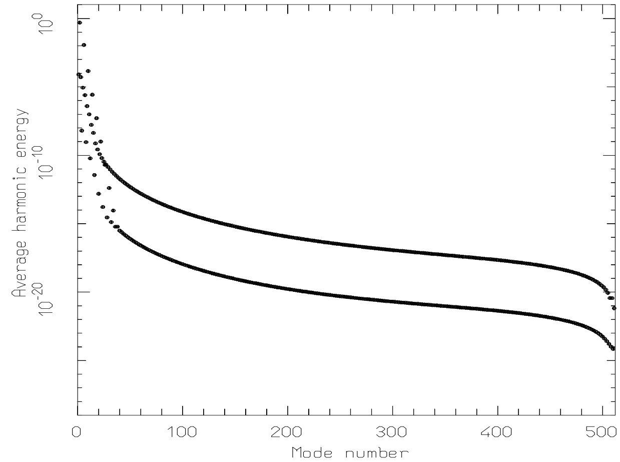

Figure 5: Average harmonic energy distribution, second mode initially excited. DBC with $N = 511$, $a = 0.5$, $\alpha = .25$, $\epsilon = 0.001$, $T = 10^5$.

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