Lab 4

The Hanging Chain and Quantum Bound States

The resonance modes that we studied in Lab 3 were simply sine functions. We can also use these techniques to analyze more complicated systems. In this lab we first study the problem of standing waves on a hanging chain. It was the famous Swiss mathematician Johann Bernoulli who discovered in the 1700s that a draped hanging chain has the shape of a "catenary", or the hyperbolic cosine function. The problem of the normal mode frequencies of a vertical hanging chain was also solved in the 1700s by Johann's son, Daniel Bernoulli, and is the first time that the function that later became known as the J_0 Bessel function showed up in physics. Then we will jump forward several centuries in physics history and study bound quantum states using the same techniques.

Resonance for a hanging chain

Consider the chain hanging from the ceiling in the classroom.[1] We are going to find its normal modes of vibration using the method of Problem 3.2. The wave equation for transverse waves on a chain with varying tension $T(x)$ and constant linear mass density μ[2] is given by

$$\mu\frac{\partial^2 y}{\partial t^2} - \frac{\partial}{\partial x}\left(T(x)\frac{\partial y}{\partial x}\right) = 0 \tag{4.1}$$

Let's use a coordinate system that starts at the bottom of the chain at $x = 0$ and ends on the ceiling at $x = L$.

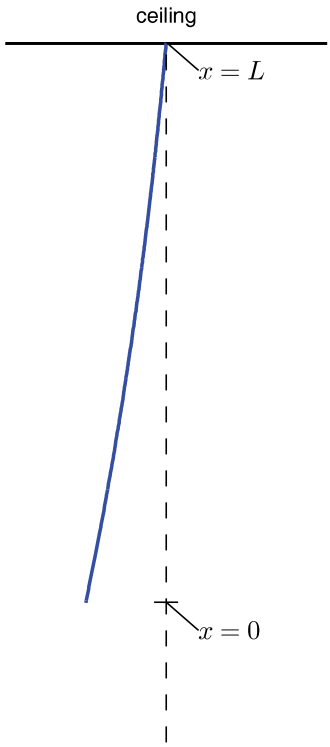

Figure 4.1 The first normal mode for a hanging chain.

P4.1 Use the fact that the stationary chain is in vertical equilibrium to help you draw a carefully chosen free-body diagram that shows that the tension in the chain as a function of x is given by

$$T(x) = \mu g x \tag{4.2}$$

where μ is the linear mass density of the chain and where $g = 9.8\ \text{m/s}^2$ is the acceleration of gravity. Then show that Eq. (4.1) reduces to

$$\frac{\partial^2 y}{\partial t^2} - g\frac{\partial}{\partial x}\left(x\frac{\partial y}{\partial x}\right) = 0 \tag{4.3}$$

for a freely hanging chain.

[1] For more analysis of the hanging chain, see N. Asmar, *Partial Differential Equations and Boundary Value Problems* (Prentice Hall, New Jersey, 2000), p. 299-305.

[2] Equation (4.1) also works for systems with varying mass density if you replace μ with a function $\mu(x)$, but the equations derived later in the lab are more complicated with a varying $\mu(x)$.

As in Lab 3, we now look for normal modes by separating the variables: $y(x,t) = f(x)\cos(\omega t)$. We then substitute this form for $y(x,t)$ into (4.3) and simplify to obtain

$$x\frac{d^2f}{dx^2} + \frac{df}{dx} = -\frac{\omega^2}{g}f \tag{4.4}$$

which is in eigenvalue form with $\lambda = -\omega^2/g$. (This relationship is different than in the preceding lab; consequently you will have to change a line in the `eigen.m` code to reflect this difference.)

The boundary condition at the ceiling is $f(L) = 0$ while the boundary condition at the bottom is obtained by taking the limit of Eq. (4.4) as $x \to 0$ to find

$$f'(0) = -\frac{\omega^2}{g}f(0) = \lambda f(0) \tag{4.5}$$

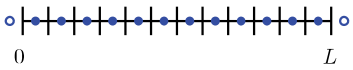

Figure 4.2 A cell-centered grid with ghost points. (The open circles are the ghost points.)

In the past couple labs we have dealt with derivative boundary conditions by fitting a parabola to the last three points on the grid and then taking the derivative of the parabola (see Problems 2.4(b) and 3.3). This time we'll handle the derivative boundary condition by using a cell-centered grid with ghost points, as discussed in Lab 1.

Recall that a cell-center grid divides the computing region from 0 to L into N cells with a grid point at the center of each cell. We then add two more grid points outside of $[0,L]$, one at $x_1 = -h/2$ and the other at $x_{N+2} = L + h/2$. The ghost points are used to apply the boundary conditions. Notice that by defining N as the number of interior grid points (or cells), we have $N+2$ total grid points, which may seem weird to you. We prefer it, however, because it reminds us that we are using a cell-centered grid with N physical grid points and two ghost points. You can do it any way you like, as long as your counting method works.

Notice that there isn't a grid point at either endpoint, but rather that the two grid points on each end straddle the endpoints. If the boundary condition specifies a value, like $f(L) = 0$ in the problem at hand, we use a simple average like this:

$$\frac{f_{N+2} + f_{N+1}}{2} = 0 \ , \tag{4.6}$$

and if the condition were $f'(L) = 0$ we would use

$$\frac{f_{N+2} - f_{N+1}}{h} = 0 \ . \tag{4.7}$$

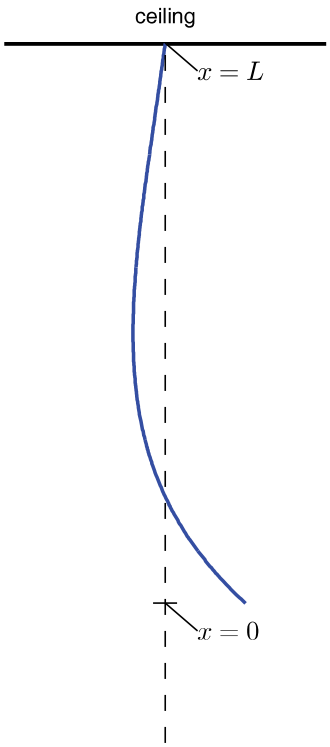

Figure 4.3 The shape of the second mode of a hanging chain

When we did boundary conditions in the eigenvalue calculation of Problem 3.2 we used a **B** matrix with zeros in the top and bottom rows and we loaded the top and bottom rows of **A** with an appropriate boundary condition operator. Because the chain is fixed at the ceiling ($x = L$) we use this technique again in the bottom rows of **A** and **B**, like this (after first loading **A** with zeros and **B** with the identity matrix):

$$A(N+2,N+1) = \frac{1}{2} \quad A(N+2,N+2) = \frac{1}{2} \quad B(N+2,N+2) = 0 \tag{4.8}$$

P4.2 (a) Verify that these choices for the bottom rows of A and B in the generalized eigenvalue problem

$$\mathbf{A}f = \lambda \mathbf{B}f \tag{4.9}$$

give the boundary condition in Eq. (4.6) at the ceiling no matter what λ turns out to be.

(b) Now let's do something similar with the derivative boundary condition at the bottom, Eq. (4.5). Since this condition is already in eigenvalue form we don't need to load the top row of **B** with zeros. Instead we load **A** with the operator on the left ($f'(0)$) and **B** with the operator on the right ($f(0)$), leaving the eigenvalue $\lambda = -\omega^2/g$ out of the operators so that we still have $\mathbf{A}f = \lambda \mathbf{B}f$. Verify that the following choices for the top rows of **A** and **B** correctly produce Eq. (4.5).

$$A(1,1) = -\frac{1}{h} \quad A(1,2) = \frac{1}{h} \quad B(1,1) = \frac{1}{2} \quad B(1,2) = \frac{1}{2} \tag{4.10}$$

(c) Write the finite difference form of Eq. (4.4) and use it to load the matrices **A** and **B** for a chain with $L = 2$ m. (Notice that for the interior points the matrix **B** is just the identity matrix with 1 on the main diagonal and zeros everywhere else.) Use Matlab to solve for the normal modes of vibration of a hanging chain. As in Lab 3, some of the eigenvectors are unphysical because they don't satisfy the boundary conditions; ignore them.

Compare your numerical resonance frequencies to measurements made on the chain hanging from the ceiling in the classroom.

(d) Solve Eq. (4.4) analytically using Mathematica without any boundary conditions. You will encounter the Bessel functions J_0 and Y_0, but because Y_0 is singular at $x = 0$ this function is not allowed in the problem. Apply the condition $f(L) = 0$ to find analytically the mode frequencies ω and verify that they agree with the frequencies you found in part (c).

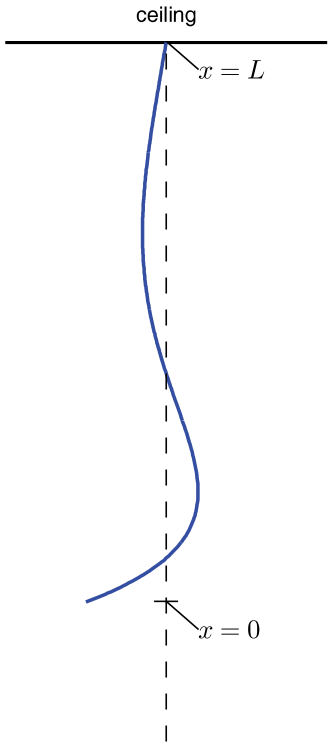

Figure 4.4 The shape of the third mode of a hanging chain

Quantum bound states

Consider the problem of a particle in a one-dimensional harmonic oscillator well in quantum mechanics.[3] Schrödinger's equation for the bound states in this well is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi \tag{4.11}$$

with boundary conditions $\psi = 0$ at $\pm\infty$. Note that k in this equation is not the wave number; it is the spring constant, $F = -kx$, with units of Newtons/meter.

[3] N. Asmar, *Partial Differential Equations and Boundary Value Problems* (Prentice Hall, New Jersey, 2000), p. 470-506.

The numbers that go into Schrödinger's equation are so small that it makes it difficult to tell what size of grid to use. For instance, our usual trick of using lengths like 2, 5, or 10 would be completely ridiculous for the bound states of an atom where the typical size is on the order of 10^{-10} m. We could just set $\hbar$, m, and k to unity, but then we wouldn't know what physical situation our numerical results describe. When computational physicists encounter this problem a common thing to do is to "rescale" the problem so that all of the small numbers go away. And, as an added bonus, this procedure can also allow the numerical results obtained to be used no matter what m and k our system has.

P4.3 This probably seems a little nebulous, so follow the recipe below to see how to rescale in this problem (write it out on paper).

(i) In Schrödinger's equation use the substitution $x = a\xi$, where a has units of length and ξ is dimensionless. After making this substitution put the left side of Schrödinger's equation in the form

$$C\left(-\frac{D}{2}\frac{d^2\psi}{d\xi^2}+\frac{1}{2}\xi^2\psi\right)=E\psi \tag{4.12}$$

where C and D involve the factors $\hbar$, m, k, and a.

(ii) Make the differential operator inside the parentheses (...) on the left be as simple as possible by choosing to make $D = 1$. This determines how the characteristic length a depends on $\hbar$, m, and k. Once you have determined a in this way, check to see that it has units of length. You should find

$$a=\left(\frac{\hbar^2}{km}\right)^{1/4}=\sqrt{\frac{\hbar}{m\omega}} \quad \text{where} \quad \omega=\sqrt{\frac{k}{m}} \tag{4.13}$$

(iii) Now rescale the energy by writing $E = \epsilon\bar{E}$, where $\bar{E}$ has units of energy and ϵ is dimensionless. Show that if you choose $\bar{E} = C$ in the form you found above in (i) that Schrödinger's equation for the bound states in this new dimensionless form is

$$-\frac{1}{2}\frac{d^2\psi}{d\xi^2}+\frac{1}{2}\xi^2\psi=\epsilon\psi \tag{4.14}$$

You should find that

$$\bar{E}=\hbar\sqrt{\frac{k}{m}} \tag{4.15}$$

Verify that $\bar{E}$ has units of energy.

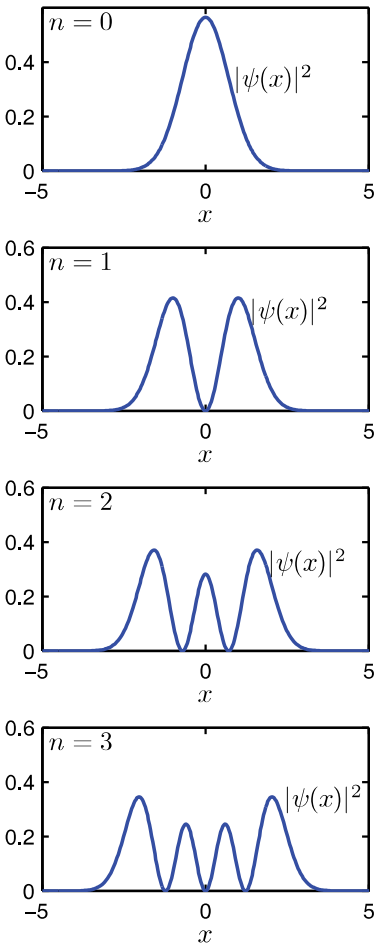

Figure 4.5 The probability distributions for the ground state and the first three excited states of the harmonic oscillator.

Now that Schrödinger's equation is in dimensionless form it makes sense to choose a grid that goes from -4 to 4, or some other similar pair of numbers. These numbers are supposed to approximate infinity in this problem, so make sure (by looking at the eigenfunctions) that they are large enough that the wave function

goes to zero with zero slope at the edges of the grid. As a guide to what you should find, Figure 4.5 displays the square of the wave function for the first few excited states. (The amplitude has been appropriately normalized so that $\int |\psi(x)|^2 = 1$

If you look in a quantum mechanics textbook you will find that the bound state energies for the simple harmonic oscillator are given by the formula

$$E_n = (n + \frac{1}{2})\hbar\sqrt{\frac{k}{m}} = (n + \frac{1}{2})\bar{E} \tag{4.16}$$

so that the dimensionless energy eigenvalues ϵ_n are given by

$$\epsilon_n = n + \frac{1}{2} \tag{4.17}$$

P4.4 Use Matlab's ability to do eigenvalue problems to verify that this formula for the bound state energies is correct for $n = 0, 1, 2, 3, 4$.

P4.5 Now redo this entire problem, but with the harmonic oscillator potential replaced by

$$V(x) = \mu x^4 \tag{4.18}$$

so that we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \mu x^4\psi = E\psi \tag{4.19}$$

With this new potential you will need to find new formulas for the characteristic length a and energy $\bar{E}$ so that you can use dimensionless scaled variables as you did with the harmonic oscillator. Choose a so that your scaled equation is

$$-\frac{1}{2}\frac{d^2\psi}{d\xi^2} + \xi^4\psi = \epsilon\psi \tag{4.20}$$

with $E = \epsilon\bar{E}$. Use Mathematica and/or algebra by hand to show that

$$a = \left(\frac{\hbar^2}{m\mu}\right)^{1/6} \qquad \bar{E} = \left(\frac{\hbar^4\mu}{m^2}\right)^{1/3} \tag{4.21}$$

Find the first 5 bound state energies by finding the first 5 values of ϵ_n in the formula $E_n = \epsilon_n\bar{E}$.

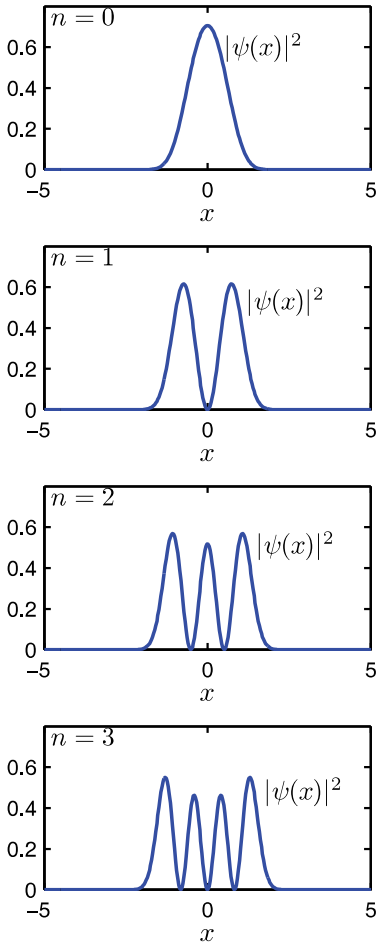

Figure 4.6 The probability distributions for the ground state and the first three excited states for the potential in Problem 4.5.