Fermi Ulam Pasta problem : A Numerical Experiment

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Abstract

This work is written as term paper done on Fermi Ulam and Pasta (FPU) problem. FPU problem is supposed to be one of the experiments which gave birth to the idea that computer simulations can play important part in understanding physical phenomena. This problem raised many puzzlels, many of which are not solved yet. The problem was reported in a Los Alamos report in May 1955 by Fermi Ulam and Pasta. It took almost 10 years to solve the so called FPU paradox, meanwhile giving birth to non-linear dynamics. In this report, first the FPU paradox will be discussed, followed by the solution to the paradox. Then, the numerical results for α and β models for FPU problem will be presented, followed by the discussion on further perspectives.

1 Introduction

Around 1950s, Enrico Fermi, John Pasta and Stanislaw Ulam were looking for a theoretical problem suitable for investigation with one of the first computers, MANIAC (Mathematical Analyzer, Numerical Integrator and Computer), which was originally built in 1952 for the Manhattan project,i.e., for the development of first hydrogen bomb. This work, which was just finished before Fermi's death in 1954, was published as Los Alamos Scientific Laboratory released technical report LA-1940, titled 'Studies of Nonlinear Problems' Authored by Enrico Fermi, John Pasta and Stanislaw Ulam. The problem they were considering was to study the ergodic properties of a linear chain of masses coupled through anharmonic springs. The idea came from Fermi who proposed to prove the ergodic hypothesis, which lies at the core of traditional statistical mechanics. The basic idea was that, in an harmonic system all normal modes are independent and hence, there is no drift of energy from one mode to another. However, an anharmonic system can allow such drift. It was expected, that if one initializes the system with a single mode, then due to anharmonic coupling terms, energy will start drifting to other modes, until equipartition of energy is achieved. However, the results they saw were totally unexpected, as we will see later. However, it is wort mentioning that, the same problem was being studied independently in 1960s by Nobohiko Saito and his PhD student Hajime Hirooka, and the result they got were similar to FPU result.

2 FPU paradox

The original idea, proposed by Enrico Fermi, was to simulate the one-dimensional analogue of atoms in a crystal: a long chain of particles linked by springs that obey Hooke's law (a linear interaction), but with a weak nonlinear (quadratic or quartic) correction. For, example the one of the possible Hamiltonians can be,

$$H = \sum_{i=0}^{N} \frac{1}{2} P_i^2 + \sum_{i=0}^{N} \frac{1}{2} (u_{i+1} - u_i)^2 + \frac{\alpha}{3} \sum_{i=0}^{N} \frac{1}{2} (u_{i+1} - u_i)^3 \tag{1}$$

$$\phi(x,t) = \frac{1}{2}\, c\, \mathrm{sech}^2 \left[\frac{\sqrt{c}}{2} (x - c\,t - a) \right] \tag{2}$$

One can go to Fourier space by doing the normal mode expansion, related to the displacement through,

$$A_k = \sqrt{2/(N+1)} \sum_{i=0}^{N} u_i sin(ik\pi/(N+1)) \tag{3}$$

with the frequencies given by $\omega_k^2 = 4sin^2(K\pi/2(N+1))$. hence the Hamiltonian can be re-written as,

$$H = \frac{1}{2} \sum_{i=0}^{N} (\dot{A}_k^2 + \omega_k^2 A_k^2) + \frac{\alpha}{3} \sum_{i=0}^{N} c_{klm} A_k A_l A_m \omega_k \omega_l \omega_m \tag{4}$$

The expected result from linearity of any equation is that, energy given to a particular mode remains in that mode. So, by introducing an anharmonic term, FPU tried to study the drift of energy from lower mode to higher modes as a function of time. The initial calculations did show the drifting of energy to higher modes, but once they left their program to run longer, even after steady state was reached, and to their surprise, after a recurrence period, almost all initial energy came back to to the initial mode (all but 3%). Thus contradictory to the predictions of statistical physics, FPU result hows that nonlinearity is not enough to ensure the equipartition of energy. Moreover, there also exist a super-period in which almost all energy (more than 99%) is returned to the initial mode.

3 Resolving the Paradox

Attempts to resolve the FPU paradox gave rise to two main lines of thoughts - the integrability of non-linear equations and dynamical chaos.

3.1 Integrability

One of the major discoveries that followed FPU paradox was the complete integrability of a class of non-linear differential equations. In 1965, Zabusky ang Krushal were able to relate the periodic behavior observed to the dynamics of solitons. They started with the one of equation of motion,

$$\ddot{u}_i = (u_{i+1} + u_{i-1} - 2u_i) + \alpha[(u_{i+1} - u_1)^2 - (u_1 - u_{i-1})^2] \tag{5}$$

They restricted their investigations to long wavelengths, and derived Korteweg-deVries equation:

$$\omega_\tau + \frac{1}{24}\omega_{\zeta\zeta\zeta} + \alpha\omega\omega_\zeta = 0 \tag{6}$$

where $\omega = \partial x/\partial\zeta$, $\zeta = z - c_0 t$, $\tau = \bar{\epsilon}t$ and $\epsilon = \frac{1}{2}\bar{\epsilon}c_0$. Here $\bar{\epsilon}$ is defined as defined as the inverse of the critical time (time at which energy in the second mode reaches its first maxima).
Numerical study of the KdV equation by Zabusky and Krushal led to discovery of solitary waves. these waves can propagate through the media without changing their forms. They preserve their shapes and velocities and, during their motion in the finite system with periodic boundary conditions, from time to time, they come back to the positions they had initially, restoring the initial condition. Specifically, it was observed by Zabusky et. al. that starting with the simplest initial condition, $x(z, 0) = Csin(\pi z)$ and initial velocities taken to be zero, solitons appear and strongly interact with each other, but preserving their identity. This explains the FPU recurrence.
It should be emphasized that the FPU paradox would probably not have been a mystery for more than 10 years if, before Zabusky and Kruskal, somebody had got the idea to look carefully at the dynamics of the nonlinear lattice as a function of the space coordinate. It was the description in terms of normal modes that caused misleading explanations and hence, the paradox.
It is worth mentioning that later, based on soliton theory, M. Toda (1978) gave the first analytical estimate of the recurrence time. His calculations were based on the exact solutions of the exponential lattice, now popularly known as Toda lattice.

$$T_R = \frac{3}{\pi^{3/2}\sqrt{2}}\frac{N^{3/2}}{\sqrt{a\alpha}}T_1 = 0.38\frac{N^{5/2}}{\sqrt{a\alpha}}T_1 \tag{7}$$

where $T_1 = 2N$ of first mode, a is the amplitude, and α is a function of non-linear coefficient. This relation by Toda rejected validity of Poincare recurrence theorem in FPU model, which says that for any dynamical system preserving phase-space volume, in its time evolution all trajectories returns close to their position, and do it ifinite number of time.

3.2 Fourier mode studies

This line of thought started with, the idea of looking for non-resonance condition that could explain inefficient energy transfer. In 1954, Kolmogorov formulated a theorem (KAM theorem), which says that "a weak nonlinear perturbation of an integrable system destroys the constants of motion only locally in the regions of resonances, and in other regions a set of points of positive measure remains for which quasi-periodic motion persists." Although its direct application to FPU problem may be doubtful, it may explain the non-ergodicity in FPU problem for weak non-linear perturbation. Moreover, the applicability of KAM theorem to the FPU Hamiltonian has been assessed only recently for the fixed end FPU-β model (Rink 2007). But, it has been questioned whether the original FPU initial condition really lies or not on a KAM torus (Casetti et al 1997). However, based on KAM theorem, Izrailve and Chirikov gave the result that that if the perturbations are so strong that non-linear resonances superpose, the FPU recurrence is destroyed and one obtains fast convergence towards thermal equilibrium.

4 Dynamical chaos

A dynamical system with a few degree of freedom may manifest quite ireegular motion. Exponential instability is a property of statistical mechanical systems. The analysis of stability of motion of particles in presence of non-linear force, led Chirikov(1959) to come with the idea of nonlinear resonances. Chirikov explained that when the non-linearity is weak, any resonance condition can be considered separately via perturbation theory. But for strong non-linearity, the resonances are very close in frequency space, and hence this overlap give rise to irregular motion. Applying this to FPU model says that if the maximum shift in the frequency of a mode is much less then the frequency difference from nearest mode, the the one can neglect neighbouring resonances. Based on these arguments, it has been concluded that α-model is more stable than β-model.

5 Numerical Results

In this work, two models were simulated for, so called α and β-models. The first one has a quadratic non-linearity while other one has cubic non-linearity. The equations of motion corresponding to these two models are:

$$\ddot{u}_i = (u_{i+1} + u_{i-1} - 2u_i) + \alpha[(u_{i+1} - u_1)^2 - (u_1 - u_{i-1})^2] \tag{8}$$

$$\ddot{u}_i = (u_{i+1} + u_{i-1} - 2u_i) + \beta[(u_{i+1} - u_1)^3 - (u_1 - u_{i-1})^3] \tag{9}$$

The algorithm used contained following steps:

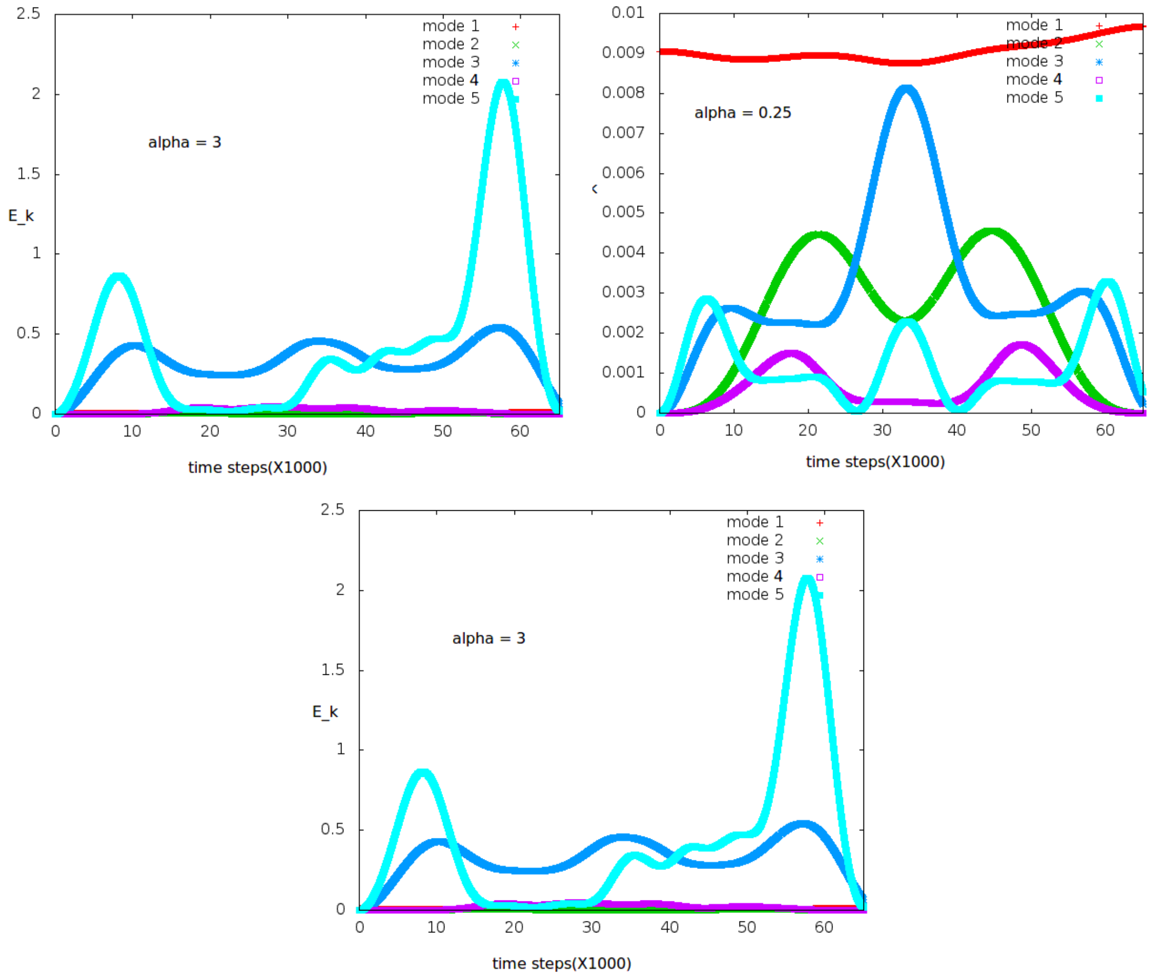
1. Start with a 2^N no. of atoms.
2. Give the initial condition (FPU initial condition; $x[i] = A\sqrt{\frac{2}{N+1}} sin\left(\frac{ik\pi}{N+1}\right)$)
3. Use fixed boundary condition.
4. Calculate the force at each site.
5. Use verlet algorithm to integrate equation of motion.

6. Find the energy in each mode.

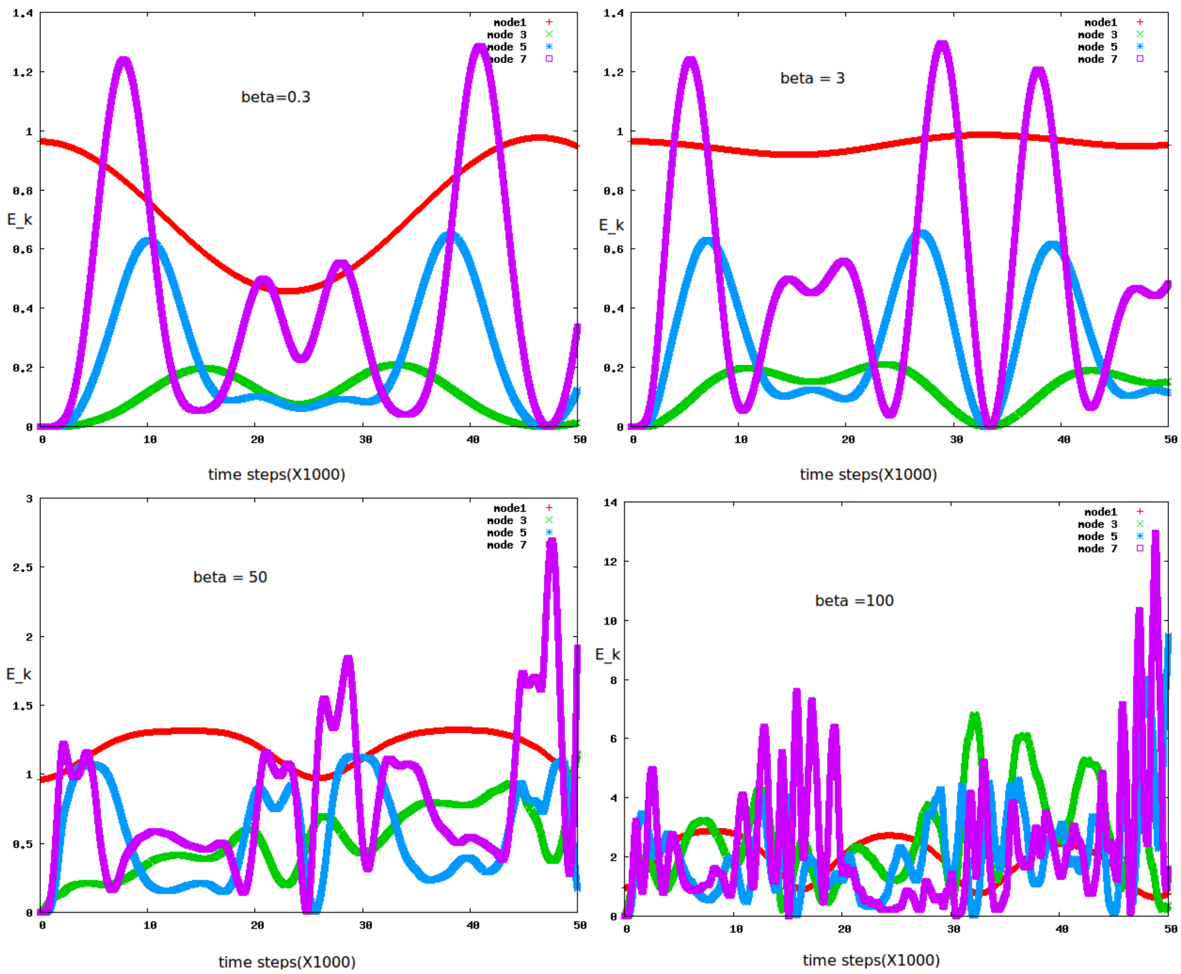
$$E_k = \frac{1}{2}[(\frac{da_k}{dt})^2 + \omega_k^2 a_k^2 \tag{10}$$

Based on above algorithms, following plots were obtained for alpha and beta model. Various curves represent energy in various modes as a function of time. In this work, we expect following observations:

1. Recurrence of energy to the first mode.
2. chaotic behaviour at large values of non-linearity constants.
3. Drifting of energy from first mode to other modes.
4. Nature of energy drift in two models.



α-model: The modes other than first one are scaled



β-model: The modes other than first one are scaled

6 Results

Hence, the energy sharing does occur in various modes as time progresses. But, after a certain period (depends on the non-linearity coefficient), the total energy comes back to mode 1, the result that Fermi, Ulam and Pasta got. Moreover, as the Non-linearity coefficient becomes larger, the energy drifting to higher modes becomes more and more. After a threshold value, equiparon of energy is obeyed and the system shows chaotic behaviour, although the corresponding linear system is completely regular and non-chaotic. It was also observed that for larger non-linearity coefficient, the recurrence time becomes smaller. Moreover, it looks like, in case of β-model enegy flow to odd modes is more.

7 Conclusion

Although FPU problem is quite old, There are many unanswered questions related to it. As stated earlier, KAM theory has not been able to assess the α-model yet. One may also ask How does recurrence time scales with the system size. Moreover, the relation between continuum and discreteness also has to answered. For, example, in FPU model considered here, only the spatial part was discrete while time and displacement field variables were continuous. One can also make models with other kinds of discretization and study the effects. Also, more careful analysis is needed for the relation between poincare cycles and energy recurrence time in FPU model.

8 References

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