Lecture Notes on the Fermi-Pasta-Ulam-Tsingou Problem

Andrew Larkoski

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Because this is a short week, we're going to just discuss some fun aspects of computational physics. Also, because last week's topic was the final homework (due the following Friday), just sit back and relax and forget about everything you have to do. ☺ Just kidding.

Today, I'm going to discuss the Fermi-Pasta-Ulam-Tsingou (FPUT) problem. Actually, Laura Freeman did her thesis on this topic at Reed in 2008; you can pick up her thesis in the lounge or on the Reed Senior Thesis digital collections if you are interested. Laura actually interviewed Mary Tsingou for her thesis, so this is actually a fascinating historical document.

In the early 1950's, Enrico Fermi, John Pasta, Stanislaw Ulam, and Mary Tsingou performed some of the earliest computer simulations on the MANIAC system at Los Alamos. (Remember MANIAC? Metropolis was the leader!) Their problem was very simple, but their results profound. They attempted to simulate a non-linear harmonic oscillator (i.e., spring) on a grid. Recall that Newton's equations for a spring on a grid is:

$$m\ddot{x}_j = k(x_{j+1} - 2x_j + x_{j-1})\,, \tag{1}$$

which is just a linear problem and so normal modes and eigenfrequencies can be found exactly, etc. The grid spacing is Δx and so position x_j is at

$$x_j = j\Delta x\,. \tag{2}$$

The problem that FPUT studied was slightly different, modified by non-linearities in x:

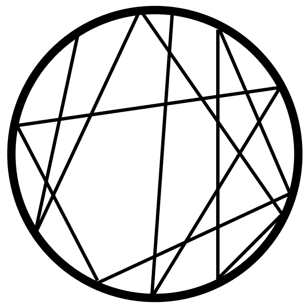
$$m\ddot{x}_j = k(x_{j+1} - 2x_j + x_{j-1})[1 + \alpha(x_{j+1} - x_{j-1})]\,. \tag{3}$$

When $\alpha = 0$, this of course returns the linear system, but for $\alpha \neq 0$ it is non-linear. The scientists coded this system up on MANIAC on a grid of 64 points (wow! tiny!) and set it running. What makes this problem so intriguing is that it defied expectation.

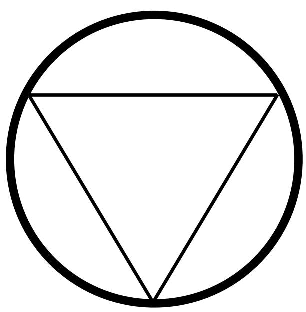
In some sense, they thought the experiment would be "boring". They had believed that the system would be ergodic. The ergodic hypothesis was introduced in the early days of statistical mechanics and is the following statement:

> Over enough time, every state of a given energy of the system will be visited an equal number of times.

The thought was that if they watched the simulation long enough, they would see this ergodicity manifest. Why is this reasonable? First, it is what is observed in most systems. For example, an ergodic system would be light trapped in a spherical reflector. Any physical reflector has imperfections, thermal fluctuations, etc., and so the light would bounce around everywhere:



If one waited long enough, then the light would visit every phase space point consistent with its energy. However, if the shell was a perfect reflector, then the reflections would not be ergodic:



For example, it's possible that the light would just bounce around in this triangular pattern *ad infinitum*. The ergodic hypothesis is absolutely fundamental for the theory of thermodynamics. An ergodic system (water, air in this room, a blackbody, the Ising model, etc.) can have a definite temperature. A system that is ergodic has thermalized: the total energy is quantified by its collective temperature and not the particular motion of each individual molecule.

A system that is not ergodic lacks a temperature because the motion of each particle is special: it is not true that, given enough time, every particle in a non-ergodic system will do what every other particle did.

So, this is the basis of the experiment. They thought, reasonably so, that their non-linear spring was an ergodic system. Amazingly, they were wrong. Actually, the story is a bit sad. Their simulations did not support ergodicity, and all were confused. Fermi, in 1954, fell ill and died before the group could reach a resolution and publish their findings. It was eventually written about a year after Fermi died, but only as a pre-print at Los Alamos (never published in a journal). Mary Tsingou was not included on the author list of the preprint.

So, what's going on? While FPUT never figured out what was happening, later people identified the source of lack of ergodicity. We'll discuss that in the rest of this class.

Unknown to them at the time, but the non-linear system they studied was actually the discrete version of a very weird non-linear differential equation called the Korteweg-de Vries equation. We can see this by massaging their problem.

As we showed earlier, the characteristic time in a harmonic oscillator is

$$t_0 = \sqrt{\frac{m}{k}}\,, \tag{4}$$

and so the characteristic velocity is just

$$c = \frac{\Delta x}{t_0} = \Delta x\sqrt{\frac{k}{m}}\,, \tag{5}$$

where Δx is the grid spacing. We can then write the FPUT problem as

$$\ddot{x}_j = c^2\frac{x_{j+1} - 2x_j + x_{j-1}}{\Delta x^2}[1 + \alpha(x_{j+1} - x_{j-1})]\,. \tag{6}$$

Expanding to fourth-order the first factor is equivalent to the Taylor expansion of:

$$\begin{aligned}\frac{x_{j+1} - 2x_j + x_{j-1}}{\Delta x^2} &= \frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2} \\ &= u''(x, t) + \frac{\Delta x^2}{12}u''''(x, t) + \mathcal{O}(\Delta x^4)\,.\end{aligned} \tag{7}$$

The term with α can be expanded to the third order as:

$$\alpha(x_{j+1} - x_{j-1}) = 2\alpha\Delta x u'(x, t) + \frac{\alpha\Delta x^3}{3}u'''(x, t) + \mathcal{O}(\Delta x^5)\,. \tag{8}$$

Then, the FPUT problem is the discretized form of

$$\frac{1}{c^2}\ddot{u} - u'' = (2\alpha\Delta x)u'u'' + \frac{\Delta x^2}{12}u'''' + \mathcal{O}(\alpha\Delta x^2, \Delta x^4)\,. \tag{9}$$

Now, we can make the substitutions that

$$\xi = x - ct\,, \qquad \tau = (\alpha\Delta x)ct\,, \qquad y(\xi, \tau) = u(x, t)\,. \tag{10}$$

This makes:

$$\frac{\partial}{\partial t} = \frac{\partial\xi}{\partial t}\frac{\partial}{\partial\xi} + \frac{\partial\tau}{\partial t}\frac{\partial}{\partial\tau} = -c\frac{\partial}{\partial\xi} + (\alpha\Delta x)c\frac{\partial}{\partial\tau}\,, \tag{11}$$

$$\frac{\partial}{\partial x} = \frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} + \frac{\partial\tau}{\partial x}\frac{\partial}{\partial\tau} = \frac{\partial}{\partial\xi}\,. \tag{12}$$

With this substitution, we then have

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) u = \left((\alpha\Delta x)^2 \frac{\partial^2}{\partial \tau^2} - 2(\alpha\Delta x)\frac{\partial^2}{\partial\xi\partial\tau}\right) y\,. \tag{13}$$

The FPUT problem them becomes

$$\frac{\alpha\Delta x}{2} y_{\tau\tau} - y_{\xi\tau} = y_\xi y_{\xi\xi} - \frac{\Delta x}{24\alpha} y_{\xi\xi\xi\xi}\,, \tag{14}$$

where $y_\xi = \partial y/\partial\xi$, and similar.

To continue, we assume that $\alpha, \Delta x \to 0$, but with the constraint that

$$\delta = \lim_{\Delta x\to 0}\sqrt{\frac{\Delta x}{24\alpha}}\,. \tag{15}$$

Taking $\Delta x \to 0$ is the continuum limit and doing this we find

$$y_{\xi\tau} + y_\xi y_{\xi\xi} + \delta^2 y_{\xi\xi\xi\xi} = 0\,. \tag{16}$$

Finally, we call $y_\xi = v$ and so

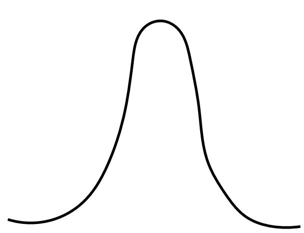
$$\boxed{v_\tau + v v_\xi + \delta^2 v_{\xi\xi\xi} = 0\,.} \tag{17}$$

So, the FPUT problem corresponds to the above non-linear partial differential equation. This equation has a name – it is the Korteweg-de Vries equation. Perhaps amazingly, this non-linear differential equation admits exact solutions. You can show by explicit calculation that

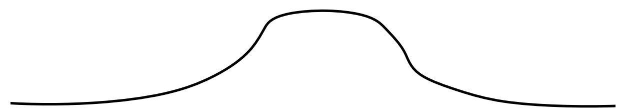
$$v(\tau,\xi) = 6\delta^{2/3}\frac{c}{2}\text{sech}^2\left[\frac{\sqrt{c}}{2}\left(\delta^{-2/3}\xi - c\tau - a\right)\right] \tag{18}$$

is a solution, for arbitrary c, a. Interpreting τ as "time" and ξ as "position", this solution moves to the right at speed $c\delta^{2/3}$. It is called a "solitary wave", or soliton.

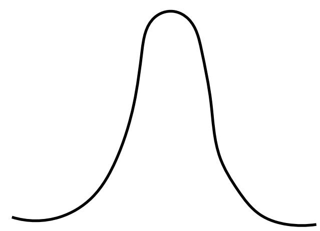
Solitons are fascinating objects that I can hardly begin to discuss here. The most striking feature of a soliton is that it is dispersionless, even though it is the solution to a dispersive partial differential equation. By dispersionless, I mean its shape is unchanged as a function of time; it just translates. Contrast this with a water wave. Say there is an initial displacement of water like such:



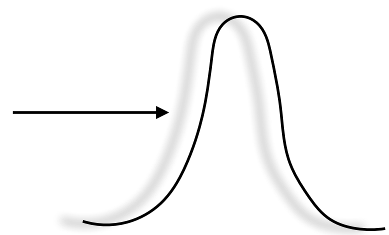
At later times, this disperses as:



i.e., the amplitude decreases, the water spreads out, maybe ripples are formed. The soliton is nothing like this. Given an initial displacement of water like such:



the soliton keeps its shape and just translates:



The shape of the soliton is conserved. In fact, associated with the Korteweg-de Vries equation, there are an infinite number of conserved quantities: things like the energy and momentum, but more exotic quantities, too. Solitons were first described as "waves of translation" by John Scott Russell who observed them produced in Union Canal, in Edinburgh, Scotland, in 1834. He was shocked at how such a disturbance didn't change shape, and was faster than his horse could carry him!

Since then, it has been noted that solitons occur broadly, in many physical systems: vortices in condensed matter systems, Morning Glory clouds, rogue sea waves, and many others.

So, what does this have to do with the FPUT problem? Well, remember their hypothesis, that the system should be ergodic; i.e., experience every phase space point consistent with the total energy? Unbeknownst to them at the time, they were actually simulating the Korteweg-de Vries equation and solitons on a grid. Once you produce a soliton in your simulation, it sticks around and does not disperse. That is, the existence of solitons inhibits the system to thermalize; it inhibits all states in the phase space from being visited.

So, this simple computer simulation turned out to have deep relationship to some really cool physics!