University of Massachusetts Amherst

Classical Mechanics 601 Presentation

The Fermi Pasta Ulam Problem

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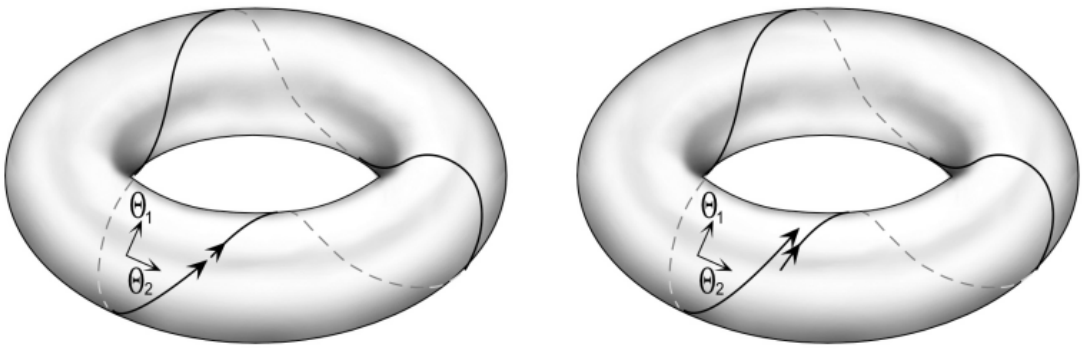

May 09, 2016

1 Introduction

By the 1950s, linearized classical mechanics was thoroughly developed but many non-linear systems were still totally inaccessible analytically. During his time at Los Alamos National Laboratory, Enrico Fermi became curious about the new possibility of numerical simulation of simple non-linear systems. With computational physicist John Pasta, mathematician Stanislaw Ulam, and computer scientist Mary Tsingou, he simulated a series of masses and springs with a quadratic (or cubic) perturbation.

$$\ddot{x}_n = \frac{k}{m}(x_{n+1} + x_{n-1} - 2x_n)\big[1 + \alpha(x_{n+1} - x_{n-1})\big] \tag{1}$$

This correction would more accurately model the behavior of a 1d crystalline lattice than the linear system. Because this perturbation mixes the modes of the linear system, Fermi expected that this simulation would exhibit ergodic behavior as the energy in one pure mode distributed to the other modes. They found that while the system initially appears to thermalize over a sufficiently long time it would exhibit periodic behavior, returning almost exactly to the initial condition. This odd behavior was robust to a range of initial conditions and parameters of the system and was unexplained in the original paper.

2 Code

This investigation by Fermi into a numerical analysis of non-linear was made possible by new computing technology developed at Los Alamos. The MANIAC-1 (Mathematical Analyzer, Numerical Integrator, and Computer), which ran from 1952-1958, was an early vacuum tube computer which allowed for extremely accurate integration of difficult differential equations.

A modern implementation of the FPU code is dramatically simpler that the original MANIAC code largely due to the lack of memory issues. Storing and accessing the mass positions quickly became incredibly time intensive especially with over 200,000 iterations.

The difficulty in our python implementation largely lies in the careful choice of an energy preserving algorithm for the iteration.

$$x'' \approx x(t + \Delta t) - 2x(t) + x(t - \Delta t) \tag{2}$$

This is implemented in lines 28-32 of the code attached below.

The other difficult step is calculating the energies of the individual modes (as was done in the original FPU paper). The simplest method is performing a Fourier transform, a

built in function for numpy, of the mass coordinates and then calculate the energies using these amplitudes and the corresponding frequencies. While this method does work, it was unavailable for the original FPU calculation which instead performed a sort of discrete fourier transform detailed in their paper.

$$a_k = \Sigma x_i \sin \frac{ik\pi}{N} \tag{3}$$

$$E_k = E_k^{kin} + E_k^{pot} = \frac{1}{2}\dot{a_k}^2 + 2a_k^2 \sin^2 \frac{\pi k}{2N} \tag{4}$$

This exact energy formula is used in our code and is implemented in lines 47-57. Note that the energy calculation only has quadratic terms (linear force terms) and therefore ignores the quadratic alpha perturbation. The FPU paper justifies this by claiming that the correction for the perturbation is relatively small, which we confirm experimentally below.

3 Results

Bellow are graphs of the energy in the first five modes of the system as a function of clock cycle. The first figure has the system initialized in the first mode, and the second in the second mode. Figure 1 from the FPU paper is of the same system as that in figure 1 below. The width of the lines in our graphs are due to the energy approximation mentioned above which causes a slight oscillation of the mode energy over each mode period.

4 Mathematical Aspects

The nonlinear "alpha" system studied by Fermi, Pasta and Ulam is a simple setup (Figure. 3) recreated by assembling a chain of alternating masses and springs.[1] This type of oscillating system is quite familiar to us, however, suppose that we were to keep not just the leading order term in the potential, but a higher order term as well. What would be the outcome of such a perturbation? The *a priori* guesswork of Fermi, Pasta and Ulam determined that the modal coupling from the nonlinear term would eventually lead to the equal excitation of all modes as required by the equipartition theorem. This assumption was not without justification; it was well known at this point that perturbations (a quadratic force in this case) to a harmonic oscillator caused highly nonlinear, ergodic behavior. It was of course found that such a thermalization process did not ultimately occur, rather quasi-periodic behavior was observed. Although the complete understanding of this process is still not known, significant progress has been made and the fundamental observations can

[1] In the original experiment, there were two setups: one with 64 masses in the chain and another with 32 masses

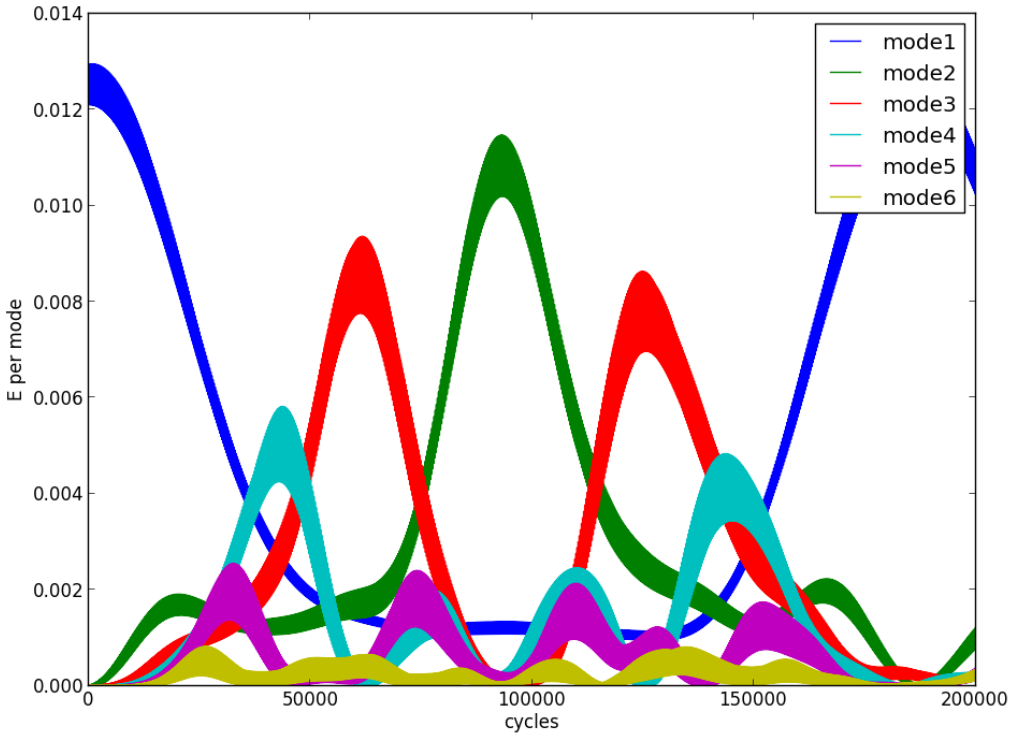

Figure 1: Excitations from mode one. Approximately one super-period

be adequately explained. It is therefore the task from here on to present only the information which is necessary to understand these concepts, and not to provide a thorough mathematical approach to solving nonlinear partial differential equations.

4.1 The Fundamental Equation

The FPU Problem is an interesting one for a variety of reasons, one of them being that the fundamental problem is so simply stated. At its core, our task reduces to solving the following differential equation

$$\ddot{x}_n = \frac{k}{m}(x_{n+1} + x_{n-1} - 2x_n)\big[1 + \alpha(x_{n+1} - x_{n-1})\big] \tag{5}$$

where each mass is m and the sping constant is k. This looks innocuous enough, though it turns out to be a rather insidious equation. In fact, this equation has proven itself to be

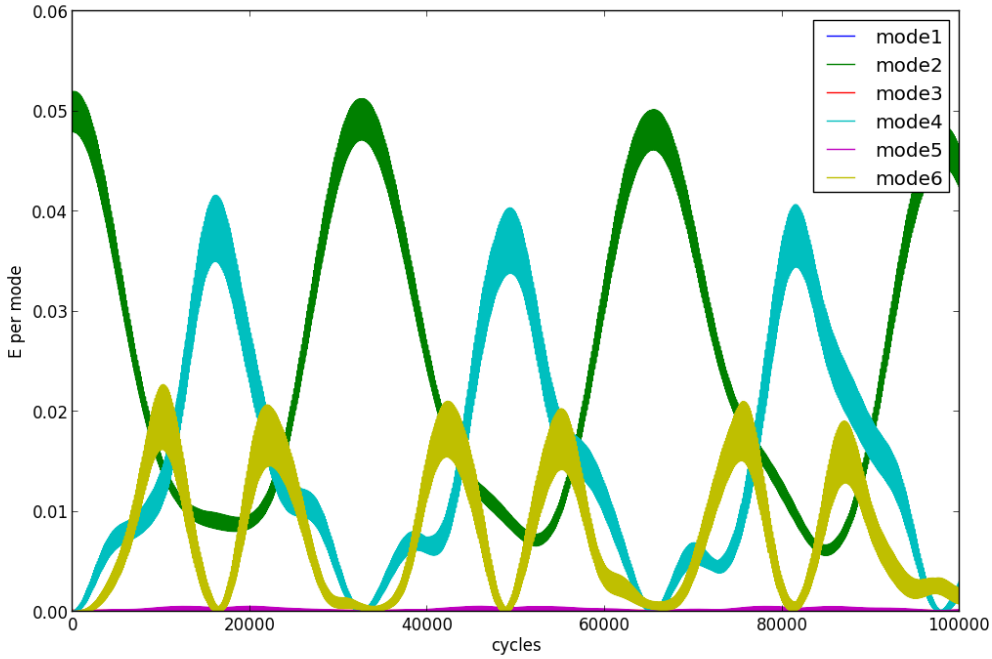

Figure 2: Excitations from mode two. Approximately three super-periods

Figure 3: The mass and spring system

insuperably difficult to solve thus far. This does not mean that we cannot make forward progress, rather only that our understanding cannot yet be considered complete.

First, note the structure of the nonlinear term. Clearly, if $\alpha = 0$, then each mode is independent and will remain so for all times. Put another way, if a particular mode were excited, the system would remain indefinitely in this mode. Now presume that $\alpha \neq 0$. Immediately we see that coupling will occur between modes and so the expectation is that the excitation of a single mode will result in the eventual excitation of *every* mode. How can such an expectation not be met when the equation seems to demand it? In order to make sense of this apparent paradox, we will assume that we may take the equations to its continuum limit. In this limit, we will explore the new equations and try to extract the relevant physics to compare with the observed behavior.

4.2 The Continuum Limit

The passage to the continuum limit is a familiar one and this approach follows the typical steps. Let the lattice spacing be a, the density be $\rho = \frac{m}{a^3}$ and the spring constant be $k = \kappa a$. In order to take the continuum limit we let the lattice spacing tend towards zero. This is equivalent to the statement that the wavelengths we consider are large relative to the lattice spacing. In other words, we will be concerning ourselves with low energy acoustic modes. In this limit, we may make the following replacement,

$$\frac{k}{m} = \left(\frac{ka^2}{m}\right)\frac{1}{a^2} = \left(\frac{k}{a}\right)\left(\frac{a^3}{m}\right)\frac{1}{a^2} = \kappa\left(\frac{1}{\rho}\right)\frac{1}{a^2} = \frac{c^2}{a^2} \tag{6}$$

The quantity c is the velocity of the wave on the continuous chain. To proceed, it is useful to rewrite (**??**) in the suggestive form

$$\ddot{x}_n = \lim_{a\to 0} c^2\left(\frac{(x_{n+1}-x_n)-(x_n-x_{n-1})}{a^2}\right)\left[1+\alpha a\left(\frac{(x_{n+1}-x_n)+(x_n-x_{n-1})}{a}\right)\right] \tag{7}$$

where use has been made of (**??**). Since the distance between any two masses is a, then if we assume that the function $h(x,t)$ solves the equation, the position x_{n+1} may be replaced by the function $h(x+a,t)$. In making these replacements we find

$$\frac{\partial^2 h(x,t)}{\partial t^2} = \lim_{a\to 0}\ c^2\left(\frac{\Big(h(x+a,t)-h(x,t)\Big)-\Big(h(x,t)-h(x-a,t)\Big)}{a^2}\right)$$
$$\times\left[1+\alpha a\left(\frac{\Big(h(x+a,t)-h(x,t)\Big)+\Big(h(x,t)-h(x-a,t)\Big)}{a}\right)\right] \tag{8}$$

We now expand the function in a Taylor series about a. The first term in parenthesis gives

$$\lim_{a\to 0}\ c^2\left(\frac{\Big(h(x+a,t)-h(x,t)\Big)-\Big(h(x,t)-h(x-a,t)\Big)}{a^2}\right)$$

$$\approx \lim_{a\to 0}\ \frac{c^2}{a^2}\left(a\partial_x h(x,t)+\frac{a^2}{2!}\partial_x^2 h(x,t)+\frac{a^3}{3!}\partial_x^3 h(x,t)+\frac{a^4}{4!}\partial_x^4 h(x,t)+\mathcal{O}(a^5)\right)$$

$$-\left(a\partial_x h(x,t) - \frac{a^2}{2!}\partial_x^2 h(x,t) + \frac{a^3}{3!}\partial_x^3 h(x,t) - \frac{a^4}{4!}\partial_x^4 h(x,t) + \mathcal{O}(a^5)\right)$$

$$= \lim_{a\to 0} \frac{c^2}{a^2}\left(a^2\partial_x^2 h(x,t) + \frac{a^4}{12}\partial_x^4 h(x,t) + \mathcal{O}(a^5)\right) \tag{9}$$

The term within the brackets in (**??**) has a plus sign between the differentials and will therefore retain only the odd terms.

$$\lim_{a\to 0} \frac{\left(h(x+a,t) - h(x,t)\right) + \left(h(x,t) - h(x-a,t)\right)}{a} \approx 2\partial_x h(x,t) + \frac{a^3}{3}\partial_x^3 h(x,t) \tag{10}$$

Putting the pieces together and excluding the explicit mention of the limit, we now have

$$\frac{1}{c^2}\partial_t^2 h(x,t) = \left(\partial_x^2 h(x,t) + \frac{a^2}{12}\partial_x^4 h(x,t)\right)\left[1 + \alpha a\left(2\partial_x h(x,t) + \frac{a^3}{3}\partial_x^3 h(x,t)\right)\right] \tag{11}$$

At this point, one may be tempted to keep terms linear in a and throw out the rest resulting in

$$\frac{1}{c^2}\partial_t^2 h(x,t) = \partial_x^2 h(x,t) + 2\alpha a\partial_x h(x,t)\partial_x^2 h(x,t) \tag{12}$$

Such an omission is not allowed! Fortunately, the reasoning is not that a mathematical misstep was made, but rather that the equation represents very different phenomena from what we are looking for. In fact, (**??**) predicts the existence of shocks which is clearly unacceptable. One must then keep terms at least up to second order in a. The resulting PDE is then

$$\frac{1}{c^2}\partial_t^2 h(x,t) - \partial_x^2 h(x,t) = 2a\alpha\,\partial_x h(x,t)\partial_x^2 h(x,t) + \frac{a^2}{12}\partial_x^4 h(x,t) \tag{13}$$

It can be shown that this equation *does* elicit the appropriate behavior for the dynamical system in question. The contribution that leads to mode mixing is obvious. As it stands, this equation is a bit unwieldy and can be recast into a much neater form via the following typical replacements: Let $\xi \equiv x - ct$ and $\tau \equiv \alpha act$ such that the function $H(\xi,\tau) = h(x,t)$. Then we may rewrite the differential equation as

$$\partial_\tau\partial_\xi H - \frac{\alpha a}{2}\partial_\tau^2 H = -\partial_\xi H\partial_\xi^2 H - \frac{a}{24\alpha}\partial_\xi^4 H \tag{14}$$

Now let $s(\xi,\tau) = \partial_\xi H(\xi,\tau)$ and let $a/24\alpha \equiv \delta^2$. With these substitutions and using the face that $\alpha < 1$, we arrive at the succinct equation:

$$\partial_\tau s + s\partial_\xi s + \delta^2 \partial_\xi^3 s = 0 \tag{15}$$

This famous equation is known as the KdV equation after Korteweg and de Vries who wrote it down in 1895.[2] This PDE has known analytical solutions. Finding a single solution is easy and may be done by ordinary methods. Finding *all* possible solutions is a bit more intensive and requires the use of inverse scattering transforms. In this case, the solution is

$$s(\xi, \tau) = 3c \operatorname{sech}^2 \left(\frac{\sqrt{c}}{2\delta}(\xi - c\tau) \right) \tag{16}$$

Given this, we then may find $H(\xi, \tau)$ if we please

$$H(\xi, \tau) = \int d\xi \, s(\xi, \tau) = 6c\sqrt{\delta} \tanh \left(\frac{\sqrt{c}}{2\delta}(\xi - c\tau) \right) \tag{17}$$

where the constants of integration have been set to zero. These solutions are simple propagating waves known as solitons. They are, in some sense, immutable as they pass right through each other with only the phase (at the most) being affected. It is the presence of these soliton solutions that causes the equipartition theorem to be violated and gives rise to quasi-periodic solutions.[3]

At this point in the discussion we have explained away the apparent paradox that the FPU Problem characterizes and are, in essence, "done." One is compelled to ask however if there was any way to know that this system would have quasi-periodic behavior, and further, what other systems *could*. To address these concerns completely, a detailed study of topology would be necessary. If we are willing to accept the results of a few key theorems however, we may get a deeper understanding as to how these quasi-periodic solutions arise in the first place.

4.3 Topological Analysis

It is worthwhile to motivate this section of the discussion with some formal definitions and theorems that will be useful in understanding what follows.

Definitions

- Diffeomorphism: Let F and G be two manifolds. If the map $R : F \to G$ and its inverse $R^{-1} : G \to F$ are both bijections and n-times differentiable, then the map R is a C^n diffeomorphism.

[2] The equation had actually already been discovered by J.V. Boussinesq in 1877

[3] N. J. Zabusky, M. D. Kruskal, *Interaction of "Solitons" in a Collisionless Plasma and the Recurrence of Initial States*, Phys. Rev. 15, 240 (1965)

- Liouville Integrability: The Hamiltonian phase space may be subdivided (foliated) by invariant manifolds such that the Hamiltonian flow associated with each invariant manifold spans the tangent distribution. In other words, consider a Hamiltonian $\mathcal{H}$. If there exists $n-1$ other Hamiltonians such that each is a constant of motion for the flow of the others, then the system is integrable.

- Canonical Transformations: Isomorphisms of smooth manifolds that preserve the symplectic manifolds that arise from the Hamiltonian flow

- Symplectic Vector Space: There are three components to this definition. Let V be a vector field and F be a field.

  1. Bilinearity: $w : V \times V \to F$
  2. Alternating: $w(\alpha, \alpha) = 0 \ \ \forall\, \alpha \in V$
  3. Non-degenerate: If $w(\alpha, \beta) = 0 \ \ \forall\, \beta \in V$, then $\alpha = 0$

Theorems

- Liouville-Arnol'd: If the level set $L_{h_i}(p,q) = \{(p,q) \mid H_1(p,q) = h_1, \ldots, H_n(p,q) = h_n\}$ has compact support, then the connected components are diffeomorphic on a n-dimensional torus. There exists a canonical transformation to action-angle coordinates (θ, a) such that $(\theta, a) : \mathbb{T}^n \times U$ where U is an open subset on $\mathbb{R}^n$. The variables are then linear in time and give $\frac{d\theta_i}{dt} = \omega_i(a)$ and $\frac{da_i}{dt} = 0$. In other words, if a Hamiltonian with n degrees of freedom has n known integrals of motion in involution, then there exists a transformation to action-angle coordinates and these canonical coordinates depend linearly in time.

- Hamiltonian Flow: Let the Hamiltonian of $2n$ symplectic variables $(p_1, \ldots, p_n)$ and $(q_1, \ldots, q_n)$ defined on the space M^{2n} have the flow ϕ_H^t where $\phi_H^t : M^{2n} \to M^{2n}$ and $t \in \mathbb{R}^n$. Then, if $(p_i, q_i) \in \mathbb{T}^d$, then $\phi_H^t(p_i, q_i) \in \mathbb{T}^d \ \ \forall\, t \in \mathbb{R}$ and $\phi_H^t(p_i, q_i) = (p(t), q(t))$

- KAM Torus: A d-dimensional invariant torus for ϕ_H^t with $2 \leq d \leq n$ is a KAM torus if the flow of ϕ_H^t on $\mathbb{T}^d$ has a linear transformation to the action-angle variables (θ, ω) where $\theta \in \mathbb{T}^d$ and $\omega \in \mathbb{R}^d$

Having made these statements, we are now in a place to understand why soliton solutions persist in a system that one would expect to be entirely ergodic. It is known that a Hamiltonian that is "completely integrable" will have (at least) quasi-periodic behavior. There are different types of integrability, and so to be clear, here we concern ourselves with Liouville integrability since we are considering Hamiltonian dynamics. If the FPU Hamiltonian is Liouville integrable, then we will have a complete understanding of the

problem. Unfortunately, the Hamiltonian in question is *not* completely integrable, though it is "close."

The operative word in the previous sentence is undoubtedly "close." It was the work of Kolmogorov, Arnol'd and Moser (worked on from 1954-1963) which later became known as the KAM Theorem, that tells us what it means to have a "nearly integrable system." Using the definition of a symplectic manifold where we may assume non-degeneracy, then according to the KAM theorem, a slightly perturbed Hamiltonian with n degrees of freedom still has a phase space which is almost completely filled by n-dimensional invariant tori. In essence, the perturbation deforms the tori in the phase space, but not enough to remove quasi-periodic behavior.

We have the necessary ingredients to understand the FPU problem:

1. The FPU Problem reduces to the KdV equation in the continuum limit
2. The KdV equation gives rise to soliton solutions which are responsible for the lack of thermalization of the modes (non-ergodicity)
3. A Hamiltonian that is completely integrable will exhibit periodic behavior (Liouville-Arnol'd Theorem)
4. Transforming and n-dimensional Hamiltonian to action-angle coordinates parametrizes the surface of an n-dimensional torus
5. The FPU Hamiltonian is not completely integrable, though it is "nearly" integrable.
6. Small perturbations of the Hamiltonian (that is, a "nearly" integrable Hamiltonian) will leave the phase space sufficiently filled by the tori such that the soliton solutions, and thus the quasi-periodic behavior, persist (KAM Theorem).

5 Conclusion

In 1954 Fermi passed away, well before the publication of the FPU paper. Although Pasta and Ulam weren't able to explain the periodicity of their simulation the paper was crucial in the early development of non-linear dynamics. By repeating the steps taken in the 50's, we were able to recreate the results that confounded so many for so long. We had the added benefit of sixty years of mathematical analysis on nonlinear partial differential equations to analytically justify the physical results of the system. The FPU Problem continues to give valuable insight into ergodic and quasi-periodic behavior though it's mathematically complete understanding remains an open problem.

References

[1] Fermi, E.; Pasta, J.; Ulam, S. *Studies of Nonlinear Problems.* (PDF). Document LA-1940. (1955).

[2] Duxois, T.; Ruffo, S. *Fermi Pasta Ulam nonlinear lattice oscillations.* Scholarpedia 3 (8): 5538 (2008)

[3] Porter, M. A.; Zabusky, N. J.; Hu, B.; Campbell, D. K. *Fermi, Pasta, Ulam and the Birth of Experimental Mathematics* American Scientist 97 (3): 214?221. (2009)

[4] Dauxois, Thierry. *Fermi, Pasta, Ulam and a Mysterious Lady* Physics Today Jan. 2008: 55-57. (2008)

[5] N. J. Zabusky, M. D. Kruskal. *Interaction of "Solitons" in a Collisionless Plasma and the Recurrence of Initial States.* Phys. Rev. 15, 240 (1965)

6 Source Code

```
import matplotlib.pyplot as plt
import numpy as np

# Parameters
m = 1        # Mass per mass
k = 1        # Spring constant
N = 64         # Number of masses
alpha = 1     # Parameter for quadratic perturbation
t_max = 200000    # Number of time steps in simulation
dt = 0.5      # Time step
num_modes = 5   # Number of modes we care about


# Initializing equilibrium
loc_init = np.linspace(0,1,N)
# Starting system in a pure mode
loc_init += 0.1*np.sin(np.pi*loc_init)

# Array that stores positions at all times
loc_arr = np.zeros([t_max, N], dtype = float)

# Starting system with no velocity
loc_arr[0] = loc_init.copy()
loc_arr[1] = loc_init.copy()

# Iterating position update over all times
for t in range(2,t_max):
  loc_init[1:-1] = 2*loc_arr[t-1][1:-1] - loc_arr[t-2][1:-1]
          + dt**2 * k/m * (loc_arr[t-1][2:]-2*loc_arr[t-1][1:-1]
          +loc_arr[t-1][:-2]
        + alpha*((loc_arr[t-1][2:]-loc_arr[t-1][1:-1])**2
              -(loc_arr[t-1][1:-1]-loc_arr[t-1][:-2])**2))
  loc_arr[t] = loc_init.copy()

# Transforming positions for easy plotting
for t in range(0, t_max):
  loc_arr[t] = loc_arr[t] - np.linspace(0,1,N)

```

```
# Array of "fourier transformed" coordinates, and derivatives
a_arr = np.zeros_like(loc_arr)
da_arr = np.zeros_like(loc_arr)
# Calculate energies of modes, not valid at t=0
e_arr = np.zeros_like(loc_arr)
index = np.arange(N, dtype = float)

# Iterating over each mode for all times to calculate a, da, e
for t in range(0, t_max):
  for K in range(0, num_modes+1):
    a_arr[t, K] = (np.sum((loc_arr[t, :])
          * np.sin((index+1)*(K+1)*np.pi/N)))

for t in range(1, t_max-1):
  for K in range(0, num_modes+1):
    #da_arr[t, k] = (a_arr[t+1, k] - 2 * a_arr[t, k] + a_arr[t-1, k
    ])/dt
    da_arr[t, K] = (a_arr[t+1, K] - a_arr[t, K])/dt
    e_arr[t, K] = (.5 * da_arr[t, K]**2
          + 2 * a_arr[t, K]**2 * (np.sin(np.pi * (K+1)/(2*N)))**2)

# Plot energies
for K in range(0, num_modes+1):
  plt.plot(np.arange(1, t_max-1), e_arr[1:-1, K], label = "mode" +
    str(K+1))
plt.legend()
plt.ylabel("E per mode")
plt.xlabel("cycles")
plt.show()
```

fpu.py