

PH427/PH527: PERIODIC SYSTEMS
COUPLED OSCILLATORS AND THE MONATOMIC CHAIN
OSU Physics, Spring 2008
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You will be using software entitled “Waves and Optics Simulations”¹, specifically the program “One dimensional Oscillator Chain”. The program simulates the motion of a number of oscillators coupled in a way that you can set, with boundary conditions and initial conditions that you can control.

To run the simulation, double-click the MS-DOS “**Chains**” icon on the desktop. A hard copy description of the program is available, but here are some basic instructions. This program, unfortunately, runs under DOS and is not supported any longer. There are efforts to port it to Java.

The basic things to do every time you run a new simulation are:

- (1) Select **Parameters** | **Number of atoms and cell** to choose the size of your chain.
- (2) Select **Boundary** | **Stationary** and then periodic, fixed, free according to your needs.
- (3) Select **Init** and then whatever initial conditions you’re interested in. You can also drag an oscillator to an initial position.

To run the simulation you use mostly the following keys:

F2 - **Run**

F7 - **Reset** (resets to $t = 0$ conditions)

While the simulation is running you’ll use

F5 - **Faster** (no loss of accuracy)

F6 - **Slower** (no loss of accuracy)

F2 - **Pause**

¹ Antonelli, et al., Consortium for Upper-level Physics Software (CUPS), Wiley, 1995.

1. INTRODUCTORY WORK

A. TWO COUPLED OSCILLATORS:

1. Set up the simulation to have 4 oscillators with 1 oscillator per unit cell.²
2. Set the boundary conditions to “fixed” at both ends. (This immobilizes both the end oscillators, and leaves us, effectively, with the configuration of 2 masses and 3 couplers.) Note that the default settings have the masses equal to 1, and the coupling strengths equal to 0.5. (You can check this by double-clicking on a mass.³) Based on the theory of coupled oscillations, predict the frequencies of the two normal modes of vibration for this system:

3. Set the initial conditions to excite the lowest frequency normal mode. Sketch the initial configuration here:

4. Run the simulation, and measure the frequency of this mode. You will find it helpful to set **Graph 1 | Displacement: $Y(t)$** and click on each of the two middle atoms. Then each displacement as a function of time will be plotted (in the appropriate colour) on graph 1.⁴

Measured frequency of lowest mode:

5. Repeat steps 3 & 4 for the high frequency normal mode.

Initial displacement:

Measured frequency:

² The number of atoms per unit cell is irrelevant here; we'll need it in the diatomic chain example.

³ There are other coefficients here to describe the nature of the force between two oscillators. You can set their values to be non zero to see how they affect the motion. Here we are concerned only with forces proportional to the **first** power of displacement.

⁴ It is instructive to plot the displacement of one atom against the other. Set **Graph 2 | $Y_2(t)$ vs. $Y_1(t)$** to do this. A plot of the velocity vs. the position of a particular atom is generated if you set **Graph 2 | Phase Space**.

What is a numerical simulation?

This exercise really has been an “experiment”. The formulae for the frequencies of the normal modes have NOT been programmed into the computer merely to spit out the correct result when you enter some numbers. The force law governing the coupling springs has been entered, and then Newton’s law ($F = d^2x/dt^2$) has been integrated. You are measuring the results of this simulation and comparing them with analytically derived formulae to give you confidence in the method before you allow the program to tell you about things that are not easy to calculate analytically.

B. FIVE COUPLED OSCILLATORS:

1. Set up 7 oscillators, and fix the two end ones, so that there are effectively 5 oscillators in your chain. Use the **Init | Modes** menu to set the system vibrating in each of mode 1 to mode 5.

For each mode,

- (i) sketch the initial displacements, and describe the motion
- (ii) calculate the wavevector for each mode (use convenient units)
- (iii) find the frequency of oscillation.

When you have done this, gather the information from all five modes and plot the frequency as a function of the wavevector.

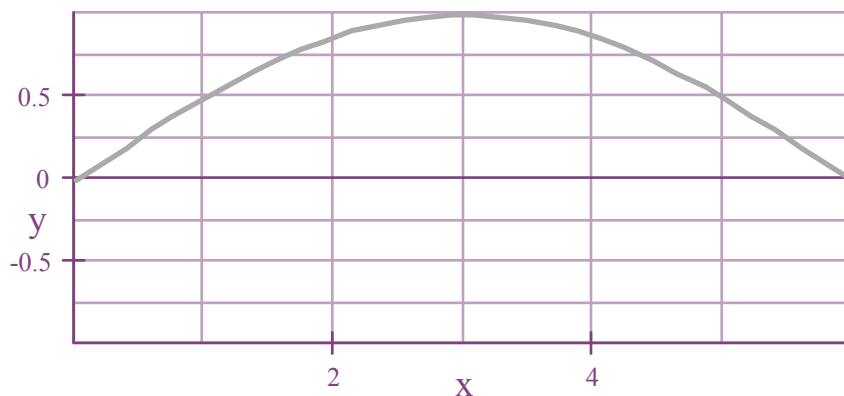
You can continue to find frequencies just as you did before, but there is another method using the FFT capability that is much quicker once you have mastered it, but it requires a little investment of time.

Using the FFT Graph - When you measure frequencies, you may find it convenient to use the FFT graph. Choosing FFT - $y(t)$ on either the Graph 1 or Graph 2 menu sets the appropriate graph to display a Fourier frequency spectrum for the chain. Unfortunately, this Fourier spectrum is not calibrated and is affected by the **Faster** and **Slower** buttons. In order to use it to measure frequencies, you must calibrate the FFT graph by making a conventional measurement of the frequency. It is very important that you do NOT subsequently hit the **Faster/Slower** buttons, as this will change the calibration of the FFT graph.

To calibrate the FFT graph, measure the frequency of a mode using the conventional period counting method and record the corresponding value for the peak in the FFT spectrum. The frequency (f) in Hz is linearly related to (ν) the value on the FFT spectrum. Thus, $f = C \nu$. Where C is the calibration constant. Use your measurements of the frequency and its corresponding FFT value to find C . Then, you can determine the frequency of a particular mode by simply examining its FFT spectrum. To ensure a sufficiently precise value for C , it is important that the FFT value of the frequency you use for calibration is somewhat large ($\nu > 20$).

MODE 1:

Initial configuration:



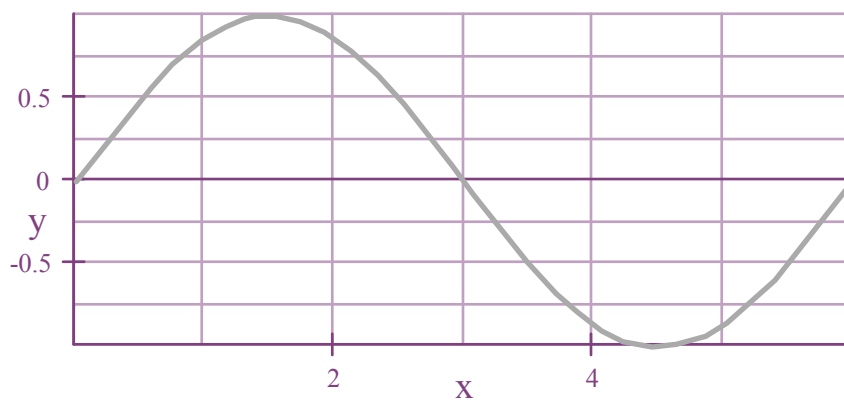
Wavevector:

Frequency:

Notes:

MODE 2:

Initial configuration:



Wavevector:

Frequency:

Notes:

MODE 3

Initial configuration:



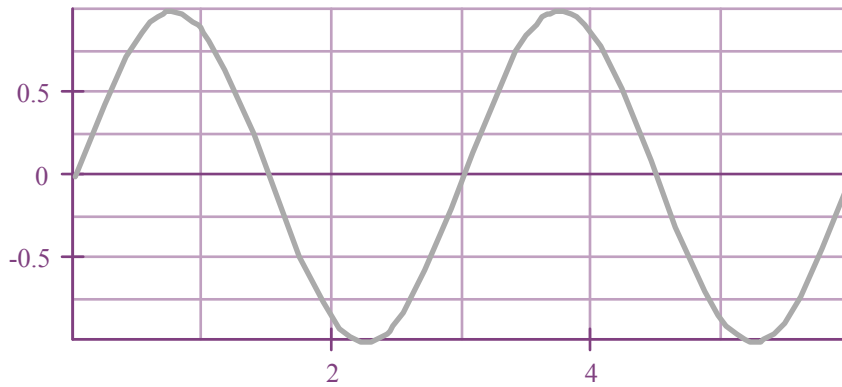
Wavevector:

Frequency:

Notes:

MODE 4:

Initial configuration:



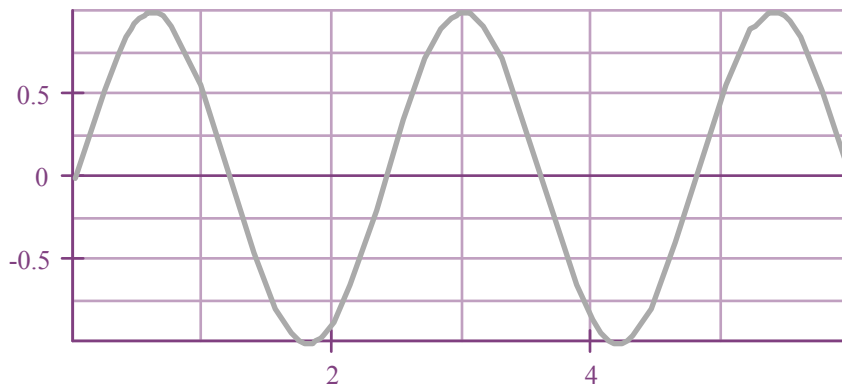
Wavevector:

Frequency:

Notes:

MODE 5:

Initial configuration:



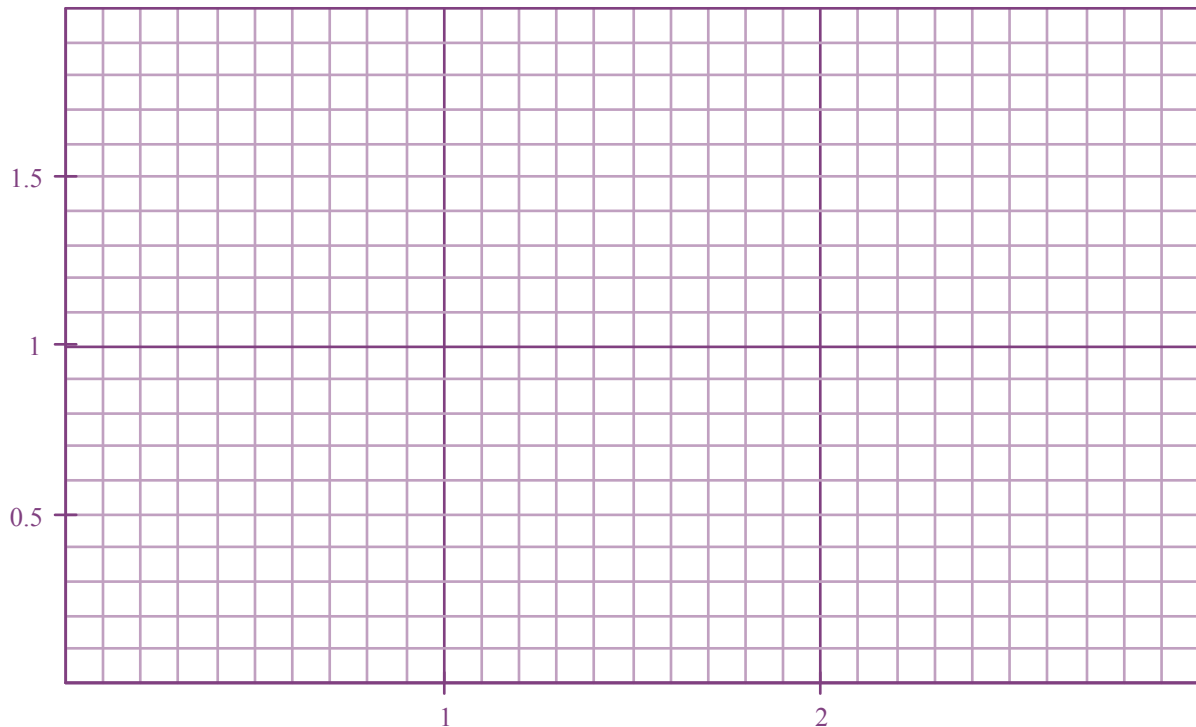
Wavevector:

Frequency:

Notes:

DISPERSION RELATION

(mode frequency as a function of mode wave vector; relabel axes as necessary)



2. EXPLORATORY WORK

A. TWO COUPLED OSCILLATORS:

Set up the 2 coupled oscillator system as above by using 4 oscillators with fixed boundary conditions.

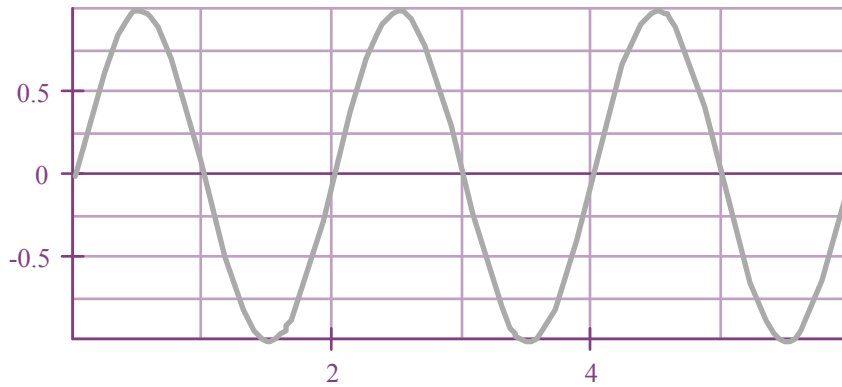
1. Set up some arbitrary initial condition and run the simulation. Predict the Fourier spectrum for this motion. Is the motion periodic?
2. Set a particular initial condition with one oscillator is displaced, while the other is not. Observe the resulting motion. You can come to look at this in more depth later.

B. FIVE COUPLED OSCILLATORS:

Set up the 5 coupled oscillator system as above by using 7 oscillators with fixed boundary conditions.

1. Predict the behaviour of modes with mode number higher than 5. Comment on your prediction and observations after you have completed the explorations.

MODE 6:
Initial configuration:

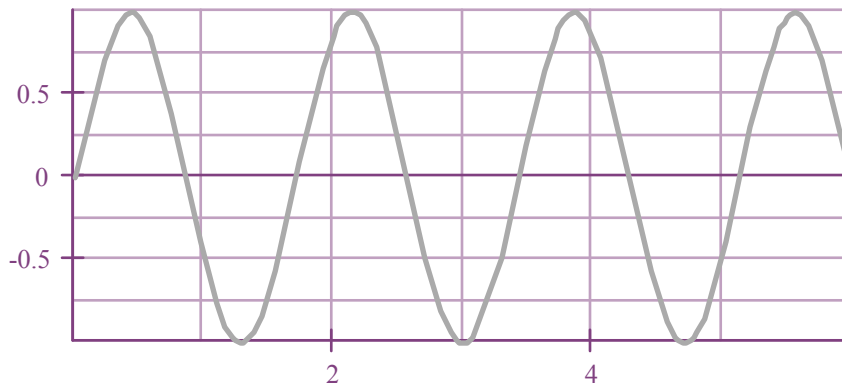


Wavevector:

Frequency:

Notes:

MODE 7:
Initial configuration:

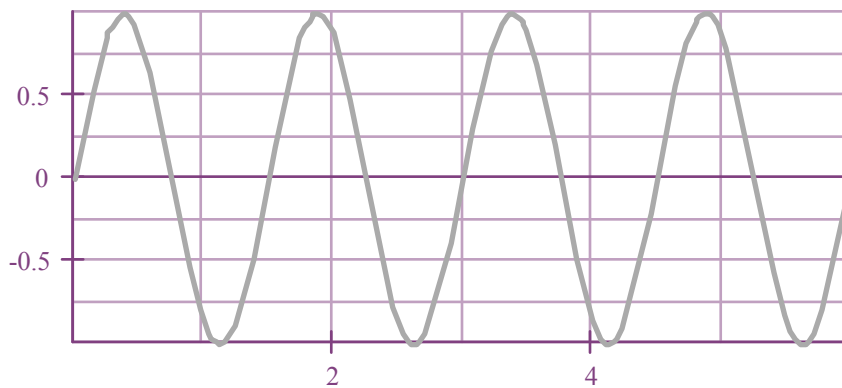


Wavevector:

Frequency:

Notes:

MODE 8:
Initial configuration:

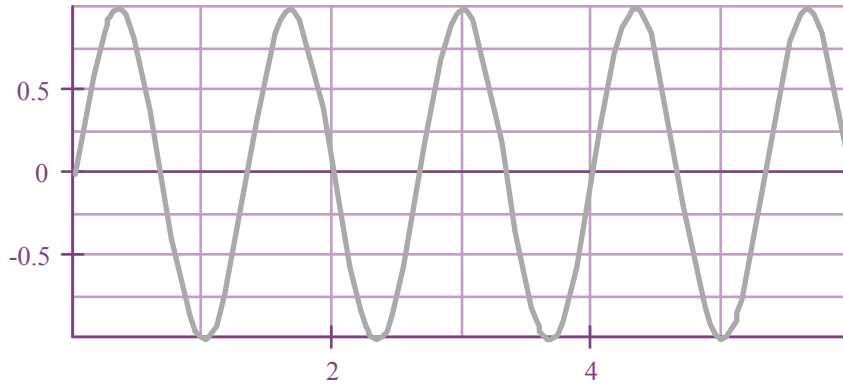


Wavevector:

Frequency:

Notes:

MODE 9:
Initial configuration:

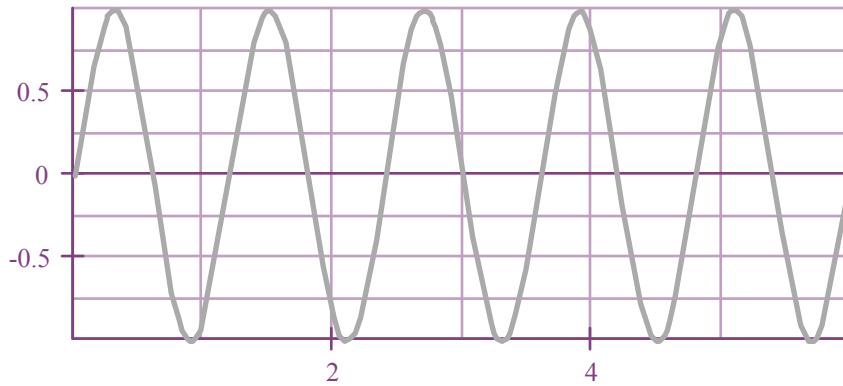


Wavevector:

Frequency:

Notes:

MODE 10:
Initial configuration:

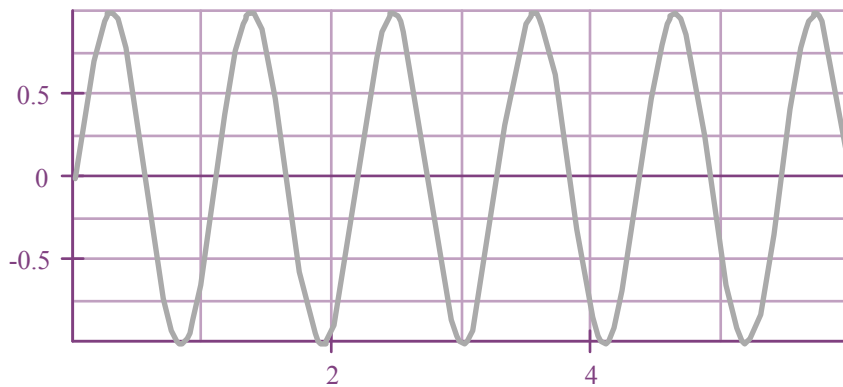


Wavevector:

Frequency:

Notes:

MODE 11:
Initial configuration:

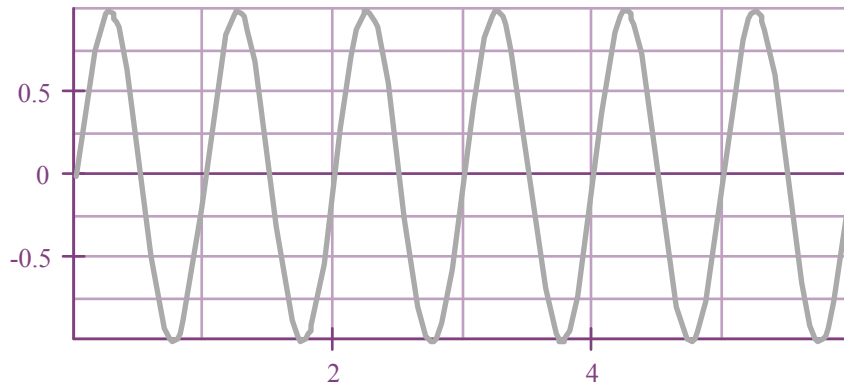


Wavevector:

Frequency:

Notes:

MODE 12:
Initial configuration:

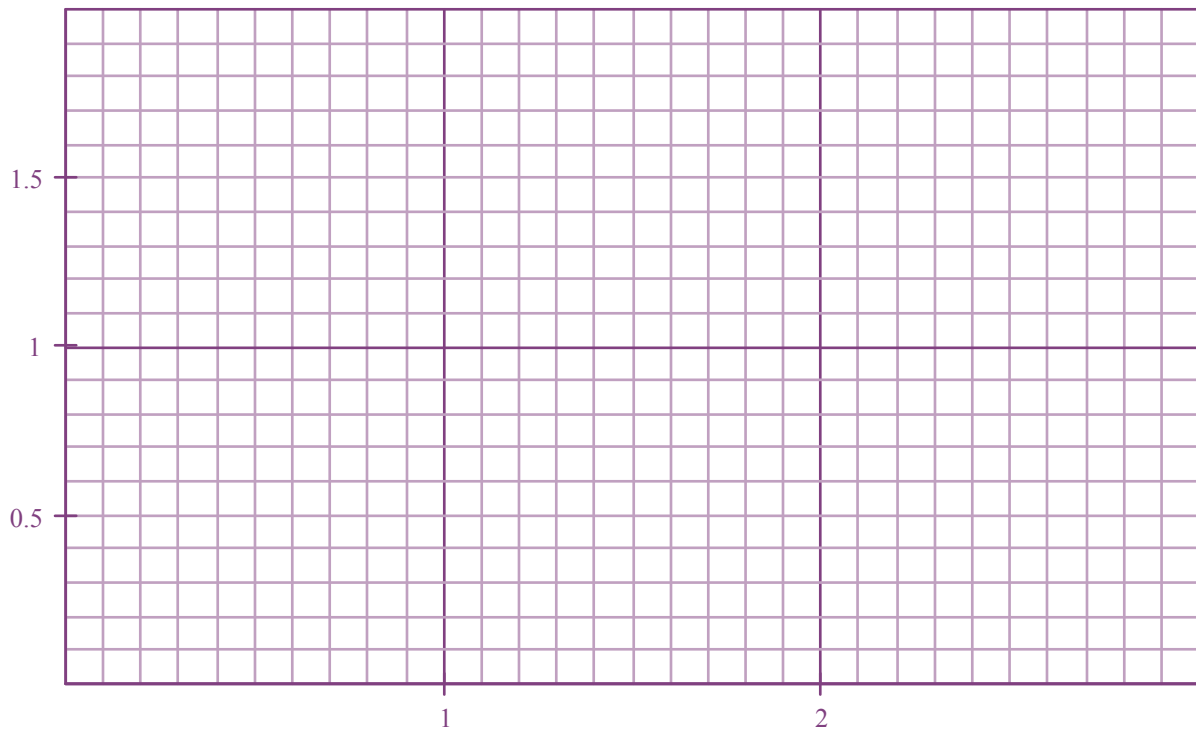


Wavevector:

Frequency:

Notes:

DISPERSION RELATION (mode frequency as a function of mode wavevector)



Notice there is a maximum frequency in the dispersion relation.
What is the wavevector (in units of π/a) at which this occurs?

What are the physical implications of such a maximum?

What would happen if you tried to drive this chain at a higher frequency (CUPS can simulate this)?

C. MANY COUPLED OSCILLATORS:

1. Set up 32 coupled oscillators with fixed boundary conditions. Predict what a few normal modes will look like and try them out. Which mode has the highest frequency? How many distinct modes are there?

2. *Periodic boundary conditions:* Fixed boundary conditions are quite restrictive. They require, for example, that atoms on the surface of a crystal remain at rest. Periodic boundary conditions can be very useful. This simply means that the masses at each end of the chain must have the same motion, but there is no requirement about what that motion is. Mathematically the statement is $\psi(n) = \psi(n+N)$ where N is the number of atoms in the crystal. We will explore this further later in the course, but for now

Change the boundary conditions from *fixed* to *periodic*. Look at a few modes and compare them to the corresponding ones with fixed boundary conditions. How is mode 1 different from mode -1?

3. FURTHER WORK:

A. TWO COUPLED OSCILLATORS:

Beats and energy transfer

Set the initial conditions so that one oscillator is displaced, while the other is not. Observe the simulation, and note how the motion of each oscillator appears in a “displacement as a function of time” plot. Measure the time it takes for the energy to be transferred from one oscillator to another. This simulation is best observed if the coupling between the oscillators is weaker than the coupling between each oscillator and the walls.

For a description of this energy exchange phenomenon, also a manifestation of the familiar problem of “beats”, see:

Main 8.1, Marion & Thornton 11.3, Crawford 1.5 & Supplementary topic 1.

The mathematics of two weakly coupled systems is not unique to classical systems that obey Newton’s law. One finds similar examples in quantum mechanics (Paradigm 5 discusses the ammonia molecule).

B. MANY COUPLED OSCILLATORS:

Tunneling

Open the file TUNNEL.CHN. Run the simulation and observe the behavior of this chain of oscillators. What form does the wave have in the region with heavy masses? Discuss the behavior of this system referring to related examples you have encountered in other Paradigms course.

2. What happens when you adjust the frequency of the driving atom? Explain this behavior.