Perturbation Methods for the Fermi-Pasta-Ulam Problem

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Abstract:

The Wigner-Brillouin perturbation method is applied to the Fermi Pasta Ulam system of coupled oscillators. The analytic solutions from the perturbation method are compared to numerically integrated solutions to check the validity of the method.

I. Introduction

The Fermi Pasta Ulam experiment was the first scientific foray into the realm of numerical experiments. Physicist Enrico Fermi was working at Los Alamos National Laboratory in New Mexico during the early 1950s when a large computer was constructed to run numerical calculations for the Manhattan Project. Fermi was given access to the computer, named MANIAC I (Mathematical Analyzer, Numerical Integrator And Computer), and decided to run "numerical experiments" on the computer. He enlisted the help of computer scientist John Pasta and mathematician Stanislaw Ulam to help him on the project.

Fermi, Pasta and Ulam decided for their first experiment to study a chain of oscillators, all with unitary mass. They wanted to investigate a system that had previously been immune to analytic solutions, which meant that they would be looking at nonlinear systems. So, in addition to the linear potential between adjacent oscillators, they studied additional nonlinear interaction potentials. One of the first that they tried, and the one that will be the focus of this paper, was the cubic potential, where the energy is dependent not only on the square of the distances between adjacent oscillators but also on the cubes of the distances between adjacent oscillators. This system is described by the Hamiltonian:

$$H = \frac{1}{2}\sum_{i=0}^{N}[\dot{x}_i{}^2 + (x_{i+1} - x_i)^2] + \frac{\beta}{3}\sum_{i=0}^{N}(x_{i+1} - x_i)^3$$

where x_i is the displacement of the ith oscillator with respect to its equilibrium position, $x_0 \equiv 0$ and $x_{N+1} \equiv 0$ as boundary conditions, and β is a dimensionless constant that regulates the size of the nonlinear term.

With this system Fermi, Pasta and Ulam hoped to simulate the thermalization of a crystal lattice as it reached equilibrium. The basic tenets of statistical mechanics led them to believe that as the system evolved it would reach an equipartition of energy, with the same amount of energy in each mode of the system. The modes of this system are precisely the

normal modes, where in each normal mode all of the oscillators have the same frequency. The process of finding these normal modes will be discussed in the next section. Once the system coordinates have been transformed into normal mode coordinates the Hamiltonian becomes:

$$H = \frac{1}{2}\sum_{i=1}^{N}[\dot{q}_i^2 + \omega_i^2 q_i^2] + \frac{\beta}{3}\sum_{i,j,k=1}^{N} c_{ijk}\, q_i q_j q_k$$

where $c_{ijk}$are constants determined by the linear transformation. It is known that a linear system, when initially excited in one of its normal modes, will stay in that normal mode indefinitely. However, in our nonlinear system, the coefficients c_{ijk} show how energy is transferred from one normal mode to another.

For their initial experiment Fermi, Pasta and Ulam set this system to run on MANIAC I with all of the energy initially in the first normal mode. They expected a slow drift of energy from the first normal mode to the other modes, until the equipartition of energy that they were expecting was reached. To their surprise, the system behaved in a much different way. FIG 1 shows a graph of the energy in the first few normal modes as a function of time. Initially all of the energy is in the first normal mode, and then the energy in this mode begins to decrease as the energies of the second, third and fourth modes begin to decrease. (Only the first four modes are shown for clarity.) But instead of leveling off at the appropriate energy level the figure shows that there is an interesting cyclical exchange of energy that occurs, with the majority of the energy cycling from the first to the fourth to the third to the second mode, and then back down again symmetrically.

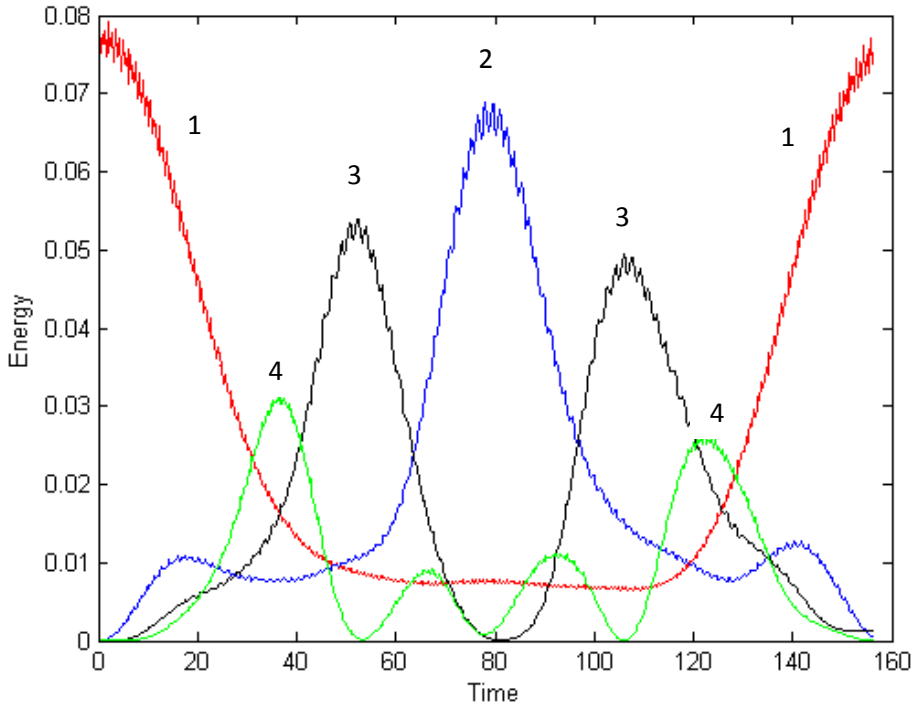

FIG 1: A plot of the first four normal modes of the Fermi Pasta Ulam system showing the recurrence of normal mode energies. This plot is for a system of 32 oscillators with cubic coupling and all of the energy initially in the first mode.

This behavior was unforeseen by Fermi, Pasta and Ulam, who wrote ”Let us say here that the results of our computations show features which were, from the beginning, surprising to us. Instead of a gradual, continuous flow of energy from the first mode to higher modes, all of the problems show an entirely different behavior.”[2] Over half a century later there still remain unanswered questions about the behavior of the system and its importance to the field of statistical mechanics.

Throughout the 1960s physicist Joseph Ford, along with other collaborators, made numerous advances in the study of the Fermi Pasta Ulam problem. What will now be presented is work based off his papers[, in particular the application of perturbation techniques to this system in an attempt to find analytical approximations to the equations of motion.

II. Perturbation Method

The process of finding an approximate analytical solution for this nonlinear system requires us to 1) find the linear transformation that can take us between the spatial coordinates and the normal mode coordinates; 2) use this transformation change Hamiltonian (1) into Hamiltonian (2); 3) apply our particular perturbation technique; and 4) solve the resulting differential equations. After the analytic solutions have been obtained some important characteristics will be pointed out graphically. Since the 2-oscillator case can easily be generalized to N oscillators, that case will be used to develop this process.

First we must find the linear transformation. In order to do this we need to simultaneously diagonalize the kinetic energy and the linear potential energy terms in the Hamiltonian that corresponds to the system

$$\ddot{x}_1 = (x_2 - x_1) - (x_1 - x_0)$$

$$\ddot{x}_2 = (x_3 - x_2) - (x_2 - x_1)$$

The resulting Hamiltonian, when written in the framework of linear algebra, becomes

$$H = \frac{1}{2}\begin{pmatrix}\dot{x}_1 & \dot{x}_2\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\dot{x}_1\\ \dot{x}_2\end{pmatrix} + \frac{1}{2}\begin{pmatrix}x_1 & x_2\end{pmatrix}\begin{pmatrix}2 & -1\\ -1 & 2\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}$$

These two matrices can be simultaneously diagonalized only if they commute. Since they do in fact commute, and since the first matrix is already diagonalized, we only need to diagonalize the second matrix. To diagonalize a matrix A we must find the matrix S such that the columns of S are the eigenvectors of A. Then the following relation holds,

$$D = S^{-1}AS$$

where the diagonal entries of matrix D are the eigenvalues of A and all other entries are zero. Additionally, we will use the normalized eigenvectors of the system. The result of this calculation is

$$\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$$

S is the transformation matrix that we need to apply to the spatial coordinate vector to find the normal coordinate vector:

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Therefore, if we substitute the expressions

$$q_1 = -\frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2$$

$$q_2 = \frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2$$

into Hamiltonian (1), we get

$$H = \frac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2 + 3q_1^2 + q_2^2) + \frac{\beta}{3}(\frac{3}{\sqrt{2}} q_1 q_2^2 - \frac{3}{\sqrt{2}} q_1^3)$$

which is of the form of Hamiltonian (2). Once we have the Hamiltonian we can easily convert this expression into the Lagrangian, and then use the Euler-Lagrange equations to yield the following equations of motion:

$$\ddot{q}_1 + 3q_1 = -\frac{\beta}{\sqrt{2}}(q_2^2 - 3q_1^2)$$

$$\ddot{q}_2 + q_2 = -\sqrt{2}\beta q_1 q_2$$

We now have the nonlinear set of equations for the normal mode coordinates q_i that we would like to solve. In order to accomplish this task we are going to approximate the solutions using perturbation theory. The particular method used is the Wigner-Brillouin method, first employed by Joseph Ford in the study of this problem in reference [4]. For this method we assume solutions of the form

$$q_1 = A_1 \cos(\Omega_1 t + \theta_1) + \beta q_{11} + \beta^2 q_{12} + \cdots$$

$$q_2 = A_2 \cos(\Omega_2 t + \theta_2) + \beta q_{21} + \beta^2 q_{22} + \cdots$$

where the Ω_i's are to be determined from the resulting equations, the A_i's and θ_i's are to be determined from initial conditions, and the q_{ij}'s can be solved for in a successive manner. By plugging these power series expansions of q_1 and q_2 into the differential equations above we obtain

$$(\omega_1^2 - \Omega_1^2)\mathrm{q}_{10} + \beta\big(\ddot{\mathrm{q}}_{11} + \omega_1^2 q_{11} + 1/\sqrt{2}(\, q_{20}^2 - 3q_{10}^2)\big) + higher\ order\ terms = 0$$

$$(\omega_2^2 - \Omega_2^2)\mathrm{q}_{20} + \beta\left(\ddot{\mathrm{q}}_{21} + \omega_2^2 q_{21} + \sqrt{2} q_{10} q_{20}\right) + higher\ order\ terms = 0$$

where $q_{10} = A_1 \cos(\Omega_1 t + \theta_1)$, $q_{20} = A_2 \cos(\Omega_2 t + \theta_2)$, and the ω_i's are the appropriate eigenfrequencies. In order for these equations to hold each power of β must independently equal zero. Notice that in order to solve for q_{11}, q_{21} we must know q_{10}, q_{20}, and to solve for q_{12}, q_{22}we must know q_{11}, q_{21}, etc. In this way we can solve for the i^{th} order of β if and only if we know the solutions for the 0^{th} through the $(i-1)^{st}$order of β.

There are various ways to solve this system of equations, the specifics of which will not be mentioned here. Solving these equations only up to first order in β yields

$$q_1 = A_1 \cos\tau_1 + \beta\left(\frac{3A_1^2 - A_2^2}{2\sqrt{2}\omega_1^2} - \frac{A_2^2 \cos 2\tau_2}{2\sqrt{2}[\omega_1^2 - 4\Omega_2^2]} + \frac{3A_1^2 \cos 2\tau_1}{2\sqrt{2}[\omega_1^2 - 4\Omega_1^2]}\right)$$

$$q_2 = A_2 \cos\tau_2 + \beta\left(-\frac{A_1 A_2 \cos(\tau_1 + \tau_2)}{\sqrt{2}[\omega_2^2 - (\Omega_1^2 + \Omega_2^2)^2]} - \frac{A_1 A_2 \cos(-\tau_1 + \tau_2)}{\sqrt{2}[\omega_2^2 - (-\Omega_1^2 + \Omega_2^2)^2]}\right)$$

$$\Omega_1^2 = \omega_1^2$$

$$\Omega_2^2 = \omega_2^2$$

where $\tau_i = \Omega_i t + \theta_i, i = 1,2$. Although it may not be readily apparent from the above equations, if we include the second order perturbation then we will find further restrictions on the Ω_i's. The above equations for q_1 and q_2 are what we sought at the beginning of this section. They are the equations of motion for the two normal modes of the system, from which we can learn more about the behavior of the system by adjusting the various parameters. Furthermore, using the linear transformation we found earlier in this section, we can transform these equations to obtain the equations of motion for the individual oscillators, which could also shed light on the behavior of the system.

It is important to keep in mind that these analytical solutions arose from the application of a perturbation technique to the given system, and therefore do not represent the true behavior of this system. Of course we hope that the perturbation method used will provide an accurate approximation to the real behavior, and to assure ourselves of this we will compare system behavior through direct numerical integration and through the perturbation method in the fourth section. One attribute we hope to recover in the system is the conservation of energy, which also serves as a simple check on the validity of the Wigner-Brillouin technique in this case. FIG 2 shows the plot of the spatial coordinate Hamiltonian

$$H = \frac{1}{2}(\dot{x}_1^2 + \dot{x}_2^2 + (x_1)^2 + (x_2 - x_1)^2 + (x_2)^2) + \frac{\beta}{3}((x_1)^3 + (x_2 - x_1)^3 + (x_2)^3)$$

where we have transformed back into the spatial coordinates and put all of the initial energy into the first normal mode. There are 0.75 units of energy in the actual system, and our perturbation approximation stays within 0.25% of this value.

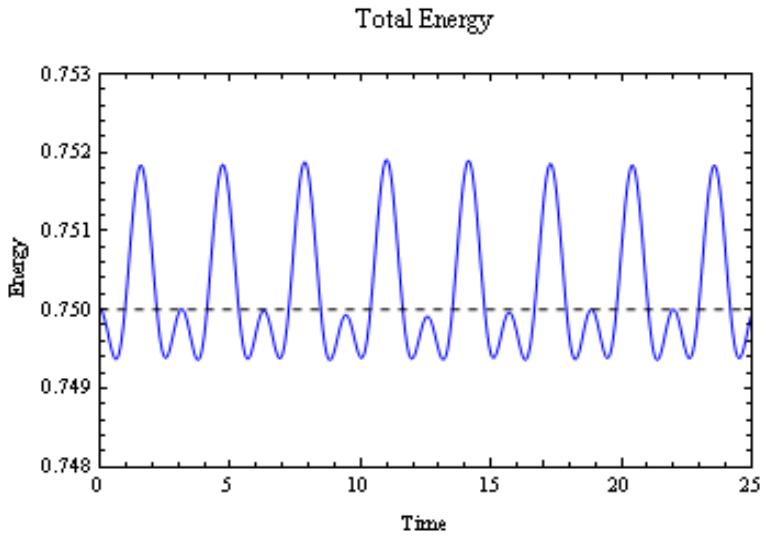

FIG 2: A plot of the total energy in the actual system (black dashed) along with a plot of the total energy from our perturbed solution (blue). Here $\beta = 0.1$. The maximum energy in the perturbed solution is 0.751835 units of energy (0.75+0.245%) while the minimum is 0.74937 units of energy

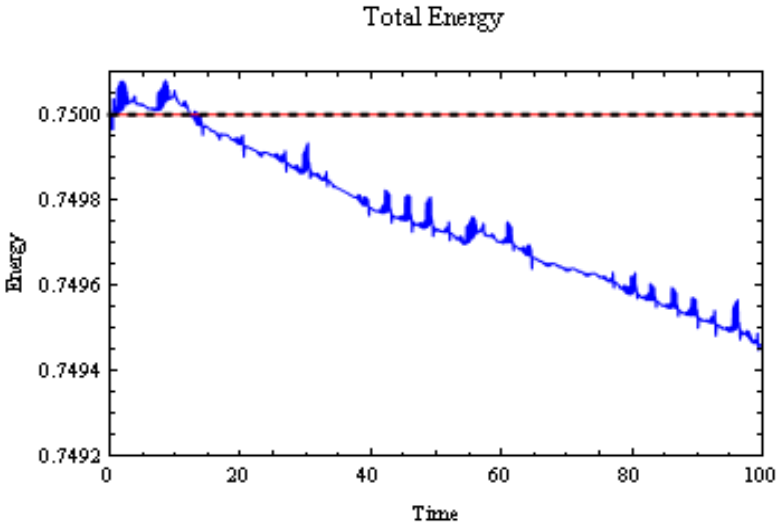

FIG 3: A plot of the total energy in the actual system (black dashed) along with a plot of the total energy from the numerical solution using 5 digits of accuracy (blue) and 10 digits of accuracy (red).

III. Numerical Integration

Next we will turn to a numerical integration scheme to approximate the solution numerically. As before we will check the validity of the resulting solution first by ensuring that the total energy of the system is conserved.

The numerical integration was performed by the Wolfram Mathematica 7.0 program, using the command NDSolve. This command takes as an argument a system of equations, including initial conditions, and the desired accuracy of the computations. Mathematica will automatically select the most appropriate numerical integration method to use, although it can use one particular scheme if desired. FIG 3 shows the total energy of the system resulting from two numerical integrations. The blue line shows the integration with 5 digits of accuracy preserved, which loses energy at a rate of 0.0086% of the initial energy per period over the interval shown.

The red line shows the integration with 10 digits of accuracy preserved, which is exactly 0.75 to within 10 digits of accuracy.

IV. Comparing Results

It now remains to be seen whether or not the perturbation approximation found in Section II accurately reflects the behavior of the system. It has already been shown that conservation of energy is maintained to within 0.25% of its initial value – but that does not shed any light on the particular dynamics of the system. In this section we will compare the analytic solutions obtained from the Wigner-Brillouin perturbation technique to the

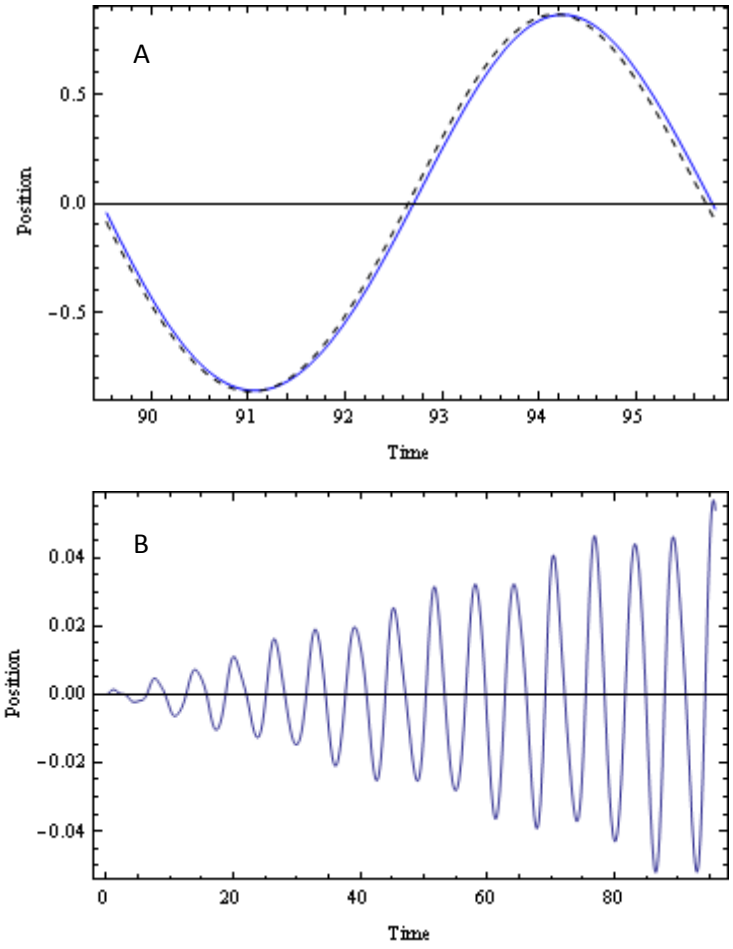

FIG 4: A) Position vs. time plot for the first oscillator. The numerical solution the black dashed line while the perturbed solution is the solid blue line. B) Position vs. time plot for the difference of the numerical and perturbed solutions.

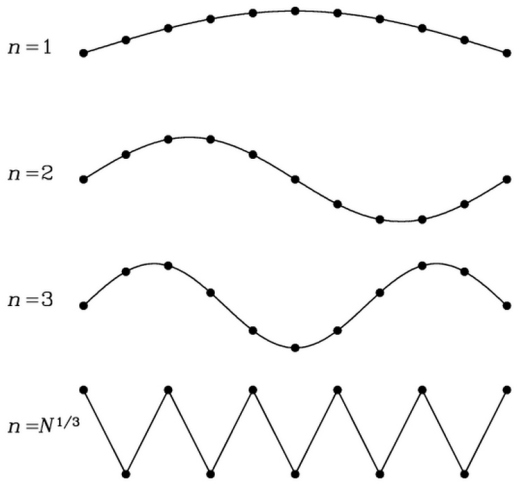

FIG 5: Normal modes for a discrete number of points, adapted from [5].

solutions obtained through numerical integration. All perturbed solutions considered in the following plots correspond to the case $\beta = 0.1$.

FIG 4A shows the numerical (dashed black) and perturbed solutions (solid blue) of the first oscillator plotted alongside each other during the 30th period of oscillation. It can be seen that the perturbed solution has started to fall out of phase with the numerical solution, which is attributed to a shift in the period that is not manifested in the first order perturbation solution. In fact, as stated in Section II, the second order perturbation will give further restrictions on the Ω_is which will shift them. FIG 4B shows the difference of the numerical and perturbed solutions plotted through 30 periods of oscillation. The growth of the oscillations in this graph indicates that the perturbed solution is diverging from the numerical solution. This fact means that in order to glean any useful observations about the behavior of the system from the perturbed solutions we must either restrict ourselves to small values of time or improve the perturbed solutions by moving to the second order.

This agreement between the solutions in the oscillator coordinates allows us to make similar comparisons between the normal mode solutions, which is what is really of interest to us. Recall that the method used by Fermi, Pasta and Ulam was to look at the normal mode energies of the system as it evolved in time. The number of normal modes in a given oscillator system is equal to the number of oscillators (see FIG 5), so in this case we have two normal modes. For initial conditions we will put all of the energy of

the system into the potential energy of the first normal mode. Corresponding to these initial conditions we expect to see all of the energy initially in the first normal mode, and then move from the first normal mode to the second normal mode through the coupling of normal modes brought about by the nonlinear interaction between them.

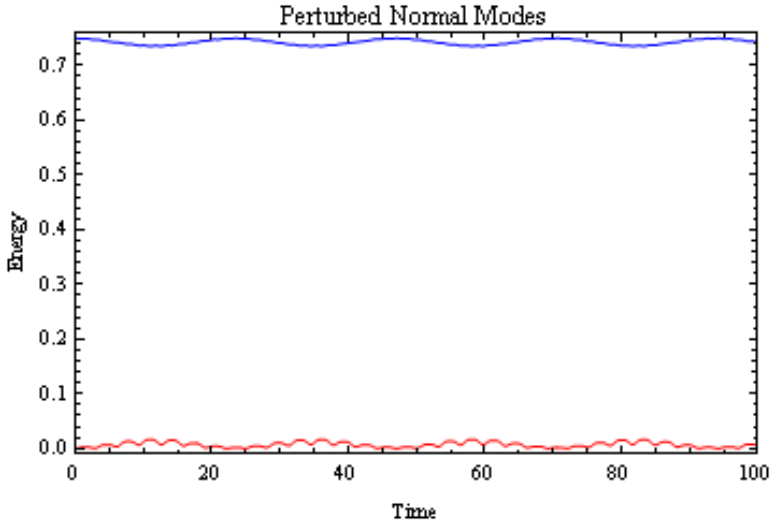

FIG 6: The two normal modes of the $N = 2, \beta = 0.1$ system. Plotted are the perturbation solutions, for the Fermi, Pasta and Ulam frequencies $\omega_1 = 1, \omega_2 = \sqrt{3}$. Different values for the frequencies will correspond to more or less energy sharing between the modes.

FIG 6 shows the two normal mode energies as a function of time over 30 periods. The entire energy of the oscillation is initially contained in the first mode, and then moves to the second mode. The energy in the second mode reaches a maximum after two periods of the system, and then begins to decrease again. The amount of energy that is transferred between modes depends on the periods of oscillation of the normal modes. Here there is a small amount of energy shared, but at frequencies closer to a resonance condition the modes can actually transfer all of the energy of the system between themselves.[4]

FIG 7A shows the amount of energy in the first mode as a function of time. The blue line corresponds to the perturbed solution while the black line corresponds to the numerical solution. As the number of periods increases the analytic solution again begins to diverge from the numerical solution. This is more easily seen in FIG 5c, the corresponding plot for the second mode energy. During the first normal …ode period the two solutions are matched almost exactly, but by the fourth considerable differences are already beginning to develop.

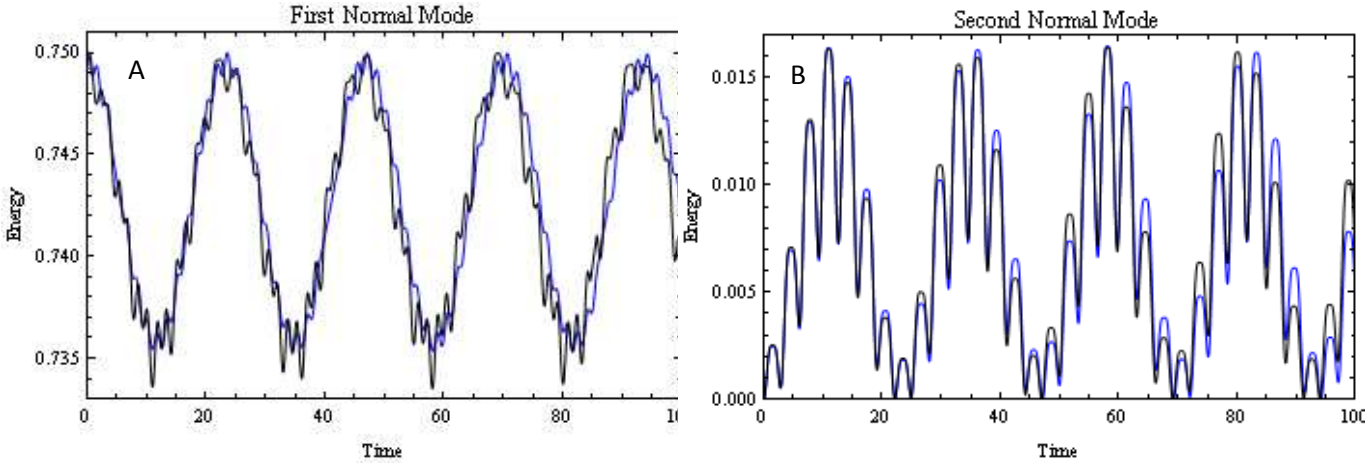

FIG 7: A) The first normal mode energy of the system, and B) the second normal mode energy of the system. In both plots the blue line corresponds to the perturbed solution and the black line corresponds to the numerical solution.

V. Conclusion

The problem initially confronting Fermi, Pasta and Ulam was to find a way to investigate a nonlinear system using new computing technologies. After they successfully translated the problem into a numerical experiment, the problem of explaining their unexpected results became a challenge to physicists, mathematicians and computer scientists alike. Although great progress was made during the 1960s and afterwards, there has yet to be a satisfactory theory that explains all of the curious aspects of this system's behavior.

The goal of this paper has been to validate the use of the Wigner-Brillouin perturbation technique with the Fermi Pasta Ulam system. After developing the method for the two oscillator case the analytic results were compared to numerically obtained results to establish whether or not this method is appropriate for the system. The perturbation solutions agree very well with the numerical solutions and conserve energy for over 30 periods to within 0.25%. However, as time increases the solutions begin to diverge from the numerical solutions, limiting their use for characterizing the system at large times. One possible approach to improve the solution would be to take the perturbation approximation out to higher orders, although even the second order perturbation becomes complicated.

There are many possible paths to follow from this point, as many aspects of this perturbation solution have not been considered here. The accuracy of the perturbation solution as a function of the perturbation parameter β needs to be considered, because the Wigner-Brillouin technique requires a small perturbation to be effective. Larger numbers of oscillators should also be considered and the resulting perturbation solutions should be compared to numerical solutions in order to verify that the theory holds independent of oscillator number. Lastly, and one of the most interesting paths, is that of finding curious behavior in these systems and attempting to pinpoint the cause of this behavior within the analytic solutions themselves. This of course could be a tedious exercise but one that might yield physical explanations for these behaviors, including energy sharing, energy recurrence, and of course the absence of any equipartition of energy within the system.

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