The Fermi-Pasta-Ulam Problem: An Exploration of the One-Dimensional Lattice

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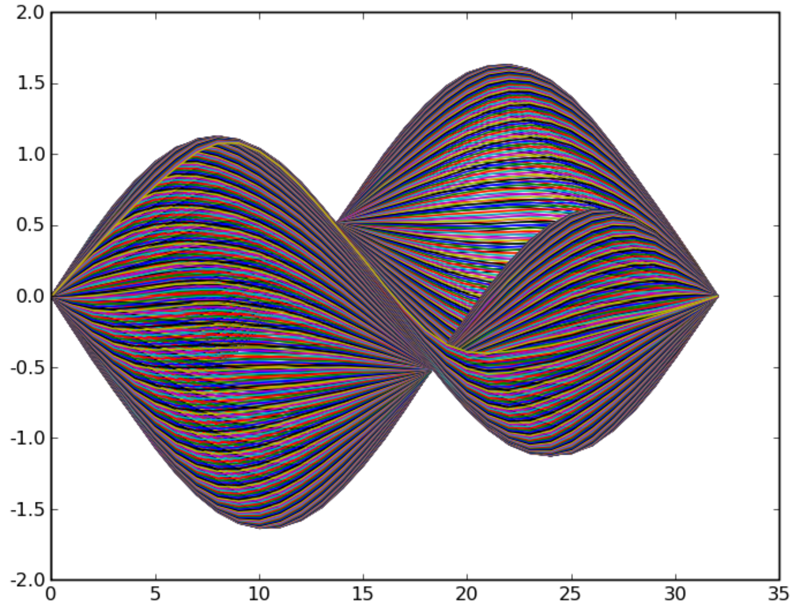
June 9, 2008



Abstract

In this paper we examine the behavior of a vibrating string with fixed endpoints under the assumption that the movement of the string must be described by some nonlinear terms. Nonlinear problems cause analytical difficulties, thus the problem was analyzed from a numerical point of view. The implementation was carried out using various parameter values and initial conditions.

Introduction

In 1952, Enrico Fermi was conducting research at the Los Alamos facility in New Mexico. He became interested in the potential of "electronic computing machines" in problems that may not have readily attainable analytical solutions. While closed solutions may not necessarily be possible, computing methods might yet yield useful numerical solutions. The obvious class of problems lacking closed analytical solutions is, of course, the class of nonlinear problems.

The one-dimensional lattice with fixed endpoints was the chosen problem. We consider some number of masses connected by springs in one-dimension, where the masses at the end have a fixed position. The interest of the problem for Fermi and company was the problem's relation to ergodic theory.

To analyze this problem numerically, we look at some number points along the string and solve for their displacement at a given time t. Generally, we take the string to have an initial displacement identical to the sine wave and no starting velocity. These initial conditions can be varied to look at the long-term behavior of the string.

The decision to view the model as a string with fixed endpoints was based on the greater ease of visualization, at least for the one-dimensional lattice. This visualization has the additional benefit of describing the motion of a plucked string instrument, such as a guitar, which will arouse greater in the general public.

Background

The necessary prerequisites to understand the problem from a physical standpoint unfortunately exceed the level of the author. As such, the problem was viewed as an opportunity to experiment with numerical methods and computer programming.

To approach this problem with only numerical interest, no background in physics is necessary. One needs only to consider the nonlinear equations described in the **Dynamical System** section and have some familiarity with the standard fourth-order Runge-Kutta. Such individuals interested in verifying the practical convergence and computational efficiency of numerical methods could use the system described to test their ideas. It is certainly substantial enough to present computational difficulties to poorly formulated algorithms.

Dynamical System

To describe the system, we consider n points along the string. Our goal is to obtain a solution for $x_i(t)$, which gives the displacement of the i-th position along the string at time t. We consider x_0 and x_n to be the fixed endpoints of the string. The only effect we consider on each point is its immediate neighbors. That is, the x_i is only affected by the positions of x_{i-1} and x_{i+1}. These neighboring points will pull x_i. The following is the equation used to describe the acceleration of each point on the string in the case of quadratic nonlinearity (with the exception of the endpoints):

$$\ddot{x}_i = (x_{i+1} - x_i) + (x_{i-1} - x_i) + \alpha \left[(x_{i+1} - x_i)^2 + (x_{i-1} - x_i)^2 \right].$$

In this instance, α denotes a parameter which determines the effect of the nonlinear terms. For the case of cubic nonlinearity, we obtain a very similar equation:

$$\ddot{x}_i = (x_{i+1} - x_i) + (x_{i-1} - x_i) + \beta \left[(x_{i+1} - x_i)^3 + (x_{i-1} - x_i)^3 \right]$$

where β is analogous to α in the quadratic case. It is worth noting that if we only consider the linear terms and allow n to approach ∞ we arrive at the standard wave equation.

It was necessary to transform the associated system of second-order differential equations into a first-order system. To accomplish this, we still treat $x_0, x_1, \ldots, x_n$ as the displacement of the string at the various points. We define $x_{n+1}, x_{n+2}, \ldots, x_{2n+1}$ to be the velocities of $x_0, x_1, \ldots, x_n$, respectively. With these variables, we derive the following system of $2n + 2$ equations:

$$\begin{aligned}
\dot{x}_0 &= 0 \\
\dot{x}_1 &= x_{n+1} \\
&\vdots \\
\dot{x}_i &= x_{n+i} \\
&\vdots \\
\dot{x}_{n-1} &= x_{2n-1} \\
\dot{x}_n &= 0 \\
\dot{x}_{n+1} &= 0 \\
\dot{x}_{n+2} &= x_2 - x_1 + x_0 - x_1 + \alpha \left[(x_2 - x_1)^2 + (x_0 - x_1)^2 \right] \\
&\vdots \\
\dot{x}_{n+k} &= x_k - x_{k-1} + x_{k-2} - x_{k-1} + \alpha \left[(x_k - x_{k-1})^2 + (x_{k-2} - x_{k-1})^2 \right] \\
&\vdots \\
\dot{x}_{2n-1} &= 0.
\end{aligned}$$

A system of this size (provided n is a worthwhile partition of the string) would cause serious analytical headaches for systems even as simple as linear with constant coefficients. In the event of nonlinearity, we must settle for a numerical approximation.

Methods

The method used to solve the system was the standard fourth-order Runge-Kutta. Had time been less of a constraint, there would have been greater exploration in the use of other numerical methods. Of particular interest would be an implementation of various multistep methods, such as an Adams-Bashforth method.

The time step used varied with the time period we were attempting to examine. The parameters α and β were generally kept very low; the effects of the nonlinear terms are not meant to overpower the linear terms. The standard testing conditions were $\alpha, \beta = .25$ with the string initially positioned as a sine wave. Generally, no initial velocity was assumed. As the experimentation proceeded, the parameters and the initial conditions were varied.

A simple program coded in Python was used to solve the system. The program allows the user to determine the number of partition points, parameter value, and the number of steps over which to integrate. The user must actually modify the source code to vary the initial conditions of the system.

Results

The first case considered is a string with no initial velocity in the sine wave position. We look at the equations with quadratic nonlinear terms where $\alpha = .25$. The behavior of the string was very "polite" oscillations for quite some time. It appeared to oscillate uniformly, returning to the initial conditions each time. However, this must have only been the appearance to the eye. Reaching upwards of 25,000 iterations the shape of the string is no longer the nice curve of a dilated sine wave. There is some disturbance. To get a better idea of the shape, look at Figure 1(a) and Figure 1(b).

Varying α from 0 to 1 yielded similar results. The more interesting (irregular) vibrations came from varying the initial velocities. The string immediately became asymmetric, though it did return to the initial conditions. It took roughly 5,000 iterations to get highly irregular motion. For a visualization of this, see Figure 1(c) and Figure 1(d).

A natural question arises: What occurs when $\alpha > 1$? Physically, such parameter values probably do not make sense for our modeling goals. However, it is still a worthwhile numerical investigation. The simple answer is: blowup. For $\alpha = 1.5$ the number of iterations decreases to about 40,000. By the time we increase to $\alpha = 2$, the blowup is catastrophic after only 245 iterations. In short, not only do larger values for α not make physical sense, they are not numerically viable options.

The same conditions were tested for the cubic nonlinear terms with the β parameter. The results were very similar, but irregularities in the behavior of the string took much longer to develop and were smaller. Initially this came as a surprise, but after some consideration this result makes sense. The distances between points must be less than one, so cubing the distance will be less than the distance squared. To view illustrations corresponding to those for the quadratic case, look to Figure 2. Ultimately, the two systems were very similar.

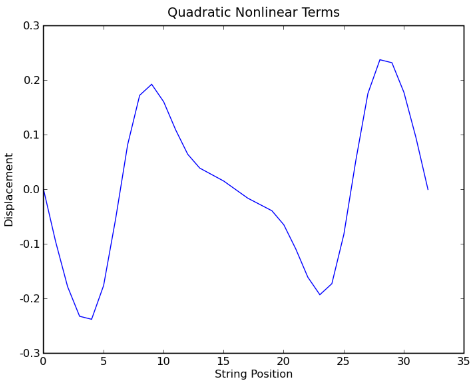
Conclusion

The movement of the string became unpredictable, but only after a great number of iterations. We could also impose some nonuniform initial condition to cause asymmetric vibrations immediately. That, however, could be deemed chaos merely for the sake of chaos. Enforcing uniform initial conditions (not simply releasing the string with no initial velocity) yielded results very similar to most basic case.

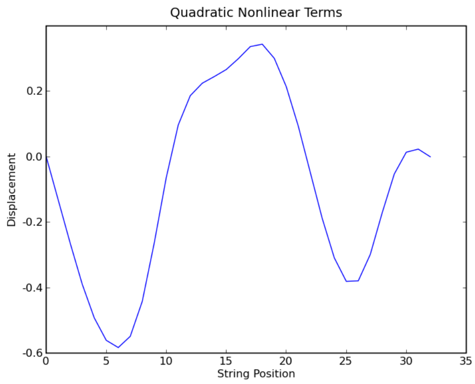
For future work a graphical display of an actual one-dimensional lattice should be created. That is, a visualization using the displacement of masses attached to springs. To progress the physical model itself, the lattice can be extended to two dimensions then three dimensions. Creation of a visualization tool for these more complicated models would be considerably more difficult to produce, and unfortunately might amount to little more than experimental toys.

Bibliography

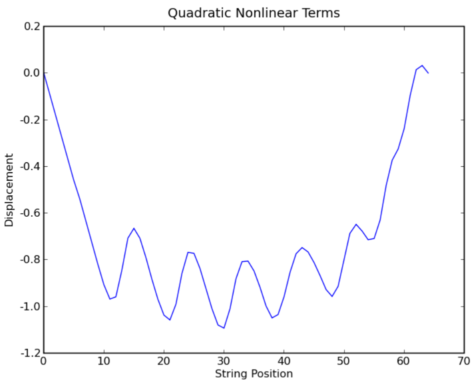
E. Fermi, J. Pasta, and H. C. Ulam, "Studies of nonlinear problems," in *Collected Papers of Enrico Fermi*, E. Segrè, ed. (U. Chicago Press, Chicago, Ill., 1965), Vol. 2, pp. 977988.



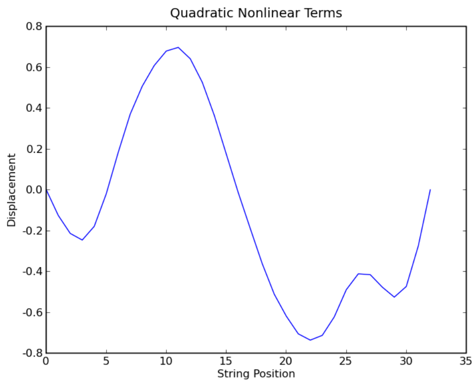
(a) Initial velocity: 0



(b) Initial velocity: 0

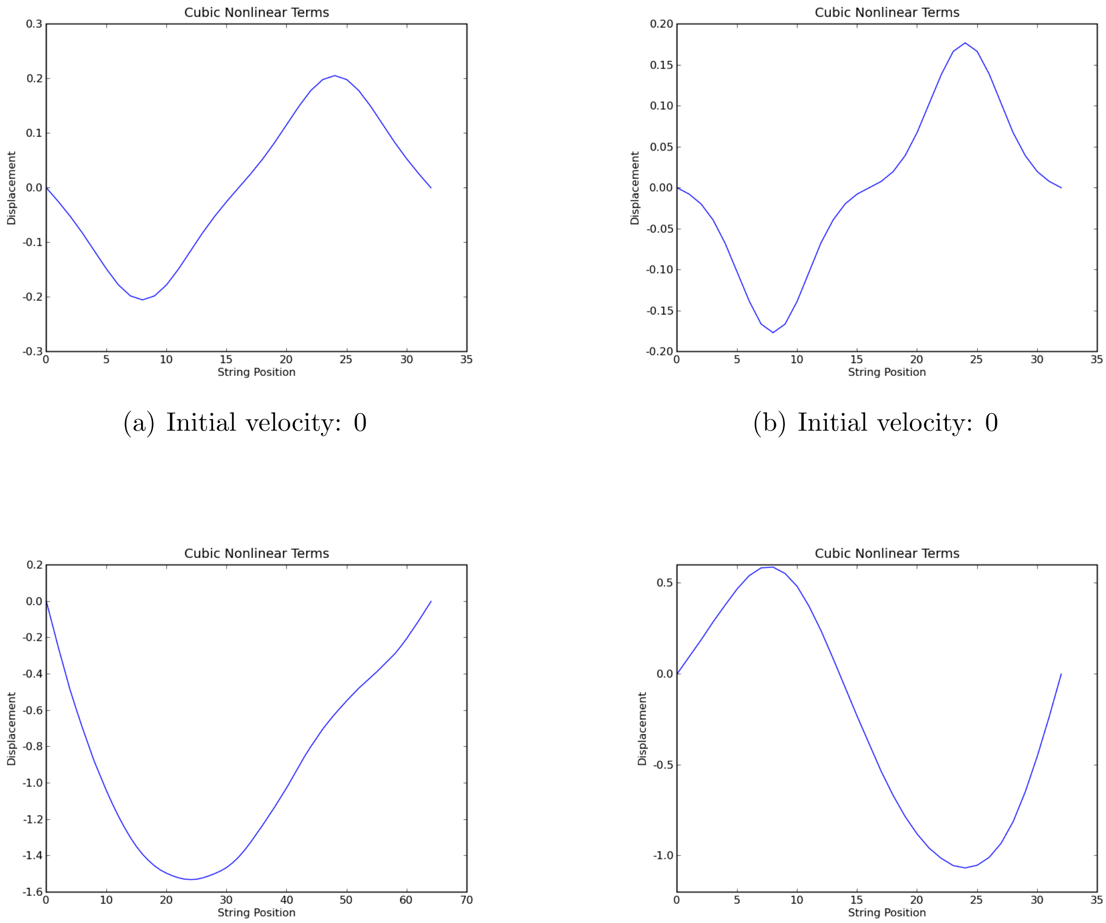


(c) Initial velocity: $-.1\,|\sin(2\pi k/n)|$



(d) Initial velocity: $-.1\,|\sin(2\pi k/n)|$

Figure 1: This set of graphs depicts the displacement of a string with quadratic nonlinear terms under various initial conditions.



(a) Initial velocity: 0

(b) Initial velocity: 0

(c) Initial velocity: $-.1\,|\sin(2\pi k/n)|$

(d) Initial velocity: $-.1\,|\sin(2\pi k/n)|$

Figure 2: This set of graphs depicts the displacement of a string with cubic nonlinear terms under various initial conditions.

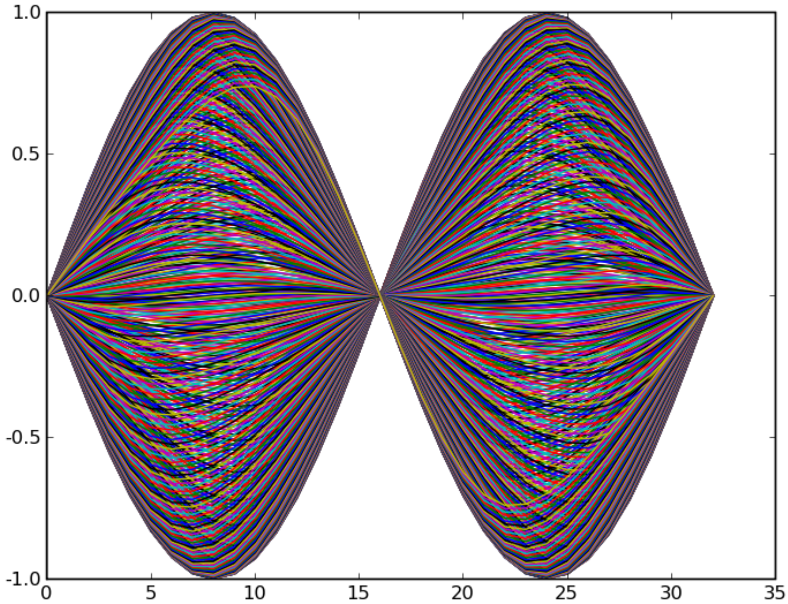


Figure 3: Here, we see 1000 iterations of the intial test superimposed on the same axes. Note the initial conditions are returned to with each oscillation.