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Dependence of the Fermi-Pasta-Ulam Model on Initial Conditions and System Parameters towards Full Equipartition of Modal Energy

Abstract

We systematically studied the dependence of the Fermi-Pasta-Ulam (FPU) model on initial conditions and system parameters, and determine how they affected the tendency towards full equipartition of energy among Fourier modes. We found a critical energy density of approximately 0.1, above which the state of energy sharing among modes became independent of initial conditions and system parameters. Below the critical energy density, the dissipation of energy was sensitive to initialisation and parameters of a system. We observed that, in general, dissipation of mode energy was more effective with larger energy densities. However, as we increased the energy density beyond 0.1, we incomprehensively noticed a slight decline in such effectiveness. We concluded that full equipartition of mode energy is never attained in the FPU model.

Keywords : FPU, equipartition, trapping time, non-linearity

1. Introduction

In 1952, Enrico Fermi and his collaborators (4) were interested in studying non-linear systems through the use of electronic computing machines. Their plan was to start with a simple physical model and then study its long-time behaviour with the expectation that the calculations would provide some hints for a future theory to explain the energy-distribution behaviour in non-linear systems. A one-dimensional dynamical system of 64 point particles with forces containing non-linear terms between neighbours was chosen. This was then studied numerically on the Los Alamos computer MANIAC I. With the total energy initially stored in the first Fourier mode, Fermi *et al.* (4) anticipated that, after a certain time, the energy would be distributed evenly among all the modes, which would allow them to calculate the rate of equipartitioning. The result, however, turned out to be rather surprising because energy equipartition never took place. Instead, most of the energy (approximately 98%) was trapped in the first few Fourier modes with other modes rarely shared any significant energy *at all.* In 1961, the same problem was revisited for longer periods of time on more advanced machines by J. Tuck and M. Menzel (6, p. 28). They found that the total energy, which was initially placed in the first mode, would be gradually distributed to a few other modes, but after some time, most of the initial energy would be drawn back to the first mode again. This confirmed that the results obtained by Fermi *et al.* were not caused by calculational errors.

In this article, we present a brief description of the Fermi-Pasta-Ulam (FPU) model. After that, we proceed to look at the dependence of dissipation of mode energy on initial conditions and system parameters. Our aim is to determine 1) how initial conditions and system parameters affect the tendency towards full equipartition of mode energy, and 2) if such full equipartition is ever accomplished at all in the FPU model.

2. The Fermi-Pasta-Ulam Model

2.1 Potential and Force Functions

The FPU model represents a one-dimensional chain of particles (See Figure 1) interacting with their nearest neighbours via a smooth pair potential function u_{ij} defined by

$$u_{ij} = \frac{1}{2}k\left(r_{ij} - r_{ij}^{0}\right)^2 + \frac{1}{4}\beta k\left(r_{ij} - r_{ij}^{0}\right)^4,$$

where k is a spring constant and β is a non-linear coefficient. r_{ij} , where $i < j$, is the instantaneous separation between particles i and j, and r_{ij}^{0} is the separation at equilibrium. Letting q_i and q_j respectively be the displacements of particles i and j, we can express r_{ij} - r_{ij}^{0} as q_j-q_i.

Let us consider the forces acting on particle i. By definition, the force on par-

ticle i due to particle j is the negative of the rate of change of u_{ij} with respect

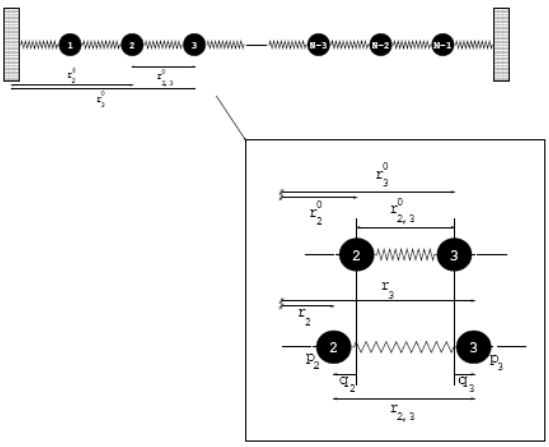

Figure 1 Schematic representation of the FPU model. Please note that the springs shown here are only schematic—they do not physically exist.

to an infinitesimal change in q_i while holding particle j fixed, i.e.

$$F_{i\leftarrow j} = -\frac{\partial u_{ij}}{\partial q_i} = k\left(q_j - q_i\right) + \beta k\left(q_j - q_i\right)^3$$

By a similar argument, the force on particle j due to i is

$$F_{j\leftarrow i} = -\frac{\partial u_{ij}}{\partial q_j} = -\left(k\left(q_j - q_i\right) + \beta k\left(q_j - q_i\right)^3\right) = -F_{i\leftarrow j} \ ,$$

Now, we can write the equations of motion of particle i as

$$\dot{q}_i = \frac{p_i}{m_i},$$
$$\dot{p}_i = F_i \ ,$$

where p_i is the momentum of particle i and $F_i = F_{i\leftarrow i-1} + F_{i\leftarrow i+1}$.

2.2 Normal Mode Transformation

If we imagine that each particle along a FPU chain represents a mass point along a string and that q_i represents a vertical displacement of each mass point, then we can visualise the FPU system as a string of a certain shape. Because the shape of a string can be understood in terms of normal (or Fourier) modes (6, p.19) among which Fermi *et al.* were interested in energy sharing, it becomes natural to present simulation results in terms of normal mode coordinates Q_k and their time derivatives $\dot{Q}_k$. We can transform any combination of particle displacements q_i to mode coordinates Q_k using the relationship

$$Q_k = \sqrt{\frac{2}{N}} \sum_{i=1}^{N-1} q_i \sin\left(\frac{ik\pi}{N}\right), k = 1,2,...,N-1.$$

Similarly, any combination of the time derivatives of particle displacements $\dot{q}_i$ can be transformed to the time derivatives

of mode coordinates $\dot{Q}_k$ by

$$\dot{Q}_k = \sqrt{\frac{2}{N}} \sum_{i=1}^{N-1} \dot{q}_i \sin\left(\frac{ik\pi}{N}\right), k = 1,2,..., N-1.$$

The total mode energy E^Q may be approximated as

$$E^Q \approx \sum_{k=1}^{N-1} \left[\frac{1}{2}\dot{Q}_k^2 + \frac{1}{2}\omega_k^2 Q_k^2 \right],$$

which is sufficiently accurate for small values of β's, and where $\omega_k = 2\sin\left(\frac{k\pi}{2N}\right)$ are the frequency of mode k.

2.3 Degrees of Energy Sharing among Modes

Throughout this work, we will be mainly interested in the degree of energy sharing among modes. We refer to the expression for the normalised effective number of modes containing energy, η^Q , as defined by (1), (2), (3) and (5), where

$$\eta^Q = \frac{1}{N-1} \exp\left(-\sum_{k=1}^{N-1} e_k \ln e_k \right)$$

where e_k is the normalised energy of mode k with $e_k = E_k^Q / \sum_{k=1}^{N=1} E_k^Q$. In this work, we define $\eta^Q \geq 0.90$ to be full equipartition.

2.4 Initial Conditions and System Parameters

We conduct computer simulation of a FPU system using two different types of initial conditions. The first one is the Kinetic Initial Condition (KIC) and the other is the Potential Initial Condition (PIC). For KIC, all particles are initially at their equilibrium positions $(q_i = 0)$ and every particle except particles 0 and N will be assigned a random momentum such that the total momentum of the system is zero and the total kinetic energy equals the total energy.[1] PIC, on the other hand, arranges the positions of particles such that at $t = 0$, the total potential energy equals the total energy of the system, leaving all particles with zero momentum $(p_i = 0)$[2] . PIC was the method chosen by (4) when they conducted their computer simulation. It is also possible to initialise a system such that its initial momentum distribution is Gaussian.[3] In this article, the symbol γ specifies the type of initial condition : $\gamma = 0$ for KIC, γ = G for KIC (Gaussian), and $\gamma = n$, where n is an integer ranging from 1 to $N - 1$, for PIC (single mode excitation).

Important system parameters are the following. The number of particles is repre-

[1] For KIC, the total energy of the system and the total kinetic energy of the system are equal at $t = 0$ because there is no contribution from potential energy.

[2] As there is no contribution from kinetic energy at $t = 0$, the total potential energy and the total energy of the system are equal.

[3] adapted from Carter's method available at http://www.bearcave.com/misl/misl_tech/wavelets/hurst/random.html

sented by N. The non-linear coefficient is β. The energy density is denoted by ε, where ε_{FPU} = 0.002 407 636 663 9 . . . (in reduced units) being the energy density used by (4). Numerical integration of Newtonian equations using Gear's 4th - order predictor-corrector algorithm is controlled by the number of time steps and the size of time step. For example, $t_{tot} = 8 \times 10^7$ @ 2.5×10^{-3} represents the number of time steps of 8×10^7 with the size of each step being 2.5×10^{-3} —the total simulation time of 2×10^5.

3. Results : Dependence of η^Q on System Parameters and Initial Conditions

We first revisited some of the simulations conducted by (4), using N = 32, $\varepsilon \geq \varepsilon_{FPU}$ and varying γ (plots not shown). When β = 0, a system is said to be harmonic (or linear) and no dissipation of mode energy is observed regardless of initial conditions and system parameters. Specifically, all energy initially assigned to certain modes is trapped only within those modes and no sharing of energy among them takes place. In such circumstances, the system trajectory is trapped or contained in a certain region of phase space, and revisits parts of the region in a highly-regular pattern. On the contrary, when anharmonicity or non-linearity is introduced into a system ($\beta > 0$), the trajectory of a system will eventually reach an irregular regime of phase space, where energy dissipation among all the modes begins to take place more readily.

We now look at how energy is distributed among modes whilst varying energy densities. We choose to study FPU systems with N = 32 and β = 1 and conduct the simulations for $t_{tot} = 8 \times 10^7$ @0.002 5, using various values of γ. For each system, we observe the time evolution of η^Q and take its time average over the last 2×10^5 time steps. We then plot η^Q versus ε as shown in Figure 2. Our choices of initial conditions include γ = 0 (black open circles), γ = 1 (red open triangles), γ = 16 (blue pluses), γ = 31 (darkgreen crosses) and γ = G (dark-red diamonds). The error bars associated with η^Q are also displayed. All lines joining adjacent data points are drawn as a guide only. The vertical line at $\varepsilon = \varepsilon_{FPU}$ represents the energy density historically used by (4). At the lowenergy end, single-mode excitations (γ = 1, 16 and 31) result in relatively small values of η^Q's, when compared against the KIC counterparts (γ = 0 and G). We observe that the values of η^Q's are not necessarily the maximum values these systems can attain.

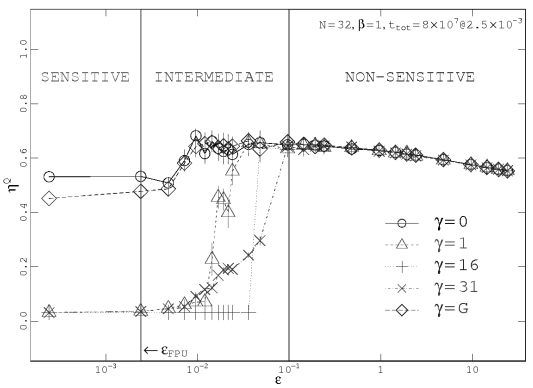

Figure 2 The sensitivity to initial conditions of η^Q at varying energy densities.

They are, as already mentioned, the averages over the last 2×10^5 computational steps. For some systems, the value η^Q displays a slowly-increasing trend when the simulation is terminated. Let us now go back to discuss other features of the figure. One of the most obvious features is the similarity between $\eta^Q_{\gamma=0}$ and $\eta^Q_{\gamma=G}$, especially when $\varepsilon > \varepsilon_{\mathrm{FPU}}$. For all initial conditions, a sudden rise in η^Q occurs approximately within the range $\varepsilon_{\mathrm{FPU}} < \varepsilon < 0.1$. Furthermore, above $\varepsilon = 0.1$, all η^Q's converge to the same value, regardless of the initial conditions. Within the range $\varepsilon_{\mathrm{FPU}} < \varepsilon < 0.1$, the dependence of η^Q on ε varies according to the initial conditions. It can be seen that, within this range, the systems with mode 16 initially excited show the strongest insensitivity to the change in ε until at $10\varepsilon_{\mathrm{FPU}}$,where $\eta^Q_{\gamma=16}$ abruptly jumps from around 0.03 to just above 0.6 over a relatively small range of energy densities. We are unable to identify any predictable pattern of how $\eta^Q(\varepsilon)$'s behave for systems with different initially-excited modes within this energy-density range. For the systems with KIC, $\eta^Q_{\gamma=0}$ and $\eta^Q_{\gamma=G}$ show a tendency to converge as ε becomes larger. Above $\varepsilon \approx 0.1$, the choice of initial conditions has no effect, and all η^Q's converge to the same value. There is a noticeable decreasing trend in the normalised effective number of modes containing energy as ε continues to increase above 0.1.

Our initial conditions can be divided into two groups. The first group is those with KIC, which include $\gamma = 0$ and G. The other group is those with PIC, namely, $\gamma = 1$, 16 and 31. For the KIC systems, the total energy is initially given to the motion of particles, as opposed to the configuration of particles for the PIC systems. According to Figure 2, when $\varepsilon \leq \varepsilon_{\mathrm{FPU}}$, a distinction can be readily identified between the two groups of initial conditions. The KIC systems exhibit a higher degree of energy sharing than the PIC counterparts. Again, we must emphasise that the systems have been observed for $t_{tot} = 8 \times 10^7$@0.002 5 due to our limitation of CPU resources. Longer observation times could have led to different results. One must keep this in mind when interpreting our results. Within the range $\varepsilon_{\mathrm{FPU}} < \varepsilon < 0.1$, the PIC systems reveal a sudden increase in the normalised effective number of modes containing enenergy. Then, $\eta^{\mathrm{Q}}_{\mathrm{PIC}}$'s reach a common plateau at approximately 0.65. Similarly for the KIC systems, a less dramatic rise $\eta^{\mathrm{Q}}_{\mathrm{KIC}}$ in is observed as ε becomes greater than $\varepsilon_{\mathrm{FPU}}$. Noticeably, the mode-energy sharing indices of the KIC systems reach the 0.65 plateau at a smaller value of energy density ($\varepsilon \approx 4\varepsilon_{\mathrm{FPU}}$), compared to the PIC systems. From these observations, we can divide our energy density into three ranges, according to the sensitivity to the initial conditions (KIC or PIC) of energy sharing among the modes. As shown in

the figure, the first range is when $0 < \varepsilon \leq \varepsilon_{FPU}$ and is marked 'SENSITIVE'. This is where a distinction can be easily made between the KIC and PIC systems. The second range is when $\varepsilon_{FPU} < \varepsilon < 0.1$ and is marked 'INTERMEDIATE'. This is where a clear distinction cannot be easily identified between the two groups of initial conditions, and where η^Q's begin to reach a common plateau at around 0.65. The third and last range is when $\varepsilon \geq 0.1$ and is marked 'NON-SENSITIVE'. Here, it does not matter how the systems are initialised; they all exhibit the same degrees of energy sharing among the modes. The most common feature of these figures is that, as ε increases, the normalised effective number of modes containing energy also increases until it reaches a common plateau. The time required to reach the plateau is inversely proportional to the energy density, as illustrated in Figure 3. Moreover,

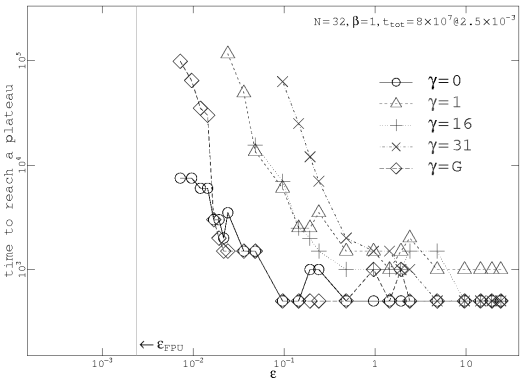

Figure 3 Time required for η^Q to reach a plateau as a function of ε.

trapping times[4] tend to be extensively long in low energy systems ($\varepsilon \leq \varepsilon_{FPU}$), as their trajectories are likely trapped in a regular regime of phase space, similar to those of harmonic systems (those with $\beta = 0$). Once a system trajectory has escaped from the regular regime and moved into an irregular regime, energy sharing among the modes starts to take place more effectively. An escape to the irregular regime tends to occur sooner in a more energetic system, hence a shorter trapping time. For all the systems which we studied, full equipartition of mode energy is never realised, and there is no tendency for η^Q to rise above the plateau of 0.65. One might argue that sufficientlylonger simulations could prove otherwise. We are inclined to believe, nevertheless, that the FPU model cannot support any higher degree of energy sharing among the modes no matter how long we conduct our simulations for, judging from the asymptotic behaviour of η^Q (t) at high energies (plots not shown).

[4] We must emphasise that the term 'trapping time' has a different meaning from 'time to reach a plateau'. Trapping time refers to the time a system trajectory spends in a regular regime of phase space. Once such trapping ceases, energy sharing starts to take place and usually η^Q has a tendency to increase with time until it reaches a plateau and fluctuates around that value. We refer to such a point in time as the time to reach a plateau. For a harmonic system ($\beta = 0$), trapping time is infinite; therefore, time to reach a plateau is not defined.

Another important question requires our attention. What happens to the dissipation of mode energy in the thermodynamic limit, where $N \rightarrow \infty$? We can seek answers to the following more specific questions of large-N behaviour: (i) keeping the excitation amplitude constant, what happens to $\eta^{Q}(\varepsilon)$ as N increases, and (ii) for kinetic initial conditions, how $\eta^{Q}(\varepsilon)$ behaves as N increases. To answer the first question, we vary N and γ systematically such that the ratio γ/N is kept at 1/16, ensuring a constant excitation amplitude. Specifically, our choices of γ/N are 1/16 (black open circles in Figure 4), 2/32 (red open triangles), 4/64 (blue pluses) and 8/128 (dark-green crosses). For generality, we use β = 1

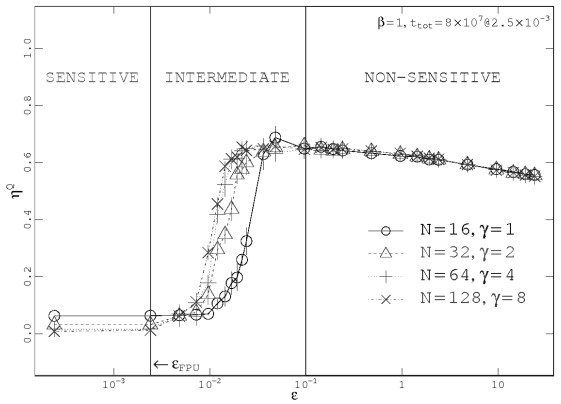

Figure 4 The thermodynamic-limit behaviour of η^{Q} (ε) at a fixed excitation amplitude and β = 1.

and t_{tot} = 8 × 10^{7} @0.002 5. At low energy densities ($\varepsilon \leq \varepsilon_{FPU}$), smaller systems tend to have slightly more rapid dissipation of energy among the modes. As ε increases, the trend reverses, and large systems have higher values of η^{Q}'s, and faster increases of η^{Q}'s as a function of ε. When ε reaches 0.1 and above, all mode-energy sharing indices become saturated at approximately 0.65 and gradually start to decrease as ε increases. To answer the second question, we study KIC systems with γ = 0, β = 1 and the same t_{tot}, while varying the number of particles. The results are reported in Figure 5 for N = 16 (black open circles), 32 (red open triangles) and 64 (blue pluses). At low energy densities

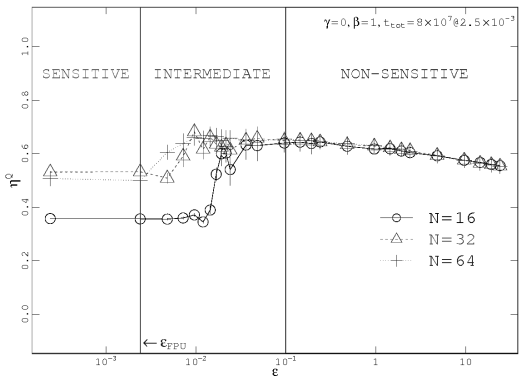

Figure 5 The thermodynamic-limit behaviour of η^{Q} (ε) for KIC systems with γ = 0 and β = 1.

($\varepsilon \leq \varepsilon_{FPU}$), the systems with N = 16 show the smallest degrees of energy sharing among the modes at around η^{Q} = 0.35, whilst those with N = 32 and 64 have essentially similar values that lie between 0.50 and 0.53 Within the intermediate energy range, the dissipation of mode energy becomes noticeably better for all

N 's as ε increases and eventually reach a common plateau at approximately 0.65, with larger systems generally being the first to reach the plateau. Again, there is an obvious convergence of all η^{Q}_{PIC} 's when $\varepsilon \geq 0.1$, with a slight decline in the values at increasing ε.

From our results, it is obvious that, above ε = 0.1, there is a saturation effect in the dissipation of energy among the modes. Regardless of the values of N , γ, β or ε , the normalised effective number of modes containing energy never exceeds 0.65. Incomprehensibly, there is a slight, yet noticeable, decline in η^{Q} as ε increases beyond 0.1, We further deduce that it is most appropriate to study the thermodynamic-limit behaviour of the FPU model at $\varepsilon \geq 0.1$, as we know that the dissipation of mode energy in systems at such energy densities will be essentially independent of initial conditions and system parameters. (4) had $\varepsilon \approx 0.0024$ and a simulation time that was too short for the true behaviour of energy dissipation among the modes to be revealed. They, however, were not incorrect in concluding that the full equipartition of mode energy was never realised.

4. Summary

Let us recapitulate what we have done in this article. Earlier, we gave a brief history of the FPU model. We then studied the dependence of η^{Q} on initial conditions and system parameters. We found that anharmonicity was a crucial ingredient for a system trajectory to eventually reach an irregular regime of phase space, where energy dissipation occurred more readily, albeit after a long time. We believed that Fermi and his collaborators did not observe their systems for sufficiently-long times to be able to identify the termination of the quasi-periodicity in their systems. Then, by studying the dependence of η^{Q} on the energy density, we were able to identify the critical energy density of approximately 0.1, above which η^{Q} became independent of N , γ , β , and ε. We also identified what seemed to be the upper limit of the state ofenergy dissipation among the modes at approximately η^{Q} = 0.65, verifying that Fermi and his collaborators were not incorrect when concluding that the full equipartition of mode energy was never attained. We cannot explain the slight decline in η^{Q} as ε increases beyond 0.1. For future work, we plan to conduct simulations with a mixture of kinetic and potential initialisation, instead of pure kinetic and pure potential initial conditions as we did in this work.

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