

Research Project-Based Learning in Practice:

Student Poster Presentations and Project
Report Example in PHYS460(undergraduate
students)/PHYS660(graduate students)
course on *Computational Methods of Physics*
<http://www.physics.udel.edu/~bnikolic/teaching.html>
conducted by the PI at the University of
Delaware in Spring 2003, 2004, and 2005



Poster Sessions of PHYS460/660 Course in Pictures:

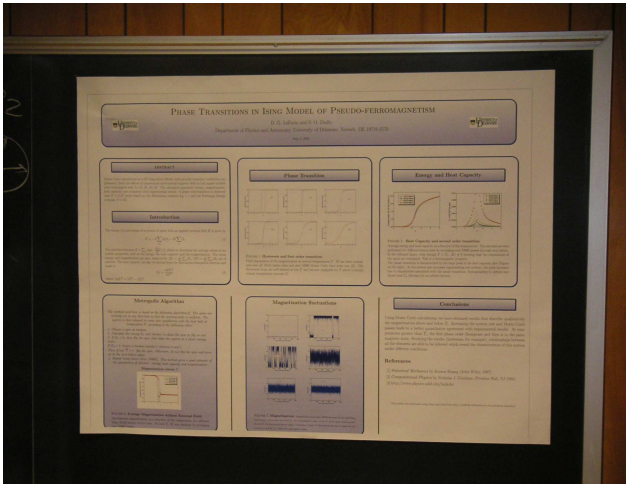


Fig. 1: Snapshots from the poster session of Computational Methods of Physics held on May 3, 2004 at the Department of Physics and Astronomy, University of Delaware. Each poster presents the results and physical insights obtained by a research team (composed of one undergraduate and one graduate student) through extensive numerical simulations of the first order phase transition in the Ising model of ferromagnetism.

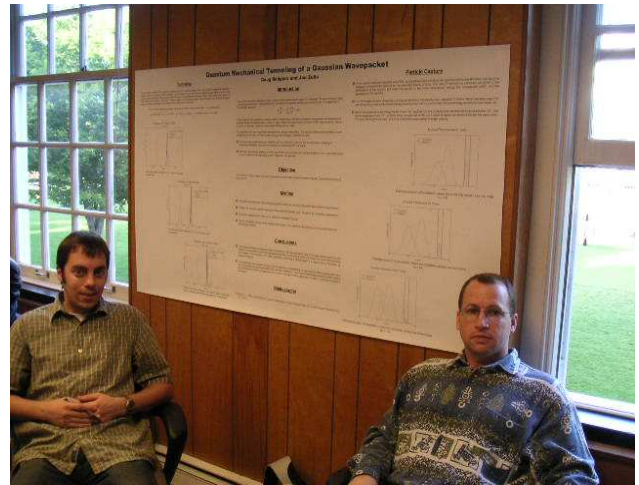
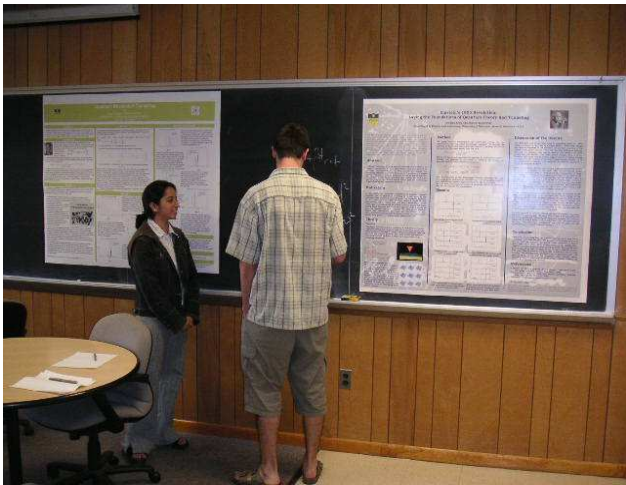


Fig. 2: Snapshots from the poster session of Computational Methods of Physics held on May 10, 2005 at the Department of Physics and Astronomy, University of Delaware. Each poster presents the results and physical insights obtained by a research team (composed of one undergraduate and one graduate student) has obtained through extensive numerical simulations of tunneling through single potential barrier and resonant tunneling through double barriers in semiconductor heterostructures.

Example of a Student Report in PHYS460/660 Course:

The report of the student Douglas Rodgers presents results on vibrations in one-dimensional model of glasses, as well as a demonstration of the resolution of the celebrated Fermi-Pasta-Ulam paradox in such systems (with non-linear interactions between the chain of atoms) when they are tuned to "strong stochasticity threshold"

Vibrational Modes of Glasses - Effects of Disorder and Nonlinearity

Douglas Rodgers

Department of Physics and Astronomy, University of Delaware, Newark, DE 19716-2570, USA

The effects of disorder and nonlinear forces on a silicon chain are examined here. Two cases are discussed: a long chain with Born-Von Karman (BVK) boundary conditions, randomized spring constants, and linear forces; and a short chain with fixed boundary conditions, uniform spring constants, and nonlinear forces.

For the first case, it is found that the mobility edge in the density of states is located at an energy of ~ 80 MeV.

For the second case, it was found that the Fermi-Pasta-Ulam (FPU) Paradox could be overcome by simply “pumping” enough energy into the system so that it could escape from the mode it originally started in, and transfer its energy through different modes (ie. solutions when linear forces are applied).

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I. INTRODUCTION

The structure of silicon “glass” can be reasonably estimated using a linear chain of N atoms connected with springs. If the so-called Born-Von Karman boundary conditions are chosen, then the ends of the chain are connected, forming a ring of oscillators with periodic boundary conditions. The force on atom i is given by:

$$m \frac{d^2}{dt^2} x_i = -K_{i-1}(x_i - x_{i-1}) - K_i(x_i - x_{i+1}) - \beta(x_i - x_{i-1})^3 - \beta(x_i - x_{i+1})^3$$

where x_i is the displacement of particle i from its equilibrium position, K_{i-1} is the spring constant of the spring preceding atom i , and β is a parameter that determines the strength of the non-linear component.

If the springs act linearly ($\beta = 0$), then the system of linear differential equations becomes:

$$\begin{aligned} m \frac{d^2}{dt^2} x_1 &= -K_N(x_1 - x_N) - K_1(x_1 - x_2) \\ m \frac{d^2}{dt^2} x_2 &= -K_1(x_2 - x_1) - K_2(x_2 - x_3) \\ &\vdots \\ m \frac{d^2}{dt^2} x_N &= -K_{N-1}(x_N - x_{N-1}) - K_1(x_N - x_{N-1}) \end{aligned}$$

This can be rearranged to obtain an eigenvalue equation. The matrix that needs to be diagonalized is:

$$\begin{pmatrix} K_N + K_1 & -K_1 & 0 & \cdots & -K_N \\ -K_1 & K_1 + K_2 & -K_1 & \cdots & \vdots \\ 0 & -K_2 & K_2 + K_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & -K_{N-1} \\ -K_N & \cdots & 0 & -K_{N-1} & K_{N-1} + K_N \end{pmatrix}$$

Its N eigenvectors correspond to the normal modes of the system, with the components of the eigenvectors being the displacement from equilibrium of each atom. The eigenvalues are equal to the square of the eigen-energies (the important quantities).

It is important to note that, if nonlinear forces are used ($\beta \neq 0$), there is no analytical solution for the modes of the chain since a set of distinct normal modes does not exist. The set of N coupled nonlinear differential equations must be integrated numerically to find the different combination of modes of the system.

We will be exploring two important cases: disorder in the springs of a long chain, and nonlinearity in the forces of a short chain.

II. DISORDER: BVK

Suppose we define some initial spring constant K_0 . We then choose some range to above and below this value, and set the spring constant to random values that fall within this range:

$$K_i = K_0 (1 + \text{rand}(-b, b))$$

where b defines the range of the random number.

We first find each mode by diagonalization of the K matrix, as well as the energies associated with these modes for “clean” ($b = 0$) and “disordered” systems. Had we chosen non-periodic boundary conditions, we would only need to diagonalize a tridiagonal matrix. However, the necessity to include traveling waves means that the cyclic tridiagonal matrix (above) is the what is required. With fairly non-sophisticated algorithms, this is a fairly arduous, but necessary task using standard Numerical Recipes routines.

In order to prevent any peculiar behavior that may arise from the discrete nature of the chain, 3000 atoms

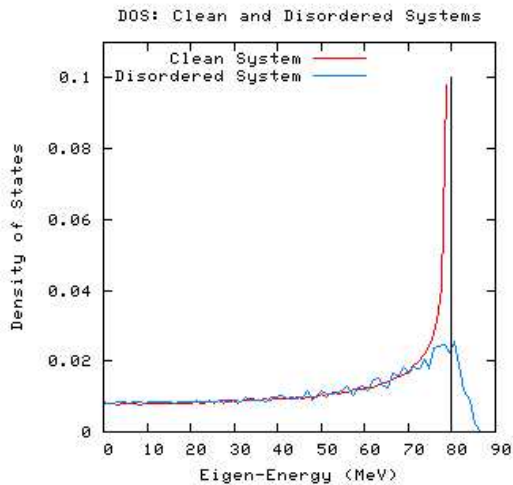


FIG. 1: The Density of States for an $L = 3000$ chain of atoms.

($L = 3000$) was deemed satisfactorily large. The initial spring constant is $K_0 = 10.6 \text{ eV}/\text{\AA}^2$, while the strength of the randomization was taken to be $b = 0.3$.

After the modes were found for the clean and disordered systems, the Density of States (DOS) was calculated by taking the eigen-energies found and counting how many fall within a certain energy range (and normalizing). The bin size was chosen large enough so that pixelization of the curves was minimized, but small enough to prevent an overly “noisy” curve.

The DOS’s for the clean and disordered systems are shown in Figure 1. The singularity in the clean system around 80 MeV locates the so-called “mobility edge.” This is the energy level at which nearly all atoms in the disordered chain are localized.

This localization becomes readily apparent when we calculate the participation ratio of as a function of the energy levels (P_i vs. ω_i). For a particular eigenstate $e_i(a)$ (which corresponds to the energy ω_i), we have:

$$P_i = \left[\sum_{a=1}^L [e_i(a)]^4 \right]^{-1}$$

This tells us the number of atoms that participates in each vibrational mode. So if, at a certain energy, every atom participates (vibrates) in the mode, then we would expect a participation ratio of 3000 here. However, if only a few atoms participate (ie. a localized mode) then we would expect a small participation ratio.

In Figure 2, we see the Participation Ratio for the clean and disordered systems. As expected, the localization around the mobility edge is extremely apparent as the participation ratio drops off as it nears the edge. Note that for clean system, only 2/3 of the atoms regularly participate in the vibration. Only for the maximum

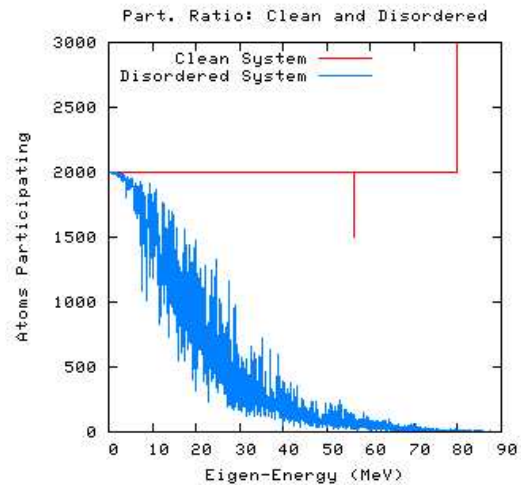


FIG. 2: The Participation Ratio for $L = 3000$.

and minimum (not apparent due to the resolution) energies do all the atoms participate. For the non-translation modes, fully 1/3 of the atoms rest on nodes of the vibration, so that they do not vibrate themselves.

Having discussed the effects on the vibrational modes due to disorder, we now turn our attention how nonlinearity effects a linear chain.

III. NONLINEARITY: FPU

When the force on an atom in the chain is nonlinear ($\beta \neq 0$), we can no longer find modes of vibration by simple diagonalization since a complete set of “localized” modes doesn’t exist.

Instead, we must integrate the equations of motion numerically, and perform a Fourier Transform to determine what modes exist in the vibration. In order to integrate the equations of motion of the particles, we first need initial conditions. The natural choice is to use one of the eigenstates of the linear ($\beta = 0$) case. Then, set β equal to a non-zero value (we choose $\beta = .2$), and then numerically integrate the equations of motion for a sufficient duration.

Performing a Fast Fourier Transform of the position of one of the atoms as a function of time allows us to see what frequencies are present in the oscillation of the particle.

For linear forces, once a system is in a certain mode, it will stay in that mode indefinitely. Fermi, Pasta, and Ulam hypothesized that, when a nonlinear system starts out in a single mode, the nonlinearity will force the system to evolve through different modes. In order to determine if this is the case, the number of atoms was taken to be $L = 128$, $K_0 = 1$, and the following procedure was utilized:

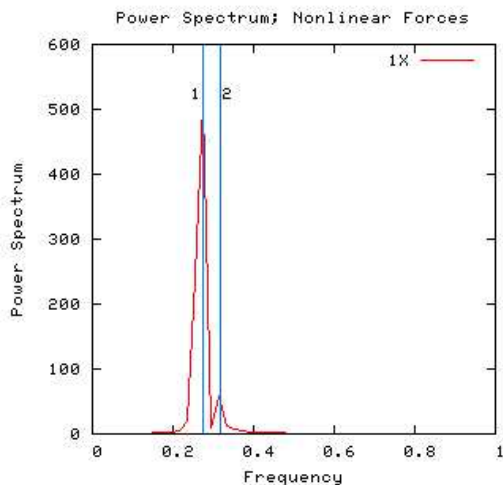


FIG. 3: Power Spectrum for $L = 128$ chain, using a 1X energy boost.

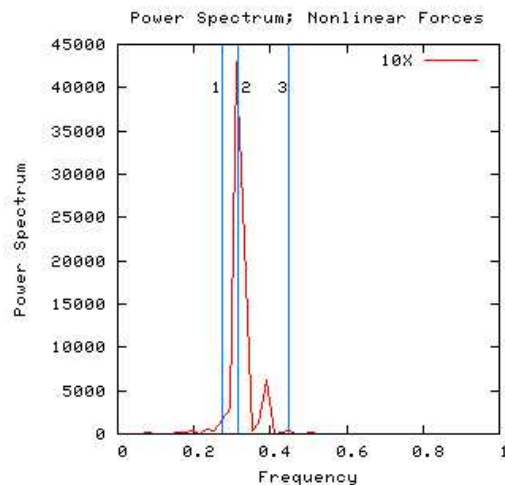


FIG. 4: Power Spectrum for $L = 128$ chain, using a 10X energy boost.

- Find the eigenstates for the linear, $\beta = 0$ case, for use as initial displacements.
- Choose an eigenstate and scale it by a factor $E = 1, 10, 20, 30, 40$. This factor determines the amount of energy “pumped” into the system.
- Using this scaled eigenstate as the initial displacements of the atoms, integrate the equations of motion (using the Verlet Method) for an extended duration using the nonlinear forces ($\beta = 0.2$).
- Finally, take the FFT of the position of one of the atoms (as a function of time) and calculate the Power Spectrum to examine the frequency distribution in the vibration of the atom.

The results are shown in Figures 3-7. The eigenstate chosen for the initial conditions from here on was chosen so that its eigenvalue fell in the middle of the range. The same eigenstate was used in every case.

In Figure 3, for a low energy system that originally started in one mode, it essentially stayed in that one mode (labeled “1”). There seemed to be some kind of spreading to another mode (labeled “2”), but just looking at this Power Spectrum is indeterminate.

Moving on to Figure 4, when the energy factor was increased to $E = 10$, we see that there seems to have been a transfer from mode 1 to mode 2. The peak for mode 1 is always completely gone, while the mode 2 peak dominates. Also highlighted is a barely visible bump labeled “3” that will make a dramatic appearance as we increase the energy further.

For $E = 20$ (Figure 5), we see now that as we transition from 10X to 20X, mode 3 becomes excited. Also notice that mode 1 has re-emerged.

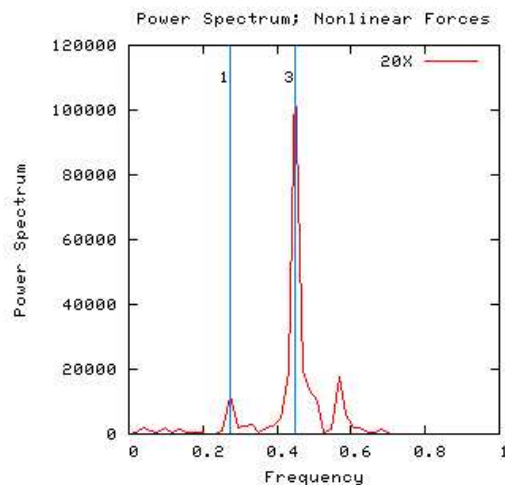


FIG. 5: Power Spectrum for $L = 128$ chain, using a 20X energy boost.

This process of transitioning through modes continues as we increase the energy input.

In Figure 6, we again see a loss of modes that previously existed, and a growth of modes that seemingly did not exist.

For clarity’s sake, I should reiterate that, for each value of E , the system was initialized in the same eigenmode (scaled by E), and allowed to evolve for equal durations.

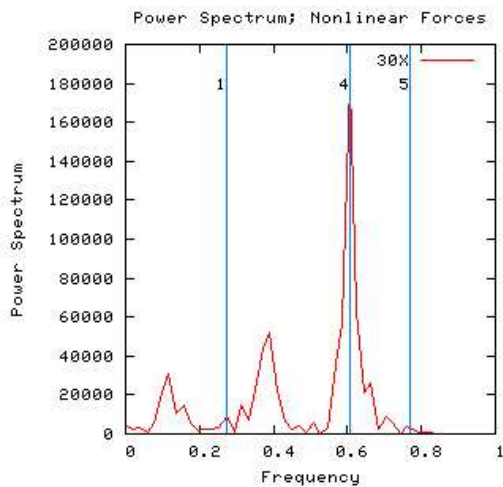


FIG. 6: Power Spectrum for $L = 128$ chain, using a 30X energy boost.

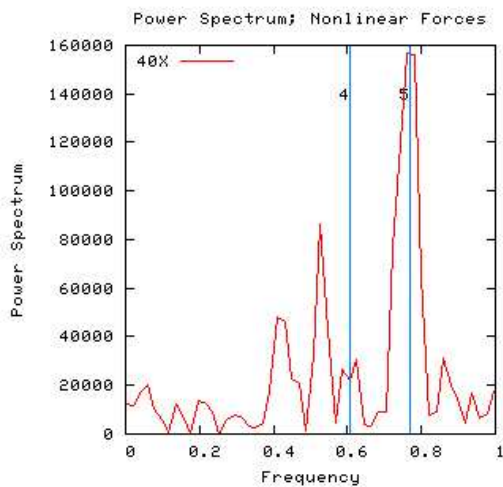


FIG. 7: Power Spectrum for $L = 128$ chain, using a 40X energy boost.

Finally, in Figure 7, we see that, for high excitation energy, the power spectrum is spread over many different modes, far more than for the lower input energies.

Figure 3 is a good approximation for a non-transitioning system, so that it can be considered the prime case of the original results that spurred the FPU Paradox.

Figure 7, which essentially began as Figure 3, shows that, when a high enough input energy is pumped in to the system, a nonlinear system that initially began in a single mode will spread out and vibrate into other modes.

IV. CONCLUSIONS

By examining disorder and nonlinearity in reality simple chains of atoms, we can gain new insight into the emerging complexities of crystalline structures.

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