MA 6307 Semester Project Report: Visualization of Ergodicity of a Nonlinear System

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Introduction

It is an experiential fact that macroscopic systems are dissipative - they converge to states that are macroscopically at an equilibrium, and eventually produce statistics of a stationary distribution. On the other hand, the fundamental physics behind the microscopic state of these systems are necessarily conserving of energy, and non-dissipative. How the convergent statistics arise from a non-dissipative system is therefore of physical interest. The ergodic behavior of nonlinear systems is relevant to statistical mechanics, to explain the unpredictable, macroscopically dissipative, and statistical behavior of deterministic systems, and whether or at what rate equipartitions of energy, or other statistical distributions among possible states are produced. Equipartition of energy is assumed in many statistical mechanics proofs of the thermodynamic behavior of systems, and these arguments depend on the ergodic behavior of the systems.

The ergodic hypothesis is a property attributed to the behavior of nonlinear ordinary differential equation systems. This property was originally proposed by Ludwig Boltzmann during the 1870's.[1]

For energy preserving dynamic systems, the state of the system is confined to a level surface of the total system energy. In linear systems, the time evolution of the system, while complex, can be factored into the time-evolution of the normal modes. For nonlinear systems, the time evolution of the system can be considerably more complex, as no independently evolving normal modes exist which can be superimposed linearly. The trajectory of the nonlinear systems were historically assumed to have the property that they "invade the energy surface densely", meaning that for arbitrarily fine resolution, the long-time averaged probability of finding the system at any point of the energy surface is nonzero. The fraction of time spent in or near any part of the energy surface is proportional to the surfaces Liouville measure.[1]

$$\frac{\int_{\Lambda} \delta(H(p,q)-E)\, dp\, dq}{\int_{\Sigma_{\mathrm{E}}} \delta(H(p,q)-E) dp dq} \tag{1}$$

Linear, Hamiltonian, time-independent systems have eigenvalues which are entirely imaginary. These correspond to non-dissipative systems, which preserve the energy of their motion. Each normal mode evolves in time in an orderly fashion. The energy in each normal mode is independently conserved, and therefore such systems cannot exhibit the ergodic property. Because the energy is conserved in each mode independently, the trajectories of the system can inhabit at most an N-dimensional surface in the 2N dimensional state-space, or the 2N-1 dimensional energy surface. For time independent systems, this takes the form of a hyper-torus in configuration space: the topological product of the circular paths taken by each set of normal-mode position and momentum coordinates.[2]

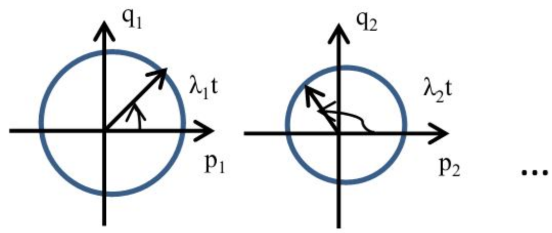

Figure 1. Depiction of evolution of normal modes with time

Enrico Fermi, John Pasta and Stanislaw Ulam in 1954 conducted a numerical experiment to investigate the rate at which a simple, weakly nonlinear system approached equipartition of energy among the normal modes of the associated linear system. [3]

The system investigated by the FPU numerical experiment was an array of nonlinear oscillators obeying an equation which was the discretization of the vibration of a linear string. Nonlinear perturbations were added to the force laws of the springs. Quadratic, cubic, and piecewise continuous terms were added to the tension model. [3]

$$\ddot{x}_i = (x_{i+1} + x_{i-1} - 2x_i) + \alpha[(x_{i+1} - x_i)^2 + (x_i - x_{i-1})^2] + \beta[(x_{i+1} - x_i)^3 + (x_i - x_{i-1})^3] \qquad (2)$$

The nonlinear model was integrated for many thousands of cycles of the model's normal modes. The sharing of energy among the various normal modes of the linear system never approached an equipartition, or even a statistically steady state. Instead, the system continued to periodically almost re-attain the initial state. High mode numbers never participated, and energy was shared significantly only between the first few modes. [3]

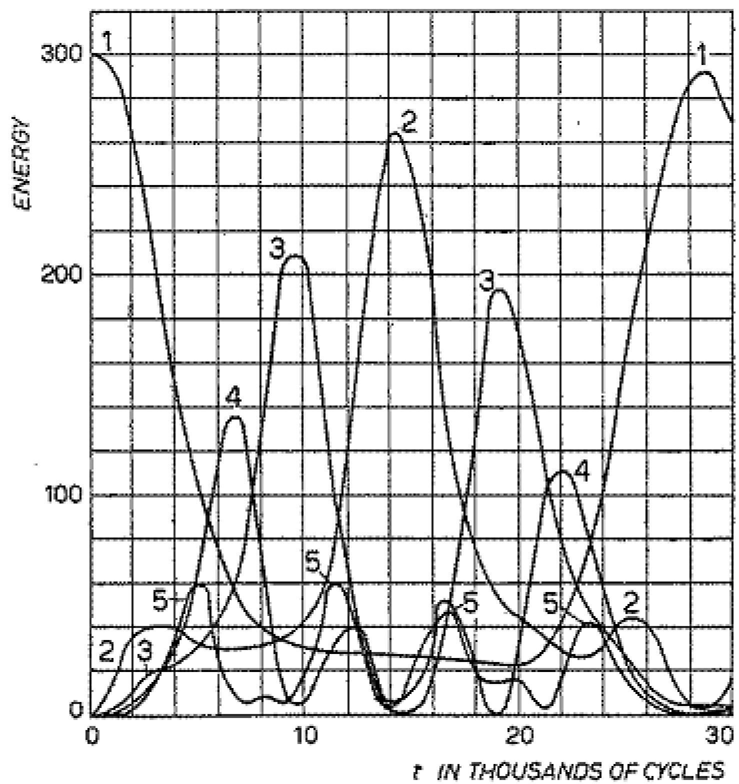

Figure 2. (Figure 1 from the FPU paper) This demonstrates the energy in each of the first few modes for 30,000 cycles[3]

The Fermi-Pasta-Ulam numerical experiment demonstrated that the ergodic property often fails to manifest for weakly nonlinear systems. It is difficult to prove that a system will eventually behave ergodically.

Numerical System, and Visualization Methods:

In this paper, a low dimensional linear system is integrated. The system has only four state variables for the purpose of visualization of the flow, and the statistics with which the flow moves across the energy surface. Nonlinear terms are added to the system and the effect on the flow and statistics are visualized.

The system chosen is that of a two-mass, two-spring network, shown below.

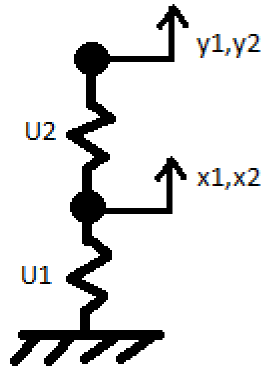

Figure 3. Low DOF nonlinear spring-mass system

The ordinary differential equations governing this system are as follows:

$$\begin{cases} \dot{x_1} = x_2 \\ \dot{x_2} = -\dfrac{\partial U_1}{\partial x_1} - \dfrac{\partial U_2}{\partial x_1} \\ \dot{y_1} = y_2 \\ \dot{y_2} = -\dfrac{\partial U_1}{\partial y_1} - \dfrac{\partial U_2}{\partial y_1} \end{cases} \tag{3}$$

$$H = \frac{1}{2}({x_2}^2 + {y_2}^2) + U_1(x_1, y_1) + U_2(x_1, y_1) \tag{4}$$

$$U_1 = \frac{1}{2} * k_{11} * {x_1}^2 + k_{12}x_1^3 + k_{13}x_1^4$$

$$U_2 = \frac{1}{2}k_{21}(y_1 - x_1)^2 + k_{22}(y_1 - x_1)^3 + k_{23}(y_1 - x_1)^4 \tag{5}$$

Choosing $k_{11} = 1$, and $k_{21} = 1$ for the linear part of the system, the following eigenvalues, corresponding to the angular rates, and normal modes are obtained:

$$\lambda_{1,2} = \pm 1.6180i$$

$$v_1 = \begin{bmatrix} 0.4427i \\ 0.7236 \\ -0.2764i \\ 0.4472 \end{bmatrix}$$

$$\lambda_{3,4} = \pm 0.6180i$$

$$v_3 = \begin{bmatrix} 0.4427 \\ 0.2764i \\ 0.7236 \\ 0.4472i \end{bmatrix}$$

These particular stiffness coefficients yield normal modes that have eigenvalues that are not rational fractions of each other. The linear system, in this case, will, in general, densely fill a 2-parameter subsurface of the 3-parameter energy surface if it is started in anything but a pure excitation of one of the normal modes.

In order to facilitate the visualization of the flow of the ODE, a nonlinear map from the four dimensional state space to an appropriate 3-dimensional space is produced. A nonlinear map is found between the state variables [x1,x2,y1,y2], and a three-dimensional, non-Euclidean set of coordinates tangent to the energy surface denoted [u1, u2, u3]. The linear system may have an easy analytical solution to parameterize the tangent space coordinates in terms of the state variables, but in general the nonlinear systems may have a more complicated shape to the energy surface. A numerical method is used to solve for the coefficients of a polynomial map, a Taylor series relative to the initial condition of the problem:

$$u^i = h_j^{1i}(x^j - x_c^j) + h_{jk}^{2i}(x^j - x_c^j)(x^k - x_c^k) \tag{6}$$

The first order terms are found by using Gram-Schmidt orthonormalization of the vectors $\{d\hat{x}^1, d\hat{x}^2, d\hat{x}^3\}$ with respect to the local gradient of the energy surface $\overrightarrow{dE}$, and each other. The remaining terms are found by transporting the basis of vectors $\{\hat{u}^1, \hat{u}^2, \hat{u}^3\}$ to several neighboring points, renormalizing their orientation with respect to the energy gradient vector $\overrightarrow{dE}$, and solving a linear-least-squares problem for the coefficients h_{jk}^{2i} which best reproduce the transported vector bases.

This gives a map to a three dimensional space, in which the flow of the ordinary differential equation system can be conveniently plotted. The polynomial map can only remain tangent to the energy surface over a finite radius of convergence which is tested via a shooting method and analyzing the relative error of the energy of the map ccoordinates to the energy at the origin of the coordinate system. Higher order terms to the map would help it converge over a larger domain, but in general it takes more than one map to completely cover a noneuclidean surface faithfully.

In the analysis, integration planes are set up in the u coordinate system. These planes count the number of times the flow of the ODE carries it past the plane in a certain small square $du^i \wedge du^j$. This is averaged over the length of time over which the system is integrated, and will help with the visualization of how densely the trajectory of the system is filling the 3-parameter energy surface.

Results and Discussion:

If initial conditions are chosen such that only one of the normal modes is excited, the trajectory of the linear ODE revisits the same point periodically. Due to the non-rationality of the eigenvalue (normal mode frequency) ratio, if the linear function is started in a mixed-mode, the trajectories densely fill a two-parameter surface, as shown below in Figure 4a for x_0 = (Normal Mode 1 + Normal Mode 2) (hereafter NM1,NM2 will refer to the real (zero phase) parts of the two normal modes of the system).

Additionally, in figure 4b, the relationship between the figure, trimmed to its range of validity, versus the complete projection of x into u is shown. The radius at which the nonlinear map is truly tangent to the energy surface is taken to be the radius at which the energy of the map significantly diverges from the energy of the energy surface. $\left|\frac{E_{map}(u(x_{limit})) - E_{surface}(x_{center})}{E_{surface}(x_{center})}\right| < 0.25$ The nonlinear map is strictly only tangent to the energy surface when the radius is less than the value produced by this. Outside of this bound, distinct flow lines may cross in the no-longer-tangent projection. Future visualizations will be limited to this radius of convergence.

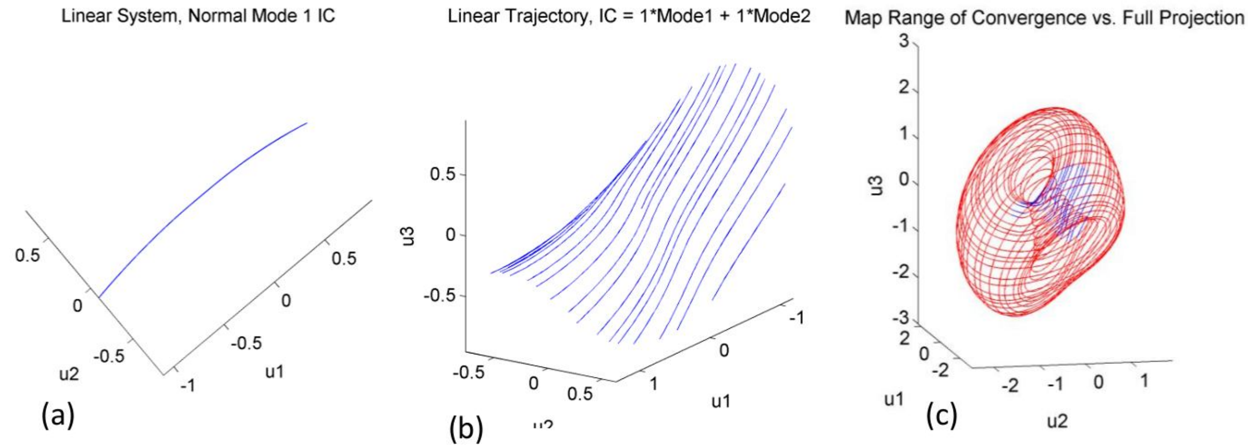

Figure 4. a) The normal modes of the linear system repeat periodically. b) The mixed modes of the linear system sweep out a 2-parameter surface within the energy-surface. c) The entire energy surface cannot be mapped with a single coordinate transformation. Outside the range of validity, the flow crosses in the projection.

Nonlinearity is added to the system of equations by setting the parameters k_{12},k_{13},k_{22}, and k_{23} equal to 0.05. With weak nonlinearity, and using initial conditions of 1x and 10x the first normal mode, the comparison between the linear and nonlinear trajectories can be seen below. The trajectories are integrated, using 4th order Runge Kutta, for a time of 150π.

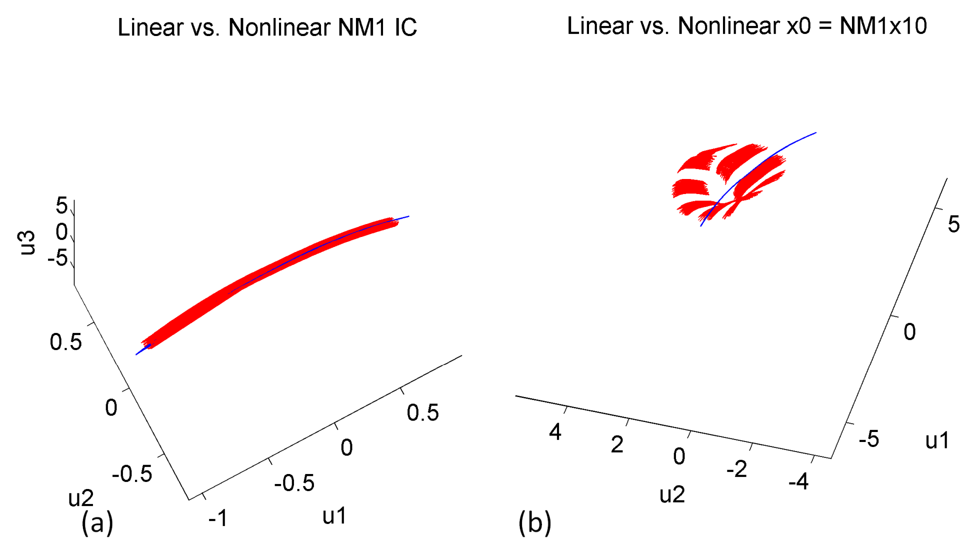

Figure 5. Linear (blue) vs. nonlinear (red) trajectories. a) 1x NM1 b) 10x NM1

The nonlinear equation's trajectory appears to be densely filling a two-parameter surface, compared with the periodic (one parameter) orbits of the linear equation's normal mode.

Looking at a mixed mode initial condition of 4xNM1+4xNM2, the nonlinear equation's trajectories still appear to densely fill only a two-parameter surface.

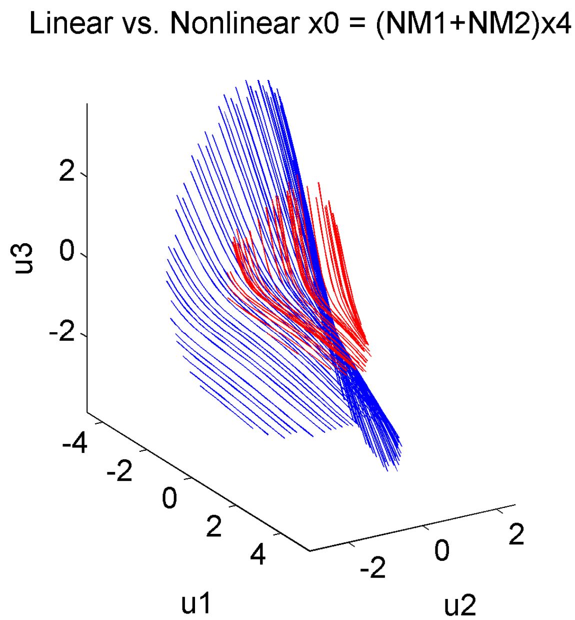

Figure 6. Linear (blue) vs. nonlinear (red) trajectory surfaces

A plane is set up along the u2-u3 axes, and the number of times the trajectory crosses the plane within a given differential area and time is counted. The time-average of plane-crossings per unit time is reported in the figures below for several initial conditions. The trajectories are integrated until t=30,000. The planes have 300x300 counting-bins in the range of the plots shown below:

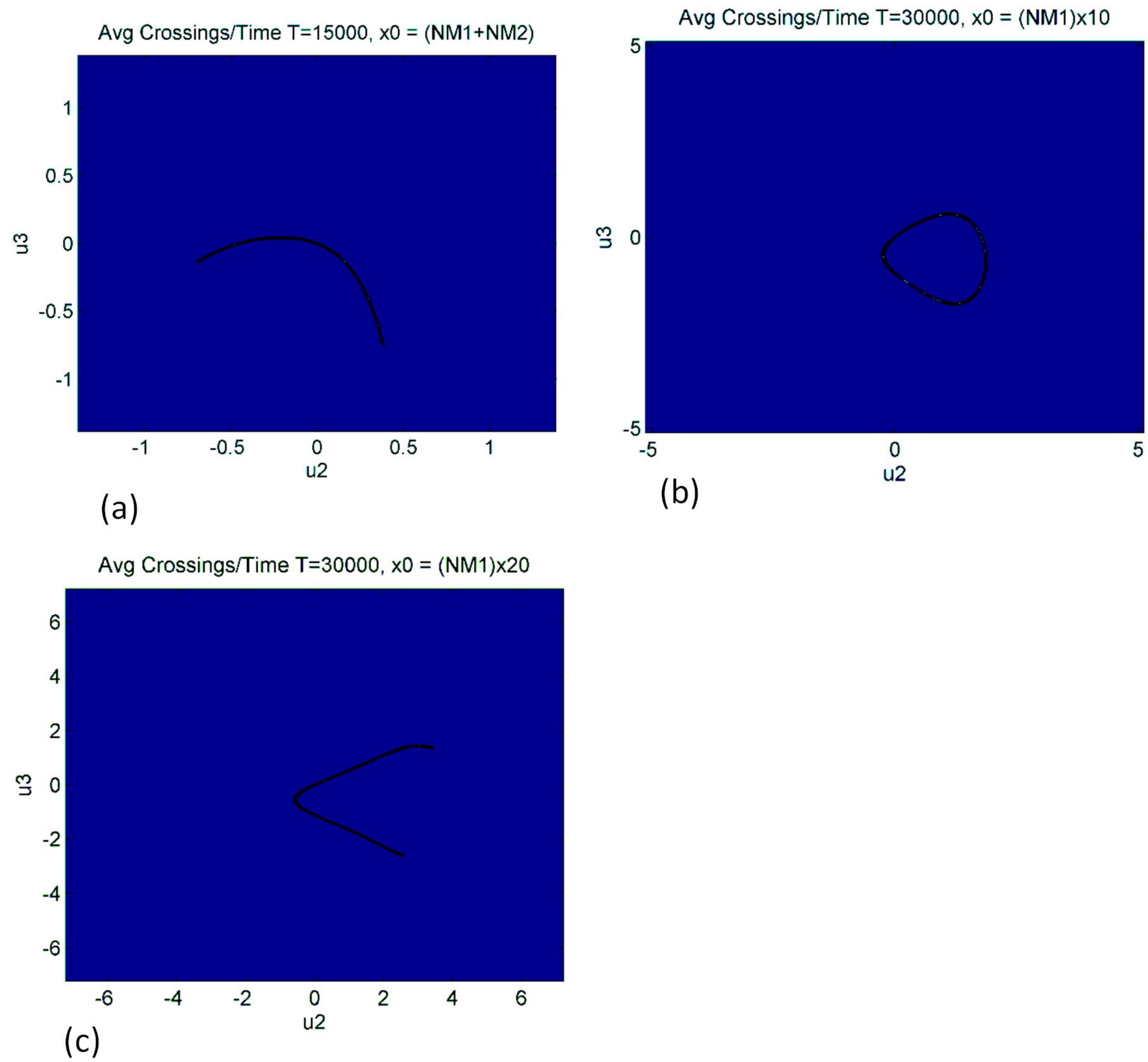

Figure 7. Long-time integrations of crossings of the u1-u2 plane, diferent ICs, nonlinear springs

These solutions are not producing the sort of even mixing predicted for an ergodic system. Only a two-parameter surface (with a one-parameter intersection with the u2-u3 plane) is being filled by the trajectories of the system, not the entire energy surface. As long as the system produces trajectories that fill only a two-parameter curve, it sugests the existence of a second conserved quantity that is not being destroyed by the nonlinearity of the force laws. The exterior force of the anchor point should be destroying the conservation of momentum symmetry.

As a last resort, the nonlinearity of the system is increased significantly. k_{12},k_{13},k_{22},k_{23} are set to 0.5, and the trajectory is integrated starting at a 20xNM1 initial condition for a period of T=300,000.

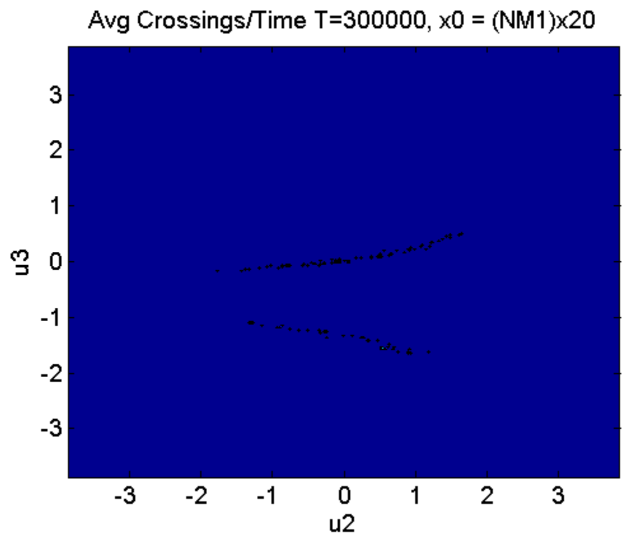

Figure 8. Highly nonlinear springs, energetic system, very long integration

Variation here is probably due to numerical error. The intersection still looks like it is a one-parameter curve.

Returning to the original set of parameters, and varying the initial condition to be several combinations of each normal mode, a nested shear of one-parameter intersections is produced. There is no inter-sheaf mixing evident.

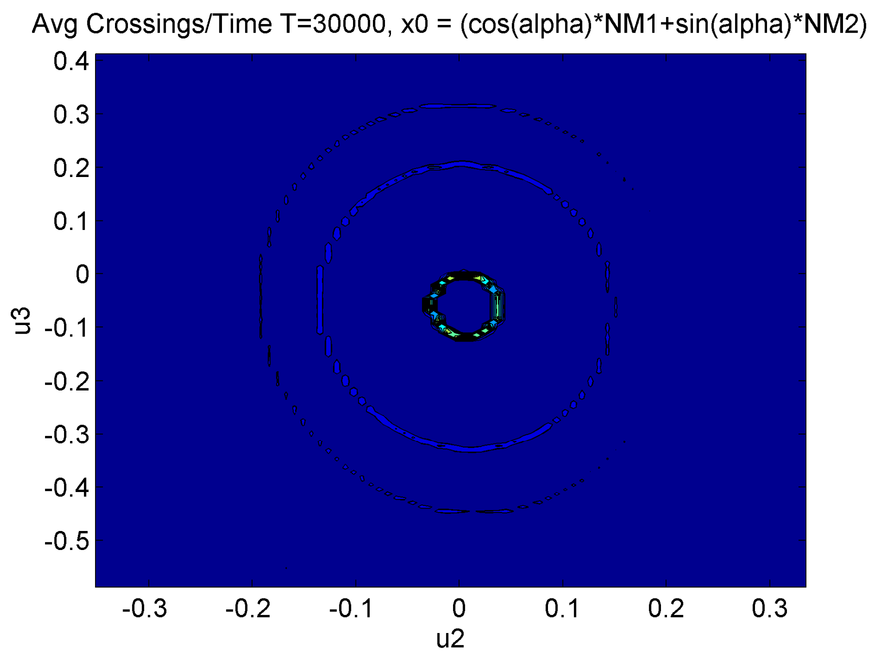

Figure 9. Nested one-parameter curve intersections of trajectories starting from different ICs, original nonlinear spring potential case

Conclusions:

In the simple nonlinear spring-mass system, the ergodic property does not obtain. The energy surface is not densely invaded by the trajectories of the system for any of the investigated conditions. Even in highly nonlinear circumstances, with high energy initial conditions, the trajectories invade at most a two-parameter surface, not the entire three parameter energy surface. The two-parameter surfaces swept out by the trajectories vary smoothly with varying the initial conditions at constant energy and appear to nest neatly.

This system must have another conserved quantity which is not destroyed by the nonlinearities in the inter-particle potentials. Chaotic or ergodic behavior is not necessarily a feature of this simple system, no matter how nonlinear. This result may be due to the simplicity of the system, or it may be akin to the Fermi-Pasta-Ulam system producing its own quasi-periodic behavior and not yielding equipartion of energy.

In my own system, $u_2=0$, $u_3=0$ represents where the trajectories cross the plane, and correspond to the initial condition. While my own system is much simpler than the FPU oscillator, the system does return periodically to being arbitrarily close to the initial conditions, even in the highly nonlinear case, a similar behavior to the FPU system.

References:

1. Gallavotti, Giovanni, Federico Bonetto, and Guido Gentile., Aspects of ergodic, qualitative and statistical theory of motion, Springer, 2004.
2. Ford, Joseph., "The Fermi-Pasta-Ulam Problem: Paradox Turns Discovery," Physics Reports (Review Section of Physics Letters) 213, No 5, (1992) 271-310.
3. Fermi, Enrico, J. Pasta, and S. Ulam. "Studies of nonlinear problems," No. LA 1940. I, Los Alamos Scientific Laboratory Report No. LA-1940, 1955.

Appendix:

The software code for this project is too long to list easily here. It is available upon request from Aaron M. Schinder, aschinder3@gatech.edu, 937-626-7651, and a software copy will be provided to Prof Raphael de la Llave, Georgia Institute of Technology along with this semester project report.