Computational Physics

PHYS-3600 (Fall 2022)

Fermi-Pasta-Ulam Experiment: Exploring its Properties

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I. INTRODUCTION

This project aims to study an experiment performed by Enrico Fermi, John Pasta, Stanislaw Ulam, and Mary Tsingou (FPUT or FPU) involving a vibrating system including a non-linear term. The experiment was conducted to investigate how non-linear systems behave and to determine whether such a system would reach thermal equilibrium.

The FPUT experiment was set up as a uniform one-dimensional chain of particles connected by springs, with the inclusion of a non-linear term with the motivation to investigate these types of systems because of how common they are in nature. The researchers conducted the experiment with the expectation of the system to thermalize, or have energy equally distributed among the particles. However, to their surprise, the energy remained concentrated within a few modes at a time and would not thermalize over time. This phenomenon, known as "energy localization", was later explained by the concept of solitons. The significant finding was that the system, after many iterations, returned to its initial condition with a small degree of error. The system displayed quasi-periodic behavior, meaning it exhibited irregular periodicity and became unpredictable over long periods. This contradicted the prevailing belief about the behavior of mechanical non-linear systems, which was that all nonlinear systems would eventually reach thermal equilibrium. It put forth the idea that perhaps non-linear systems retain memory of how they were initially configured. These findings sparked further research into the dynamics of nonlinear systems, chaos theory, and the study of solitons.

This report will explore the FPUT experiment in greater detail, examining the experiment's design and methodology, along with its results. We will simulate the experiment and explore the effects the non-linear terms and the initial configuration has on the modal energies. We will first replicate FPUT's findings, and then explore various configurations to determine how changing the initial conditions affects the results. More specifically, can the period of the system be predicted at short times? How does the initial distribution of energy change the total energy distribution over time? How do the quadratic and cubic terms affect the system? We will delve into this famous experiment and answer these and other questions.

II. BACKGROUND

A. Springs with non-linear terms

Our system has a series of N oscillators equally spaced by a distance Δx. This distance has no effect on the system and its behavior, so the distance is set for aesthetic purposes in the simulation. We can describe our equilibrium position of the i-th oscillator with:

$$\mathrm{P}_i = i\Delta x \qquad i = 0,1, \dots, N-1$$

We can describe spring motion of an oscillator's displacement from equilibrium x_i with a non-linear term using Newton II:

$$m\ddot{x}_\iota = k(x_{i+1} + x_{i-1} - 2x_i) + \epsilon(x_i) \tag{1}$$

where $\epsilon(x_i) = \alpha[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2]$ for quadratic non-linearity

or $\epsilon(x_i) = \beta[(x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3]$ for cubic non-linearity

where we have our standard notation as m being mass and k being our spring constant. In the simulations being performed, m and k are each set to 1 for convenience as they have irrelevant effect on the system's attributes of interest. Our non-linear coefficients α and β are chosen so the non-linear displacement term is of order 10^{-2} of the linear term. Since motion involving springs is relative to a particle's distance from its equilibrium position, a way of describing overall position of the i-th particle is the sum of the equilibrium position and its displacement:

$$X_i = \mathrm{P}_i + x_i$$

The above equations can be used to set up our spring and, provided initial conditions of position and speed, the FPUT experiment can be replicated [5].

B. FPUT Simulations & Energy Distribution

The experiment was conducted with the expectation of the system reaching thermal equilibrium, such as a gas having energy equally distributed among all degrees of freedom

(directions of translation and rotation). The system has two main components that affect the periodic behavior: the initial configuration and the nonlinear term.

The first, and most remarkable condition, was one where the system was configured to be one-half of a sine wave with a quadratic coefficient $\alpha = 0.25$. In this configuration, all the energy is set in the first mode. As the simulation runs, the energy is exchanged into the second mode, then the third, and so on. It was found that over many iterations through time the system would return to its initial condition within 1% of error (as seen in Figure 1). We can also see that over a large amount of time ($\frac{\omega}{2\pi} \approx 6000$) the system starts to lose its periodic behavior. Since our system is chaotic because of the nonlinear term, it is harder to predict the outcome at long times [1].

While testing different conditions, it seemed that this was not a consistent result. Plotting different conditions did not repetitively give some sort of quasi-periodicity. In the system, it is more appropriate to say that there are multiple special cases that give a result worthy of noting. This fact made it hard to summarize results. Although, one element to consider is that this effect is seen in the double pendulum [1]. With just two degrees of freedom, the double pendulum transfers energy back and forth between the two instead of sharing it. This effect is seen in the FPUT system as well, even with 16 or more degrees of freedom.

Now, a large question that was neglected when discussing above, is how are the modal energies calculated? The answer is Fourier modes and Lagrangian change of variables [2]. We can introduce new variables, a_k and $\dot{a}_k$ where:

$$a_k = \sum x_i \sin\left(\frac{ik\pi}{N}\right) \tag{2}$$

These new variables are written in terms of the k-th mode of our system. Using these new expressions, we can describe our energy as:

$$E = \frac{1}{2}(\dot{a}_k^2 + \omega_k^2 a_k^2) \tag{3}$$

$$\text{where } \omega_k = 2\sin\left(\frac{k\pi}{2N}\right)$$

Using these equations, we can plot (Figure 2) for the first few modes that display the quasi-periodicity of the system under our conditions.

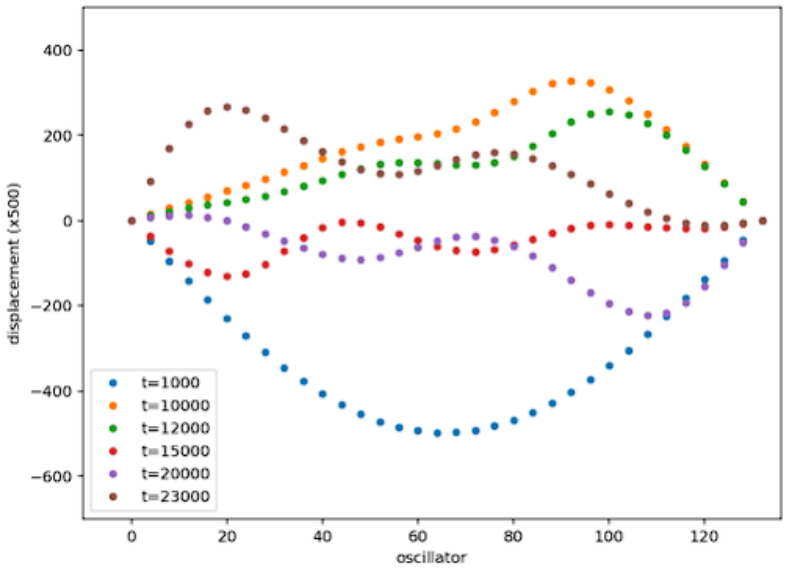

FIG. 1. Oscillators and their displacements (displacements increased by a factor of 500) at different times.

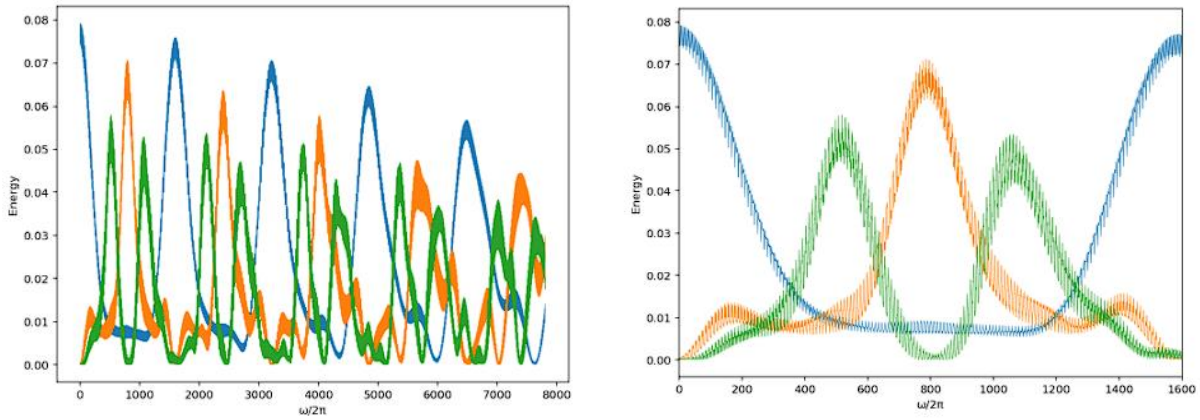

FIG. 2. (Left) Plot of the modal energies over $\frac{\omega}{2\pi}t$ (ω is frequency) with 500000 time iterations. The $\frac{\omega}{2\pi}$ factor does not affect the overall shape of the graph, but allows for more convenient reading of the plot when dealing with larger time intervals. (Right) Same graph as left image, but with only one quasi-period shown. This was done with $\alpha = 0.25$, $N = 32$ and the initial configuration as half of a sine wave.

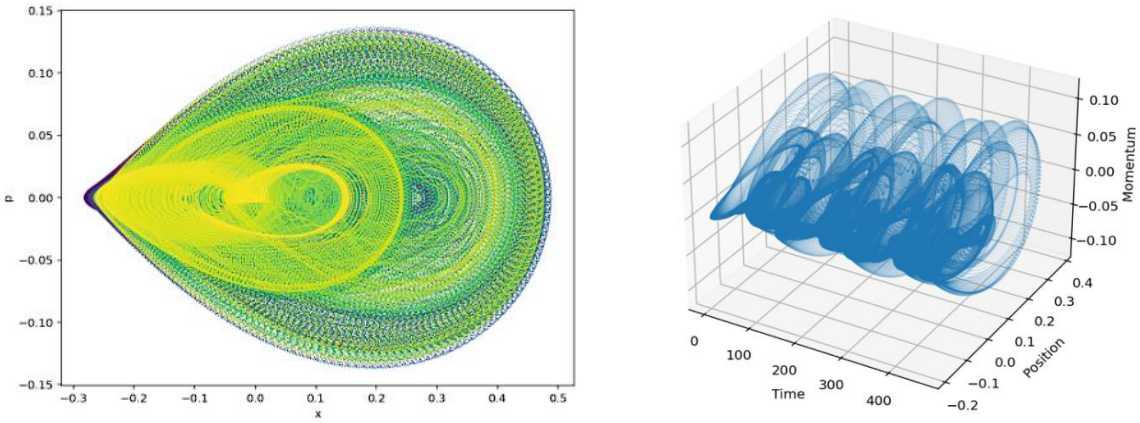

FIG. 3. (Left) Phase space of every time layered on top of one another for the fourth particle ($N = 32$). The colourmap used changes as time increases. (Right) Phase space of the same particle with the time dimension included (Follows the same conditions as Figure 1).

C. Korteweg-De Vries and Solitons

The Korteweg-De Vries (KdV) is a partial differential equation that is used to describe the behavior of long, shallow water waves. Of course, that is not the topic of interest, but it can be related to FPUT's system. Our system is long relative to the modes, and the displacement is small, relating to the shallow component of KdV. Using these approximations one can find the KdV equation, which is as such [6]:

$$v_r + vv_\xi + \delta^2 v_{\xi\xi\xi} = 0$$

What does this mean though? Yes, the connection between FPUT and KdV exists, but how are they related?

As mentioned earlier, our system behaves the way it does due to solitons. Solitons are a type of wave that can travel for long distances without losing their shape or energy. Often, solitons are found in physical systems that can be described using non-linear partial differential equations. Our KdV equation so happens to be just that.

A soliton is a self-reinforcing wave that maintains its speed and shape as it propagates. Solitons are characterized by their stability, localization, and the ability to interact with other

solitons without losing any of its own characteristics. These three characteristics appear in our experiment [4].

Stability refers to the fact that solitons maintain their shape and speed as they propagate. This means that they are not subject to the same kinds of dissipative effects that are typically seen in other waves, where they would lose energy and disappear. The localization of solitons is the fact that solitons are well-defined, isolated waves that do not spread out as they propagate. Again, this property is not seen in other types of waves, which will disperse over time. Lastly, a solitons ability to interact with other solitons without losing its identity refers to the fact that when two or more solitons collide, they pass through each other and emerge on the other side with individual shapes and speeds unchanged.

Since the FPUT experiments relation to the KdV equation and thus solitons are true, we can use these characteristics to help understand the behavior of our vibrating string. The above characteristics assist in explaining how our wave can return to its initial configuration with such small error. The stability, localization, and interaction of our waves are somewhat seen in our experiment, but not during long times (Figure 4).

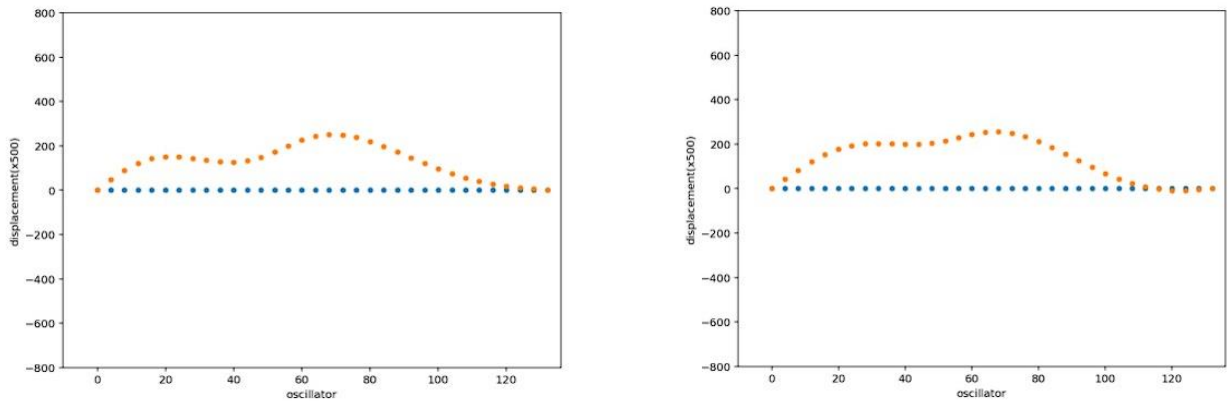

FIG. 4. (Left) Displacement of string at $t = 53190$. (Right) Displacement of string at $t = 53850$.

III. PROPERTIES OF THE FPUT EXPERIMENT

A. Initial Configurations

The first "variable" we can experiment on is the initial configuration of the system. Since we have a chaotic system, we know that very small differences will produce very unpredictable results. However, it was found that if we keep the initial configuration in some form of a wave, we almost always experience some sort of quasi-periodic behavior.

The first condition that was examined was the following:

$$x_i = \frac{1}{\sqrt{N+1}} \sin\left(log\left(\frac{x\pi}{N+1}\right)\right)$$

this could also be described as a "check-mark" (Figure 7). It was found that this condition had the system behave in a quasi-periodic behavior, as expected. The first modal energy was repeating in triplets of waves, where it would repeat the same three waves periodically (Figure 5). One can also note the decrease in the amplitude of the modal energy, showing how the first modal energy transfers some of its energy to other modes and will continue to do this as time goes on.

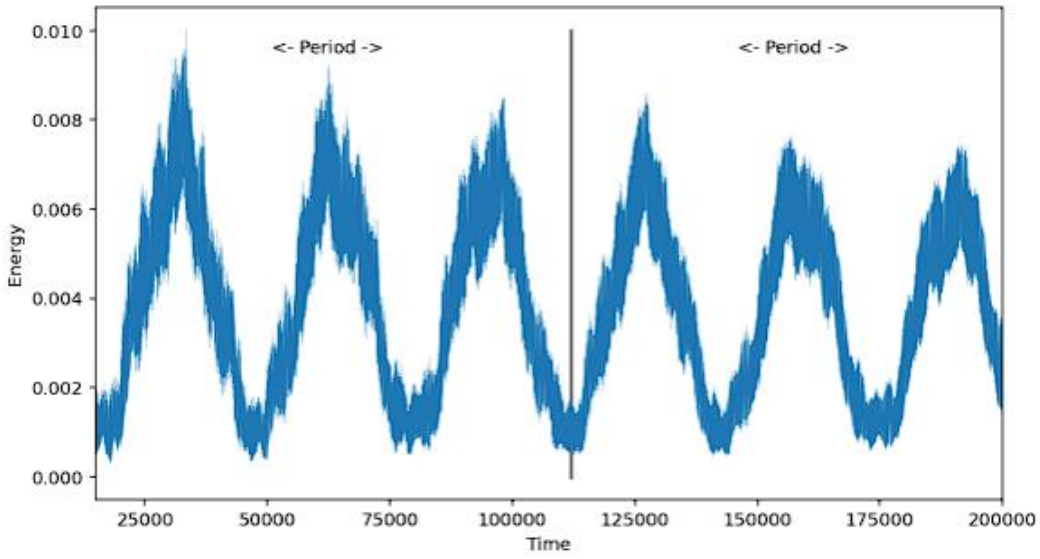

FIG. 5. First modal energy of the "check-mark" configuration.

It is important to emphasize that here we are just displaying how drastic changing the initial configuration has an effect the system and its behavior. Giving the 5th particle an extra push of $+0.1$, we can compare it to the configuration without this extra push and notice the difference (Figure 6). Although it doesn't look like much, our energies in mode 1 and 3 are not quite the same.

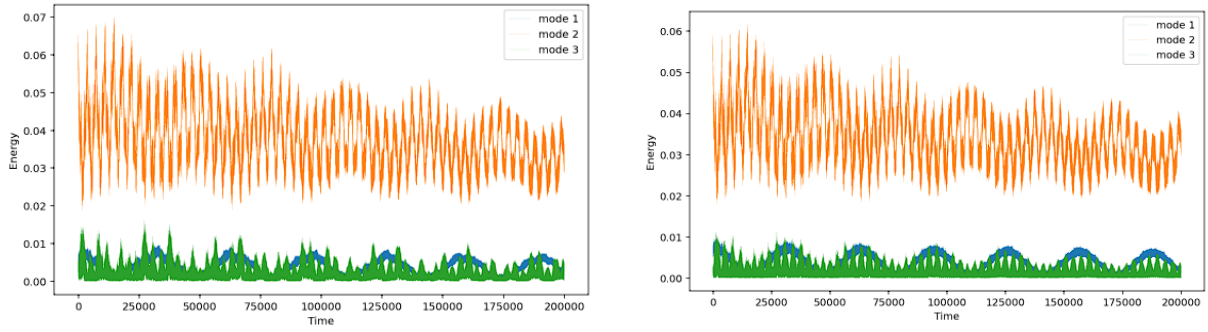

FIG. 6. (Left) "Check-mark" modal energies. (Right) "Check-mark" modal energies along with a small displacement of the 5th particle.

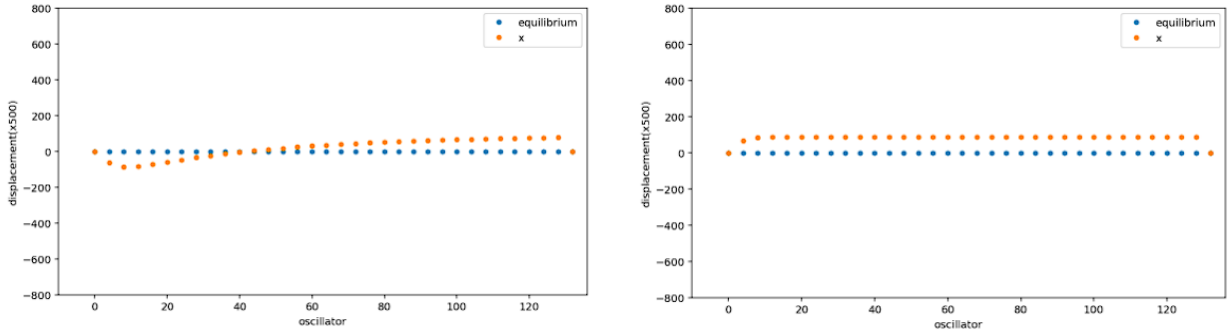

FIG. 7. (Left) Initial configuration of the "check-mark". (Right) Initial configuration of a normalized hyperbolic tan function.

The second configuration we examined was:

$$x_i = \frac{1}{\sqrt{N+1}} \tanh(i)$$

This was also described as a normalized hyperbolic tan function (Figure 7). Overall, our energies repeat periodically just as they did in the first configuration. We still see the behavior in the first modal energy where we have three distinct waves that repeat themselves periodically (Figure 8).

Something to note in both, is the modal energy, and which one holds most of the energy throughout the simulation.

In the first configuration, we see that all the energy starts in mode 2. Looking at Figure 6, we can see that the second modal energy continues to hold most of the energy even as time goes on. This is a replication of what FPUT discovered, they found that the energy would return to its initial mode at long enough time periods. Then again, in the second configuration, we start with all the energy in mode 1 and then continue to have most of the energy be held in the first mode (Figure 9).

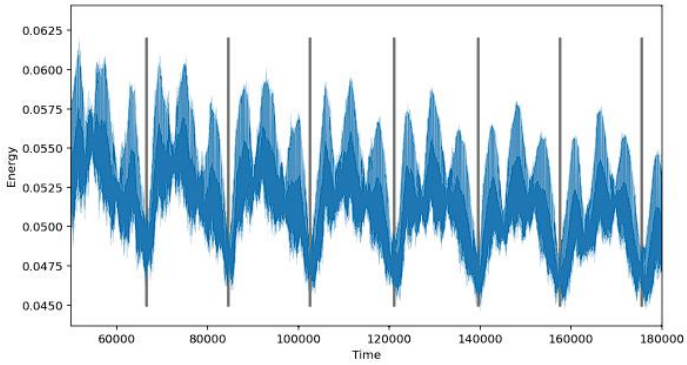

FIG. 8. First modal energy of normalized hyperbolic tan function.

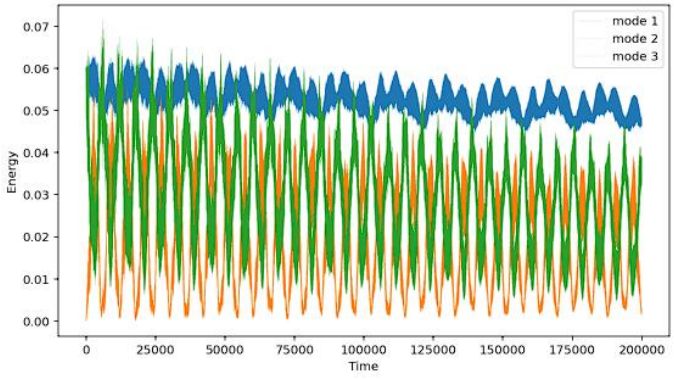

FIG. 9. Modal energies of normalized hyperbolic tan function.

B. Nonlinear Terms

Another component of this system we can vary is the non-linear term. This will not produce as chaotic results as varying the initial configuration did, so there is potential to find some sort of

a relation between what happens when we change the non-linear term and how the system behaves. To do this, we must hold all the other components of the system to be constant. The half-sine wave configuration was chosen, along with $N = 32$.

The first non-linear term considered was the quadratic term. The idea here was to find what would happen if we varied this number and examine the energies. Just as explored above, the first quadratic term examined was $\alpha = 0.25$. Two more simulations were explored, while increasing the quadratic term by 0.05 in each one. So, we had three data sets to look at: $\alpha = 0.25, 0.30, 0.35$. Examining the frequency of the first modal energy in each simulation produced an interesting result: each simulations energy began together, with the same amplitude at $t = 0$. As time progressed, it was found that the energy would oscillate more frequently and decay faster in its amplitude for a system with a higher quadratic term. The modal energy waves would stray away from each other, but after some time they would all return to a maximum at the same time (near $t = 155000$) (Figure 10). The interesting thing to note though, was that each system reached this point almost exactly one period in difference from the others. So, for our $\alpha = 0.25$, we saw that it reached this point in 13 periods. Then for $\alpha = 0.30$, we saw it reach this in 14 periods, and for $\alpha = 0.35$ it reached it in 15. A trend could be noticed here, where each increase of a twentieth in our quadratic term would have it reach this critical time value in one less period. This was tested again for $\alpha = 0.40$, and the same trend followed. So, for our simulations, we could describe the trend with N_{max}:

$$N_{max} \equiv 20\alpha + 8$$

this would roughly predict how many periods a half-sine-wave-with-$N = 32$'s first modal energy would reach $t \approx 155000$.

Then, the cubic term was studied. The same method was used, where it was examined how many iterations it would take for the system's first modal energy to reach alignment with the other systems. This time, we started with $\beta = 3.00$, and increased our term by a half for two more simulations. It was noted that almost the same occurrence happened, although a bit sooner ($t \approx 148000$) (Figure 11). The same trend occurred as well, although our β increments were increased by a factor of ten.

For $\beta = 3.00$, we saw the number of periods to be 15. For $\beta = 3.50$ the number of periods was 16, then for 4.00 the number of periods was 17. This linear relation is described as:

$$M_{max} \equiv 2\beta + 9$$

This trend was tested for $\beta = 4.50$ and the result was as expected (Figure 11).

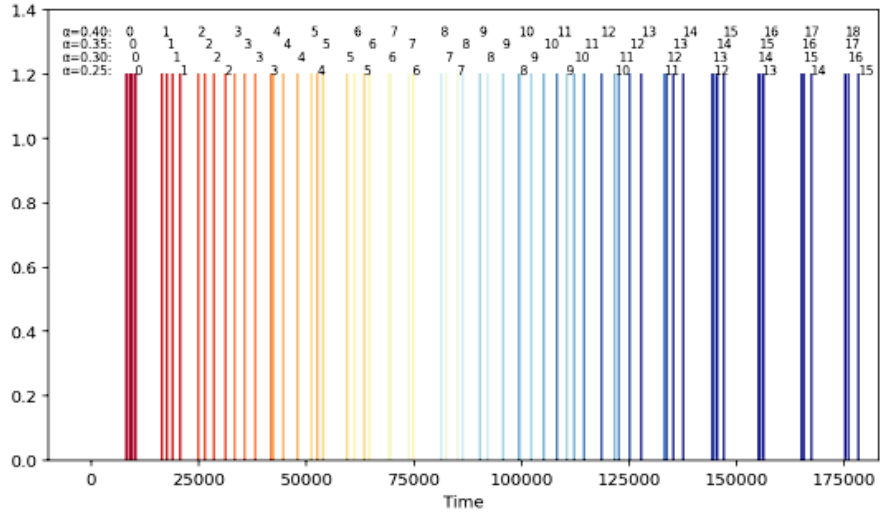

FIG. 10. Maxima of the first modal energy for a half-sine wave with $N = 32$. The period number is displayed above each maximum for convenience. Each color represents the period number of each wave.

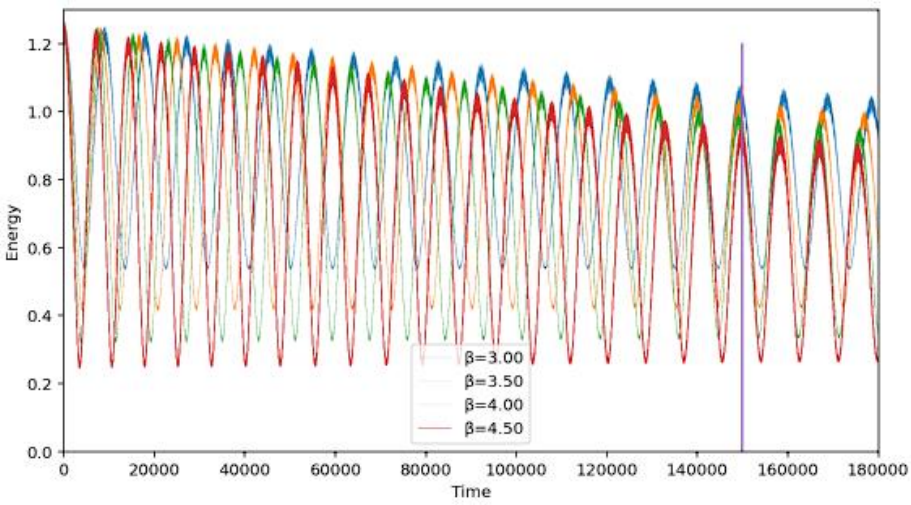

FIG. 11. First modal energy for $\beta = 3.00$ (blue), $\beta = 3.50$ (orange), $\beta = 4.00$ (green) and $\beta = 4.50$ (red). The purple line represents where the energies return to alignment.

C. Frequency over Small Periods

Based off the fact that the non-linear term has some measurable effect on the system, the behavior we are going to examine in this section is how fast a maximum appears in the first modal energy wave (besides at $t = 0$) based off the non-linear term.

First, we examined our base case that has been covered numerous times in this paper, the half-sine wave with $\alpha = 0.25$. It was noted that the first maximum to appear was at $t = 9900$. Another simulation was run, with $\alpha = 0.75$ and the first maximum occurred at $t = 5000$. So, the trend that should be seen is that a higher quadratic term produces a maximum quicker than lower terms.

To examine this further, 15 simulations were run. Each simulation had α vary from 0.1 to 1.5 and the first maximum for each was calculated. These two data sets were plotted against each other, and the result was as follows (Figure 12):

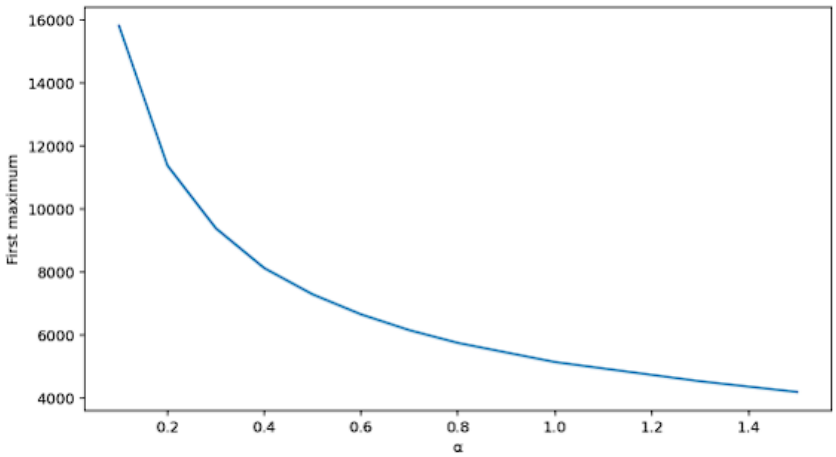

FIG. 12. First maximum occurrence for difference α-systems

A fit can be made to this graph, which worked out to be:

$$E_{max} \equiv 5142\alpha^{-0.488}$$

Using this relation, different α values were tested, and it was verified that the relation was true (Figure 13). Although, as α became larger, the accuracy decreased. We can conclude that the first period could be predicted based off the α value.

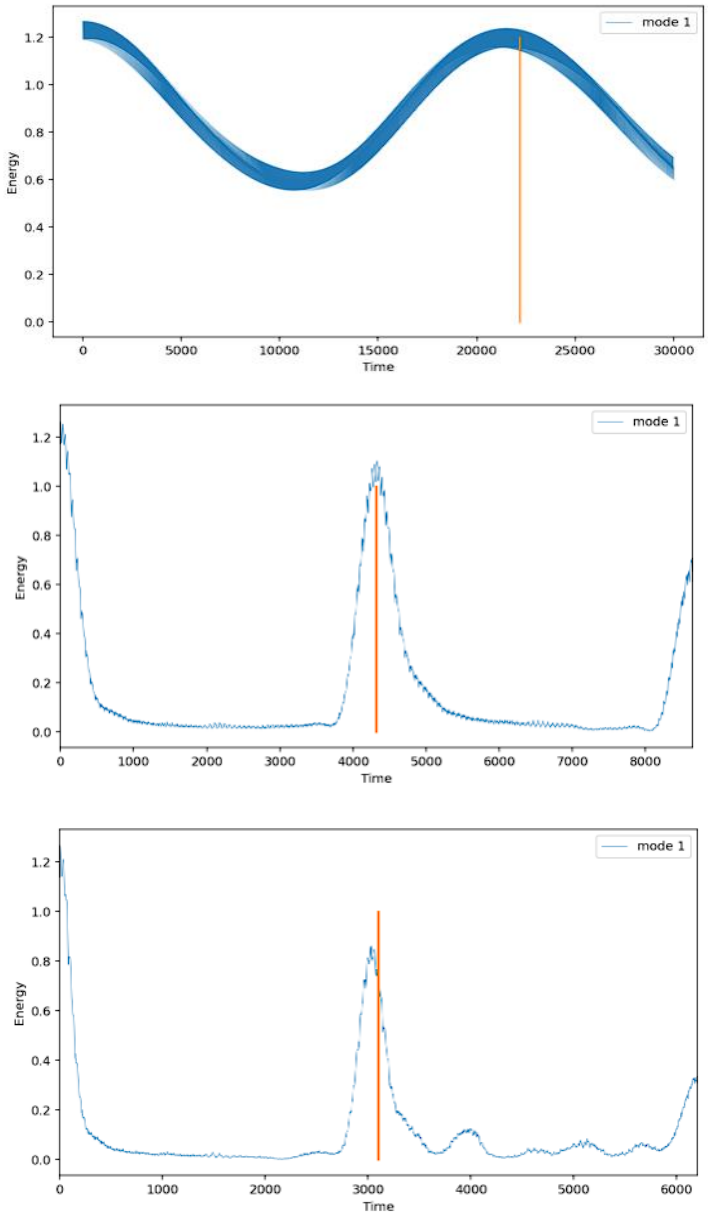

FIG. 13. (Top) First modal energy for a system with $\alpha = 0.05$, with the orange line being $E_{max}(0.05)$. (Middle) The same as the top but with $\alpha = 1.43$ and the orange line being $E_{max}(1.43)$. (Bottom) The same as the top and middle but with $\alpha = 2.82$ and the orange line being $E_{max}(2.82)$

IV. METHODS

To simulate the FPUT experiment, we exploited the fact that our system has conservation of energy. This meant we could use a symplectic integrator, which was convenient because of the provided equation of motion being a force expression. Using the general expression for momentum, we could derive the two Hamiltonian functions that are needed to implement a symplectic method.

There was some modification that had to be done to the symplectic integrator for the simulation to directly replicate the experiment. In the integrator, a few lines of code were added to fix the ends of the string so they would not move. This would ensure our simulation would run as desired.

In the original paper FPU published [1], the most common time step used was $\delta t = \frac{1}{\sqrt{8}} \approx 0.3$. Acknowledging the fact that computers have become more advanced since 1955 (the distribution year of the paper), our time step was chosen to be $\delta t = 0.1$ which was successful in yielding results as expected. It was noted that when dealing with the cubic non-linear term, as time evolved to $t > 350000$ the energies became unstable (Figure 14).

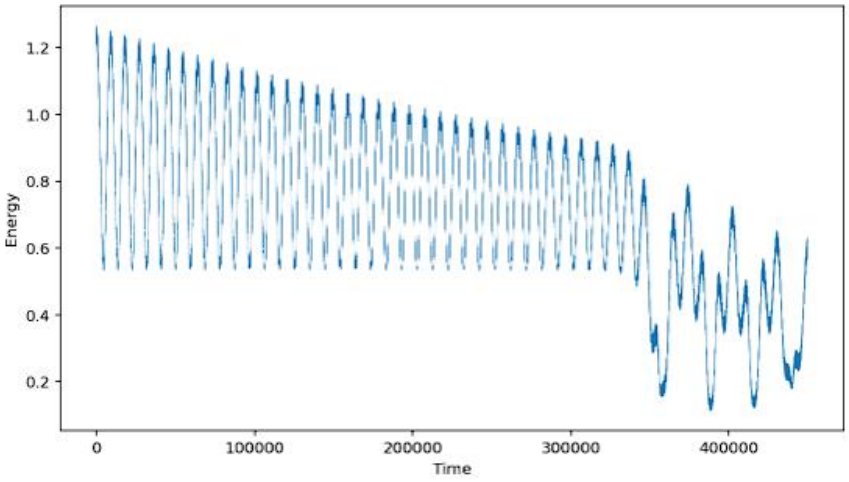

FIG. 14. Modal energy for an $N = 32$ system with $\beta = 3.00$

[1] Fermi, Enrico, et al. *Studies of the nonlinear problems*. No. LA-1940. Los Alamos National Lab. (LANL), Los Alamos, NM (United States), 1955.
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[3] Scholarpedia, Fermi-Pasta-Ulam nonlinear lattice oscillations – Scholarpedia (2011), [Online; accessed 5-December-2022]
[4] Zabusky and Porter. Soliton - Scholarpedia (2010), [Online; accessed 20-December-2022]
[5] Wikipedia, Fermi-Pasta-Ulam-Tsingou problem – Wikipedia (2022), [Online; accessed 5-December-2022]
[6] Wikipedia, Korteweg–De Vries equation (2022) [Online; accessed 18-December-2022]