

A first study of the Fermi-Pasta-Ulam problem

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1 Introduction

The Fermi-Pasta-Ulam (FPU) experiment is a classical problem in nonlinear physics. The unexpected results obtained by the three scientists triggered a whole new interest in classical physics, which eventually led to the development of dynamical chaos theories and the integrability of some nonlinear equations.

As it will be discussed, the FPU problem is also relevant from the point of view of statistical mechanics. Fermi himself was interested in proving the ergodic hypothesis which lies at the basis of classical statistical mechanics.

Moreover, the development of nonlinear physics stimulated the use of computers to study the behavior of many-body systems and/or complex systems in general. FPU were among the first to perform *experiments* on a computer: this idea is now commonly accepted and scientists and mathematicians do use the tools of computer science to investigate problems otherwise unsolvable analytically.

The interest here is in the 32-particle chain with both fixed and free ends. A small computer code has been written to simulate this system and reproduce the original results obtained by FPU in their seminal paper appeared in 1955 [3]. The role of time integration has been studied. Two algorithms have been implemented:

a *standard* velocity Verlet scheme and a fourth order symplectic scheme (Forest-Ruth). The influence of the parameter that governs the strength of the nonlinearity has also been addressed, especially with respect to some analytical results [2] for its critical value. The fundamental importance of the initial conditions imposed on the system with respect to its chaotic behavior are also stressed, along with the identification of a stochasticity threshold [6], that successfully explained the FPU paradox.

2 The FPU system

The FPU system simply consisted of a linear chain of particles which interacted with their nearest neighbor only by elastic springs. The ends are kept fixed. The interatomic forces had a linear component determined by the constant χ . The potential energy was therefore given by

$$V(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^N \sum_{j \in nn(i)} \chi(x_i - x_j)^2, \quad (1)$$

where $\mathbf{x} \equiv \{x_1, x_2, \dots, x_N\}$, being $N = 32$ for all simulations performed here. x_i is the displacement of the i -th particle from its original position; $nn(i)$ is the set containing the nearest neighbors of particle i .

The idea of FPU was to modify the potential energy for the system to include a cubic or a fourth order term:

$$V(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^N \sum_{j \in nn(i)} \chi(x_i - x_j)^2 + \frac{1}{2} \sum_{i=1}^N \sum_{j \in nn(i)} \frac{\alpha}{3} (x_i - x_j)^3, \quad (2)$$

$$V(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^N \sum_{j \in nn(i)} \chi(x_i - x_j)^2 + \frac{1}{2} \sum_{i=1}^N \sum_{j \in nn(i)} \frac{\beta}{4} (x_i - x_j)^4. \quad (3)$$

The resulting equations of motion for the two models (respectively the α - and β -model) are:

$$\ddot{x}_i = (x_{i+1} - 2x_i + x_{i-1}) + \alpha[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2], \quad (4)$$

$$\ddot{x}_i = (x_{i+1} - 2x_i + x_{i-1}) + \beta[(x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3], \quad (5)$$

where the double dotted quantities are double derivatives with respect to time, and m and χ are taken unity. Equations (4) or (5) are then integrated and the evolution of the system is tracked. This was indeed one of the first MD simulations performed ever.

When the potential energy is given by eq. (1), the system is simply a collection of independent harmonic oscillators. The exact solution for the equations of motion can be then expressed as a superposition of normal (or fundamental) modes $Q_k(t)$:

$$Q_k(t) = \sqrt{\frac{2}{N}} \sum_{i=1}^N x_i(t) \sin\left(\frac{\pi ki}{N}\right), \quad (6)$$

which can be viewed as a Fourier (sine) transform of the displacements $x_i(t)$. Given the initial conditions $x_i(0)$ and $\dot{x}_i(0)$, the energy *stored* in a mode k is expressed as:

$$E_k = \frac{1}{2}(\dot{Q}_k^2 + \omega_k^2 Q_k^2), \quad (7)$$

whereas the equations of motion (in this normal mode representation) are given by

$$\ddot{Q}_k + \omega_k^2 Q_k = 0. \quad (8)$$

Equations (7) and (8) show that the model is integrable and energy sharing between normal modes is not allowed. The motion of the system is periodic in time

with the discrete spectrum (eigenfrequencies) given by[2]

$$\omega_k = 2\sin\left(\frac{\pi k}{2N}\right), \quad (9)$$

with $k \in \{1, 2, \dots, N\}$.

By adding a weak nonlinearity, FPU expected that the system would exhibit an ergodic behavior. In particular, their belief was that energy initially stored in a particular (linear) mode Q_k , would be eventually transferred to all other modes, hence revealing a transition to thermal equilibrium.

When a nonlinear interaction is present, equation (8) is modified in the following way (for the α -model the result is similar [2])

$$\ddot{Q}_k + \omega_k^2 Q_k = \beta \sum_{i,j,k=1}^N D_{ijk} Q_i Q_j Q_k, \quad (10)$$

where D_{ijk} [4] are complicated coefficients that show the coupling between the i -, j -, and k -th modes.

3 Results

Equation (4) or (5) were integrated in 1955 on the computer MANIAC available at LLNL. Here, a small code has been developed to integrate eq. (5), which will be the only one considered. The system is composed of 32 particles. The ends of the chain are kept either fixed or free. Only sinusoidal normal modes are allowed for the linear system¹, i.e., either superposition of pure sines or cosines (respectively for fixed and free ends). Along with much of the literature on this problem, k and m

¹Here and in the following discussion, the adjective linear is referred to the nature of the springs and not the space dimensionality of the system, that being 1D.

are set unity. The particles are initially given a displacement according to the first fundamental mode²

$$x_i(0) = A\sqrt{\frac{2}{N+1}}\sin\left(\frac{\pi ki}{N+1}\right) \quad (11)$$

for fixed ends, and

$$x_i(0) = A\sqrt{\frac{2}{N+1}}\cos\left(\frac{\pi ki}{N+1}\right) \quad (12)$$

for free ends, where A is set equal to 10.0 units of length. The time step Δt is set to 0.05 units of time.

The eigenmodes and their corresponding eigenfrequencies are evaluated by solving the classical eigenproblem numerically [1]:

$$-m\frac{\omega^2}{\omega_0^2} a_i = K_{ij}a_j, \quad (13)$$

where $\omega_0 = \sqrt{2k/m}$, \mathbf{K} is the dynamical matrix for the linear system, and \mathbf{a} are the eigenvectors ($i = 1, 2, \dots, N-1, N$). Figure (1) shows the excited ground eigenmode for the free- and fixed-end chain, while in figure (2) the eigenfrequencies as a function of the mode index can be seen, for the case of fixed-end chain.

A first simulation has been performed setting $\beta = 0.3$, using a simple integration scheme, known as velocity Verlet. The equations of motion were integrated for more than 500 periods³ of the ground mode. As it can be seen in figures (3) and (4), the total energy of the system E_{tot} , initially stored entirely in the ground mode (E_k , with $k = 1$), rapidly flows into modes $k = 3$ and $k = 5$. This would not be surprising, and it was something FPU expected, as it was supposed that energy would get partitioned among all the modes allowed for the system. Two things are,

²Eq. (11) and (12) are continuum solutions, i.e., when N is very large. That is why the fundamental modes are calculated numerically. See what follows.

³The period of any (linear) mode is $T_k = 2\pi/\omega_k$, with $\omega_k = 2\sin\left(\frac{\pi k}{2N}\right)$. In all the figures, time is scaled with $T = \frac{2\pi}{\omega_0}$ where $\omega_0 = \sqrt{2k/m}$.

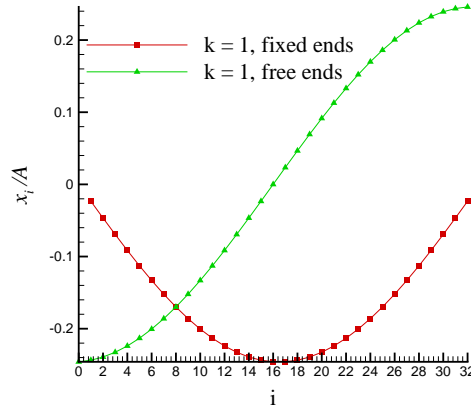


Figure 1: Excited ground mode for the free- and fixed-end chain.

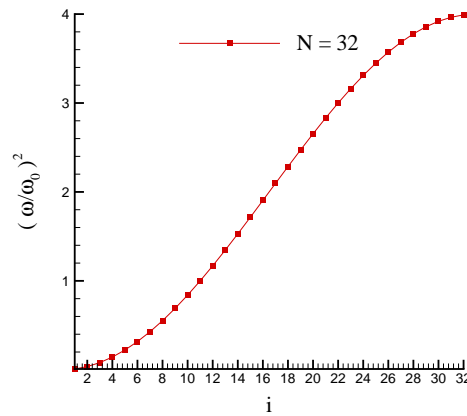


Figure 2: Eigenfrequencies as a function of the mode number.

however, *suspicious*:

- the energy starts flowing into only the odd modes, leaving the even modes empty (within the accuracy imposed by the integration scheme);
- the energy returns almost entirely into the ground mode within a thousand periods. Moreover, this trend is recurrent, revealing a quasi-periodic behavior for the system.

This simple simulation did trigger a great interest in this problem. However, the very first attempts to explain it were aimed at *trivializing* the results of the simulations. In particular, the accuracy of the numerics was questioned. It was in fact observed that only a fraction of the energy (even though a large fraction, as it can be seen in figures (3) and (4)) would return in the first mode. It can also be noted that the

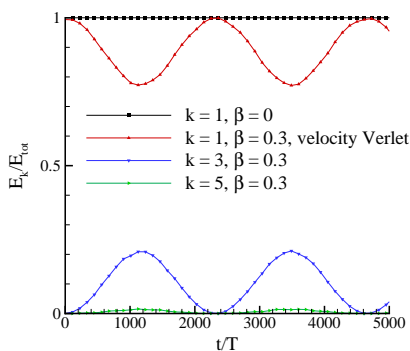


Figure 3: Energy per mode of a fixed-end chain of 32 atoms for $\beta = 0.3$.

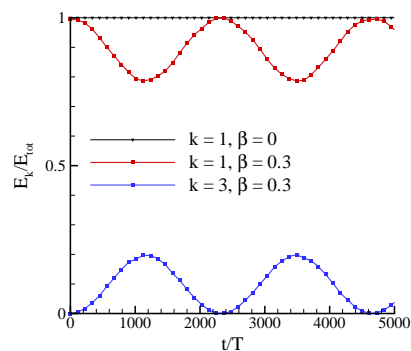


Figure 4: Energy per mode of a free-end chain of 32 atoms for $\beta = 0.3$.

results for the free-end and fixed-end chains are qualitatively the same.

Tuck in 1961 [5] performed more accurate computations, revealing the existence of a *super period* of about 80000 linear cycles, T_1 . More than 99% of the energy would go back into the first mode after this super period.

A similar investigation has been performed here. In particular, a higher order scheme was implemented and compared with the traditional velocity Verlet. The Forest-Ruth algorithm is a 4th order integration scheme, which is symplectic (i.e., it preserves energy), but highly intensive from a computational viewpoint. To integrate the equations of motion (5) over a time step Δt , four force calculations are required. As well known, the heaviest part of any MD code is the force calculation for each particle.

Results obtained and shown in figure (5) reveal that the discrepancy between the

two algorithm is negligible and hardly detectable. Both reveal the same periodicity in the energy recurrence. This demonstrates that something more profound was to

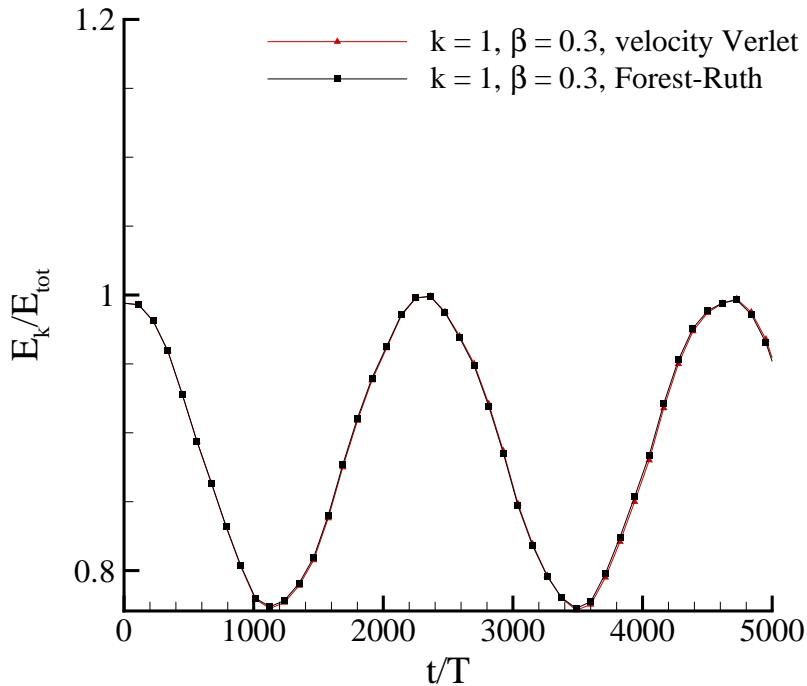


Figure 5: Comparison between velocity Verlet and Forest-Ruth integration schemes for a fixed-end chain of 32 atoms with $\beta = 0.3$.

be found in the behavior of the FPU system.

In particular, it was observed that upon increasing the strength of the nonlinearity, the sharing of energy between the modes becomes more and more important, as shown in figures (6) and (7) for $\beta = 1$. The results obtained are, however, qualitatively similar to those obtained previously, when $\beta = 0.3$. When setting $\beta = 3$, something dramatic happens. The energy suddenly fills all modes, being distributed among them. Two observations can be made, by looking at figures (8) and (9):

- even modes are now populated;

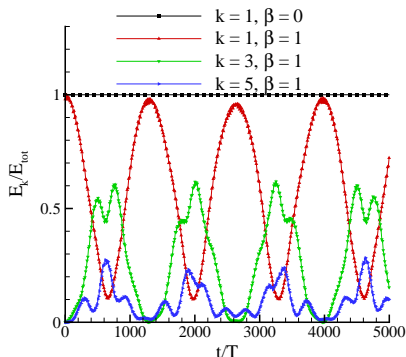


Figure 6: Energy per mode of a fixed-end chain of 32 atoms for $\beta = 1.0$.

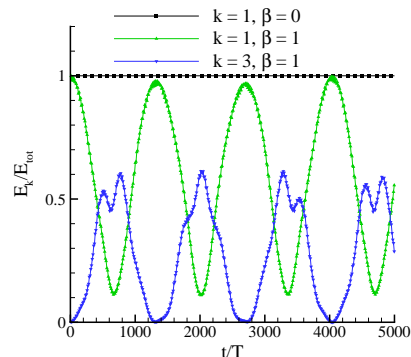


Figure 7: Energy per mode of a free-end chain of 32 atoms for $\beta = 1.0$.

- no (quasi-) periodicity can be observed: the behavior seems to be chaotic.

It also seems that the flow of energy from the initially excited mode to the other modes is faster in the fixed-end chain than in the free-end one. However, the two results are qualitatively similar.

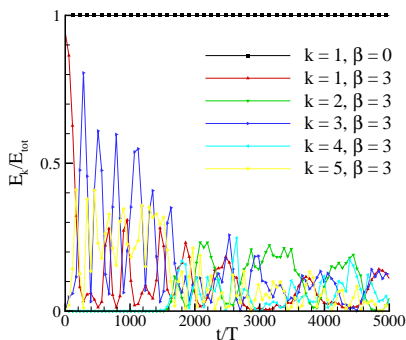


Figure 8: Energy per mode of a fixed-end chain of 32 atoms for $\beta = 3.0$.

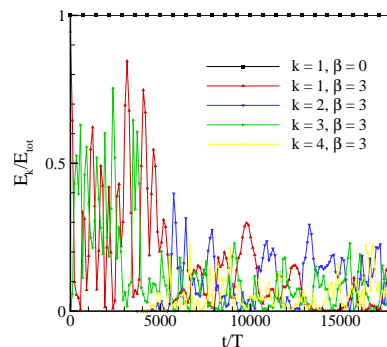


Figure 9: Energy per mode of a free-end chain of 32 atoms for $\beta = 3.0$.

Finally, as shown in figure (10), when $\beta = 3$ energy fills all modes, being almost evenly distributed among them (something that Fermi was expecting to see even for the lowest values of β). Analogous results are found for the free-end chain.

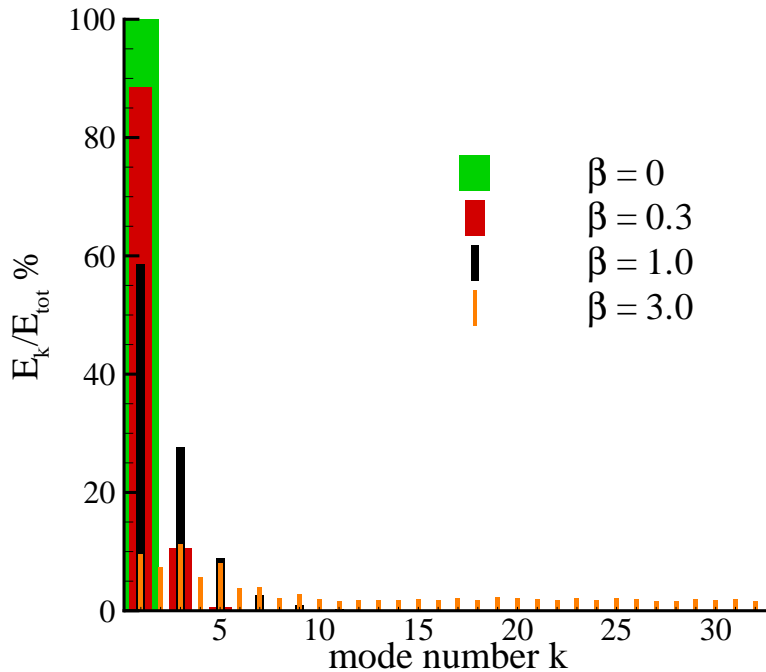


Figure 10: Energy spectrum for the fixed-end chain.

3.1 Dynamical chaos and the stochasticity *border*

Deterministic dynamical systems, like the FPU one, are reversible in principle. Reverting time leads the system to the initial conditions. This is true *analytically*, when no such considerations like the time integration accuracy and the round-off errors are taken into account (i.e., when the dynamics is traced on a computer⁴). However, some systems may exhibit an exponential sensitivity to the initial conditions. The separation $\Delta(t)$ between two neighboring phase space trajectories has an exponential growth $\Delta(t) \sim \Delta(0) \exp(ht)$ [2], where h is called *dynamical entropy*. For such systems, any small perturbation (for example due to the round-off error,

⁴As previously said, the FPU problem is relevant as it was a numerical experiment performed on one of the first computers ever built (the MANIAC, at LLNL in the early fifties), beside the theoretical aspects.

or a weak nonlinear interaction between the particles, like the FPU system) can not be neglected.

The analysis of the stability of motion for many-body problems led Chirikov [6] in 1959 to the identification of a so-called *stochasticity border* and a criterion to determine under which conditions dynamical chaos occurs in nonlinear systems.

The application of Chirikov's criterion to the FPU model allows the identification of a critical value for the strength of the nonlinear interaction β_{cr} [2]

$$3\beta_{cr}\frac{E}{N} \sim 3\frac{\sqrt{\Delta k}}{k}, \quad (14)$$

where E/N is the energy per normal mode and Δk is the number of initially excited modes around the central k -th mode.

This criterion successfully explained the FPU paradox. It turned out that when only the lowest mode is excited ($k = 1$, like in the original FPU simulation), only a strong perturbation can prevent the recurrent behavior observed by FPU, as shown by the computations performed here as well (see figures (3) or (4)). That means that the FPU model was *below* a stochasticity threshold, above which it would have shown the chaotic behavior that FPU had expected to see.

As shown by relation (14), if higher modes (k) are initially excited, one needs a weaker and weaker nonlinear perturbation for the system to reveal a chaotic behavior. Dynamical chaos is revealed and, therefore, the system can be characterized with statistical tools (from the statistical mechanics point of view, one could say that the system is ergodic).

Two simulations have been performed, now exciting the 3rd mode (see figure (11)), instead of the ground one ($k = 1$). As opposed to the results shown in figures (3) or (4), for $\beta = 0.3$ the FPU system now already lacks the recurrent

behavior exhibited when the ground mode was initially excited. Hence, a much

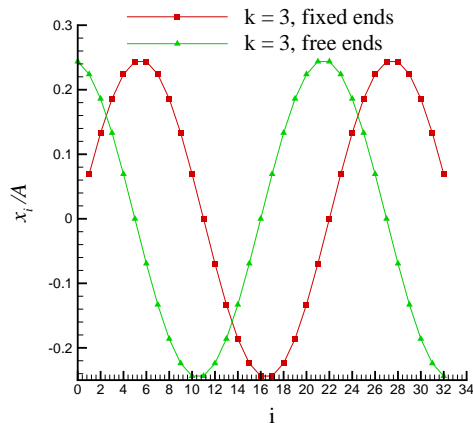


Figure 11: Mode $k = 3$ for the free- and fixed-end chain.

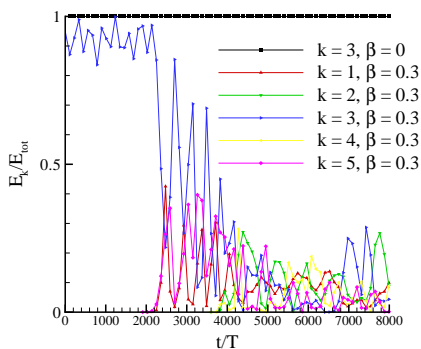


Figure 12: Energy per mode of a fixed-end chain of 32 atoms for $\beta = 0.3$, when the 3rd linear mode is initially excited.

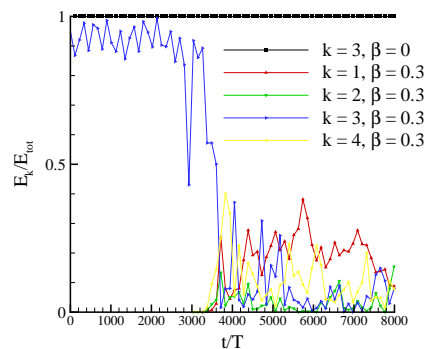


Figure 13: Energy per mode of a free-end chain of 32 atoms for $\beta = 0.3$, when the 3rd linear mode is initially excited.

smaller nonlinear perturbation was necessary to trigger a chaotic behavior: this is well predicted by relation (14). Moreover, the behavior of the chain is qualitatively the same, both with free and fixed ends.

Upon decreasing β to 0.1, one can still see an aperiodic behavior, even though it seems more regular than $\beta = 0.3$ during the first 10000 periods, with a strong return of the energy in the initial mode (figures (14) and (15)).

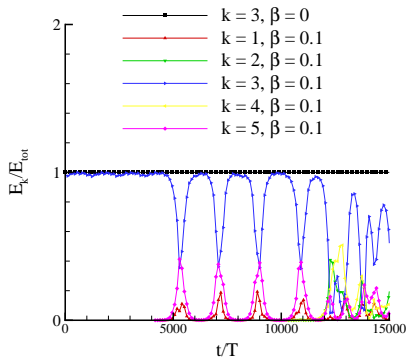


Figure 14: Energy per mode of a fixed-end chain of 32 atoms for $\beta = 0.1$, when the 3rd linear mode is initially excited.

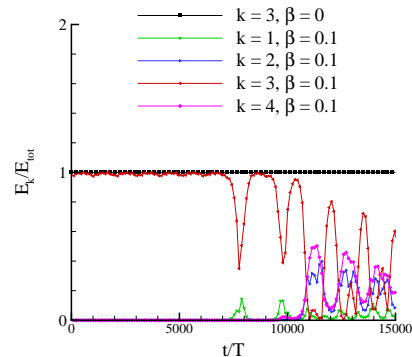


Figure 15: Energy per mode of a free-end chain of 32 atoms for $\beta = 0.1$, when the 3rd linear mode is initially excited.

Interestingly, when β is further decreased to 0.01, energy gets transferred from the initial mode ($k = 3$) at a faster rate, the periodicity of the recurrence in the energy back to the initial mode being shorter. However, the fraction of energy transferred to the other modes (not shown in figures (16) and (17)) is way smaller than the previous cases ($\simeq 0.1\%$).

This shows that the identification of the stochasticity threshold is hard to determine: as made clear in [2], “*the border of stochasticity between quasi-periodic and stochastic motion is not sharp. Rather, it is relatively wide and has a very complicated structure.*”

3.1.1 Linearly compressed chain

A particularly interesting case is when the free-end chain is linearly compressed. It is known that when the system is linear, any configuration can be expressed as a linear superposition of the fundamental modes.

The initial displacements are shown in figure (18). The overall compression of the chain is around 1.7%. The energy spectrum associated with this initial configuration

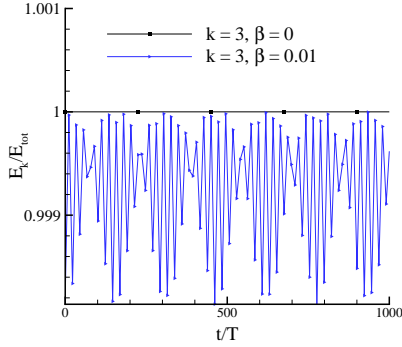


Figure 16: Energy per mode of a fixed-end chain of 32 atoms for $\beta = 0.01$, when the 3rd linear mode is initially excited.

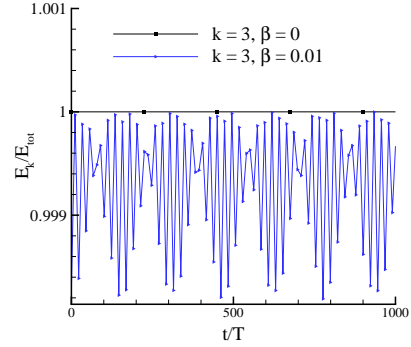


Figure 17: Energy per mode of a free-end chain of 32 atoms for $\beta = 0.01$, when the 3rd linear mode is initially excited.

is shown in figure (19): from there, it can be seen that most of the energy ($\simeq 80\%$) is stored in the first mode, with a non-negligible contribution from modes 3, 5, 7. Figure (19) also shows the energy spectrum when only modes 1, 3, 5 are excited (in such a way that the energy spectrum is similar to that of the linearly compressed chain).

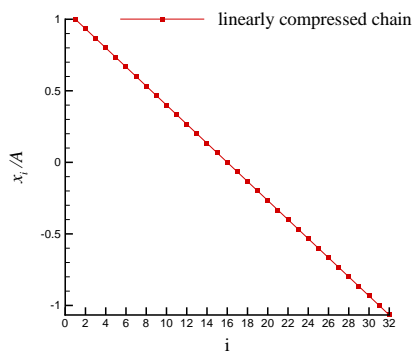


Figure 18: Initial configuration for the linearly compressed free-end chain of 32 atoms.

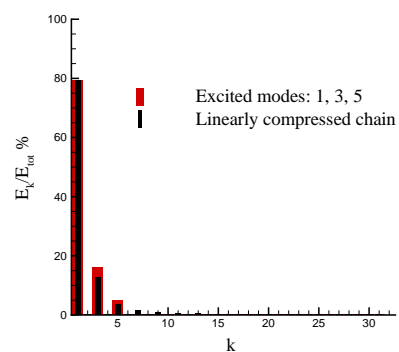


Figure 19: Energy spectrum of the linearly compressed free-end chain of 32 atoms.

Figure (20) shows the energy sharing between the modes: it can be seen that, despite the fact that higher modes are initially excited, the initial modes are pre-

served, and the system retains a recurrent behavior. That is because most of the energy is initially stored in the ground mode, being the excitation of higher modes insufficient to trigger a chaotic behavior for the system. Moreover, the behavior of the system is comparable to the same system when only modes 1, 3 and 5 are excited, with the same value for β (see figures (20) and (21)).

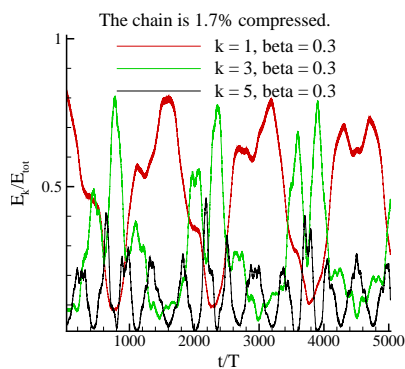


Figure 20: Energy per mode of a free-end linearly compressed chain of 32 atoms for $\beta = 0.3$.

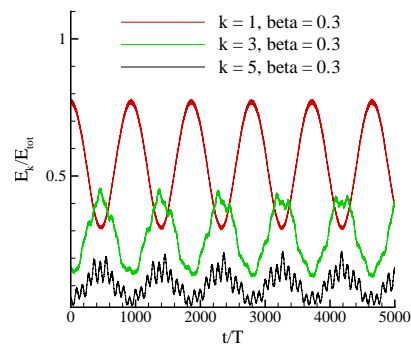


Figure 21: Energy per mode of a free-end chain of 32 atoms for $\beta = 0.3$, when only modes $k = 1, 3, 5$ are initially excited.

4 Summary and conclusions

Despite its (apparent) simplicity, the FPU model has posed many questions, many of which are still open today, after more than 50 years.

The simple computations developed here have shown that the 32-particle chain, both with free and fixed ends, in the presence of a weak nonlinear interaction shows a recurrent behavior, unexpected when looking at equation (10). In fact, FPU were expecting a flow of energy from the initially excited mode, to all the modes allowed for the system. Fermi wanted to use this result to further study the problem of thermal equilibrium with respect to the ergodic problem, which he tried, unsuccessfully, to prove rigorously.

The simulations performed here show, instead, a recurrent behavior of the energy flow from the ground mode to the higher modes. Energy gets first transferred to higher modes: given sufficient time, though, it flows almost entirely back into the initially excited mode. This trend seems quasi-periodic. Calculations have also shown that the behavior of the chain is the same, independently of the boundary conditions, even though quantitative discrepancies can be observed. In particular, it seems that when higher modes are excited, stronger differences can be seen between the free- and fixed-end case.

The FPU paradox was successfully explained by using concepts which were being developed in the context of dynamical chaos. Chirikov's criterion to determine a so-called *stochasticity threshold* was successfully applied to the FPU model. It also shed light on the strong influence of the initial conditions on the chaotic (or recurrent) behavior of the FPU system.

The application of Chirikov theory leads to the identification of a critical parameter (β_{cr}), which is tightly related to the initially excited mode (14): when $\beta < \beta_{cr}$ the model has a quasi-periodic behavior. As calculations performed here have shown, when the initially excited mode is higher than the ground one, one finds a smaller β_{cr} . Hence, smaller values for β are necessary to trigger a chaotic behavior, in agreement with equation (14).

As previously said, this problem has still many unanswered questions. For example, it is still unclear if it is possible to identify a *weak chaos border* for systems in the limit $N \rightarrow \infty$ [2].

This problem can also be extended to more complex geometries to study vibrational modes: for example, nanotubes hit by laser pulses, breathers in crystals, and nanostructures in general. Even though the mathematics is extremely complicated, and often no analytical solutions are available, the FPU has taught us that computer

science and numerical modeling can be used as predictive tools, often unveiling new and unexpected results.

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