Computational Physics – PH 354

Homework due on 22nd Feb 2022

Exercise 1: Quadratic equations

a) Write a program that takes as input three numbers, a, b, and c, and prints out the two solutions to the quadratic equation $ax^2 + bx + c = 0$ using the standard formula
$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$
Use your program to compute the solutions of $0.001x^2 + 1000x + 0.001 = 0$.

b) There is another way to write the solutions to a quadratic equation. Multiplying top and bottom of the solution above by $-b \mp \sqrt{b^2 - 4ac}$, show that the solutions can also be written as
$$x = \frac{2c}{-b \mp \sqrt{b^2 - 4ac}}.$$
Add further lines to your program to print out these values in addition to the earlier ones and again use the program to solve $0.001x^2 + 1000x + 0.001 = 0$. What do you see? How do you explain it?

c) Using what you have learned, write a new program that calculates both roots of a quadratic equation accurately in all cases.

This is a good example of how computers don't always work the way you expect them to. If you simply apply the standard formula for the quadratic equation, the computer will sometimes get the wrong answer. In practice the method you have worked out here is the correct way to solve a quadratic equation on a computer, even though it's more complicated than the standard formula. If you were writing a program that involved solving many quadratic equations this method might be a good candidate for a user-defined function: you could put the details of the solution method inside a function to save yourself the trouble of going through it step by step every time you have a new equation to solve.

Exercise 2: Calculating derivatives

Suppose we have a function $f(x)$ and we want to calculate its derivative at a point x. We can do that with pencil and paper if we know the mathematical form of the function, or we can do it on the computer by making use of the definition of the derivative:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}.$$

On the computer we can't actually take the limit as δ goes to zero, but we can get a reasonable approximation just by making δ small.

a) Write a program that defines a function `f(x)` returning the value $x(x-1)$, then calculates the derivative of the function at the point $x = 1$ using the formula above with $\delta = 10^{-2}$. Calculate the true value of the same derivative analytically and compare with the answer your program gives. The two will not agree perfectly. Why not?

b) Repeat the calculation for $\delta = 10^{-4}$, 10^{-6}, 10^{-8}, 10^{-10}, 10^{-12}, and 10^{-14}. You should see that the accuracy of the calculation initially gets better as δ gets smaller, but then gets worse again. Why is this?

Exercise 3: Consider the equation $x = 1 - \mathrm{e}^{-cx}$, where c is a known parameter and x is unknown. This equation arises in a variety of situations, including the physics of contact processes, mathematical models of epidemics, and the theory of random graphs.

a) Write a program to solve this equation for x using the relaxation method (another name for fixed point iteration method) for the case $c = 2$. Calculate your solution to an accuracy of at least 10^{-6}.

b) Modify your program to calculate the solution for values of c from 0 to 3 in steps of 0.01 and make a plot of x as a function of c. You should see a clear transition from a regime in which $x = 0$ to a regime of nonzero x. This is another example of a phase transition. In physics this transition is known as the *percolation transition*; in epidemiology it is the *epidemic threshold*.

c) Write a program (or modify the previous one) to solve the same equation $x = 1 - \mathrm{e}^{-cx}$ for $c = 2$, again to an accuracy of 10^{-6}, but this time using fixed point iteration with acceleration. Have your program print out the answers it finds along with the number of iterations it took to find them.

Exercise 4: The biochemical process of *glycolysis*, the breakdown of glucose in the body to release energy, can be modeled by the equations

$$\frac{dx}{dt} = -x + ay + x^2 y, \qquad \frac{dy}{dt} = b - ay - x^2 y.$$

Here x and y represent concentrations of two chemicals, ADP and F6P, and a and b are positive constants. One of the important features of nonlinear linear equations like these is their *stationary points*, meaning values of x and y at which the derivatives of both variables become zero simultaneously, so that the variables stop changing and become constant in time. Find the stationary points of these glycolysis equations

a) Demonstrate analytically that the solution of these equations is

$$x = b, \qquad y = \frac{b}{a + b^2}.$$

b) Show that the equations can be rearranged to read

$$x = y(a + x^2), \qquad y = \frac{b}{a + x^2}$$

and write a program to solve these for the stationary point using the relaxation method with $a = 1$ and $b = 2$. You should find that the method fails to converge to a solution in this case.

c) Find a different way to rearrange the equations such that when you apply the relaxation method again it now converges to a fixed point and gives a solution. Verify that the solution you get agrees with part (a).

Exercise 5: Wien's displacement constant

Planck's radiation law tells us that the intensity of radiation per unit area and per unit wavelength λ from a black body at temperature T is

$$I(\lambda) = \frac{2\pi hc^2 \lambda^{-5}}{e^{hc/\lambda k_B T} - 1},$$

where h is Planck's constant, c is the speed of light, and k_B is Boltzmann's constant.

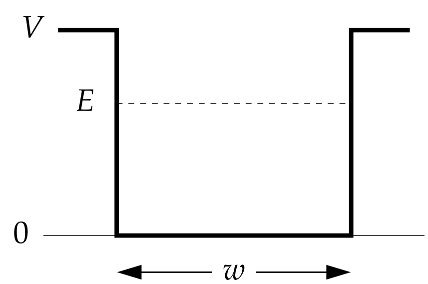
a) Write a program to calculate the wavelength λ at which the emitted radiation is strongest. Solve the resulting equation to an accuracy of $\epsilon = 10^{-6}$ using the bisection method, and hence find a value for the displacement constant. Note: The wavelength of maximum radiation obeys the *Wien displacement law*:

$$\lambda = \frac{b}{T},$$

where the so-called *Wien displacement constant* is b.

b) The displacement law is the basis for the method of *optical pyrometry*, a method for measuring the temperatures of objects by observing the color of the thermal radiation they emit. The method is commonly used to estimate the surface temperatures of astronomical bodies, such as the Sun. The wavelength peak in the Sun's emitted radiation falls at $\lambda = 502\,\text{nm}$. From the equations above and your value of the displacement constant, estimate the surface temperature of the Sun.

Exercise 6: Consider a square potential well of width w, with walls of height V:



Using Schrödinger's equation, setup the equations for the allowed energies E of a single quantum particle of mass m trapped in the well.

a) For an electron (mass $9.1094 \times 10^{-31}\,\text{kg}$) in a well with $V = 20\,\text{eV}$ and $w = 1\,\text{nm}$, write a Python program to calculate the values of the first six energy levels in electron volts to an accuracy of $0.001\,\text{eV}$ using false position method.

Exercise 7: The roots of a polynomial

Consider the sixth-order polynomial

$$P(x) = 924x^6 - 2772x^5 + 3150x^4 - 1680x^3 + 420x^2 - 42x + 1.$$

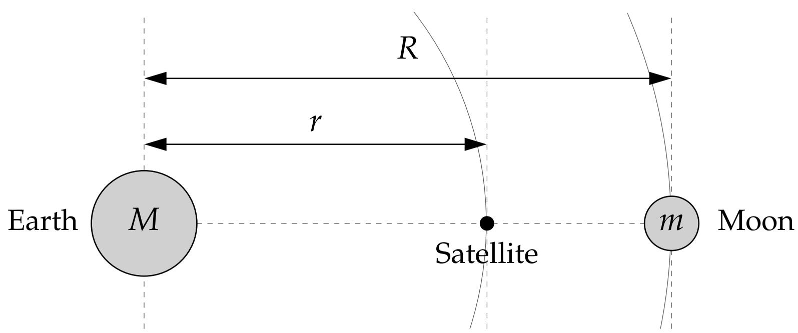
There is no general formula for the roots of a sixth-order polynomial, but one can find them easily enough using a computer.

a) Make a plot of $P(x)$ from $x = 0$ to $x = 1$ and by inspecting it find rough values for the six roots of the polynomial—the points at which the function is zero.

b) Write a Python program to solve for the positions of all six roots to at least ten decimal places of accuracy, using Newton's method.

Exercise 8: The Lagrange point

There is a magical point between the Earth and the Moon, called the L_1 Lagrange point, at which a satellite will orbit the Earth in perfect synchrony with the Moon, staying always in between the two. This works because the inward pull of the Earth and the outward pull of the Moon combine to create exactly the needed centripetal force that keeps the satellite in its orbit. Here's the setup:



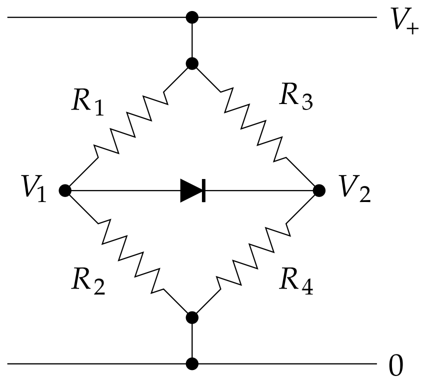
a) Assuming circular orbits, and assuming that the Earth is much more massive than either the Moon or the satellite, find the distance r from the center of the Earth to the L_1 point. Write a program that uses the secant method to solve for the distance r from the Earth to the L_1 point. Compute a solution accurate to at least four significant figures.

The values of the various parameters are:

$$
\begin{aligned}
G &= 6.674 \times 10^{-11}\,\mathrm{m^3 kg^{-1} s^{-2}}, \\
M &= 5.974 \times 10^{24}\,\mathrm{kg}, \\
m &= 7.348 \times 10^{22}\,\mathrm{kg}, \\
R &= 3.844 \times 10^{8}\,\mathrm{m}, \\
\omega &= 2.662 \times 10^{-6}\,\mathrm{s^{-1}}.
\end{aligned}
$$

Exercise 9: Nonlinear circuits

Consider the following simple circuit, a variation on the classic Wheatstone bridge:



The resistors obey the normal Ohm law, but the diode obeys the diode equation:

$$I = I_0(e^{V/V_T} - 1),$$

where V is the voltage across the diode and I_0 and V_T are constants.

a) Write a program to calculate the voltages V_1 and V_2 with the conditions

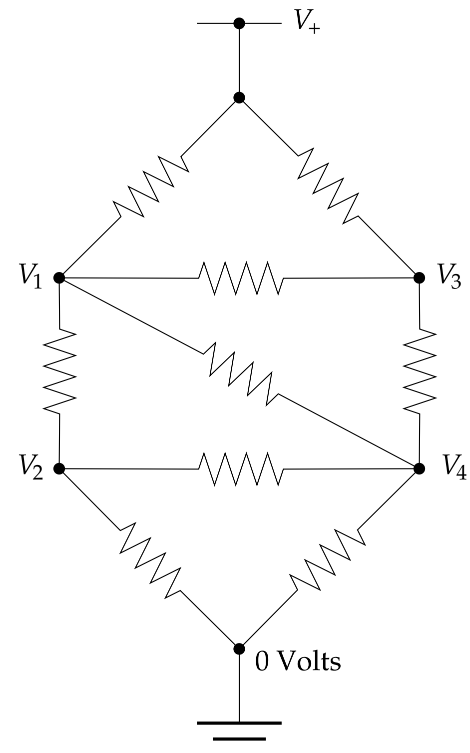
$$\begin{aligned} V_+ &= 5\,\mathrm{V}, \\ R_1 &= 1\,\mathrm{k\Omega}, \qquad R_2 = 4\,\mathrm{k\Omega}, \qquad R_3 = 3\,\mathrm{k\Omega}, \qquad R_4 = 2\,\mathrm{k\Omega}, \\ I_0 &= 3\,\mathrm{nA}, \qquad V_T = 0.05\,\mathrm{V}. \end{aligned}$$

You can use Newton's method to solve the equations.

b) The electronic engineer's rule of thumb for diodes is that the voltage across a (forward biased) diode is always about 0.6 volts. Confirm that your results agree with this rule.

Exercise 10: A circuit of resistors

Consider the following circuit of resistors:



All the resistors have the same resistance R. The power rail at the top is at voltage $V_+ = 5\,\text{V}$. What are the other four voltages, V_1 to V_4?

To answer this question we use Ohm's law and the Kirchhoff current law, which says that the total net current flow out of (or into) any junction in a circuit must be zero. Thus for the junction at voltage V_1, for instance, we have

$$\frac{V_1 - V_2}{R} + \frac{V_1 - V_3}{R} + \frac{V_1 - V_4}{R} + \frac{V_1 - V_+}{R} = 0,$$

or equivalently

$$4V_1 - V_2 - V_3 - V_4 = V_+.$$

a) Write similar equations for the other three junctions with unknown voltages.

b) Write a program to solve the four resulting equations using Gaussian elimination and hence find the four voltages (or you can modify a program you already have, such as the program `gausselim.py`).

Exercise 11:

a) Modify the program `gausselim.py` to incorporate partial pivoting (or you can write your own program from scratch if you prefer). Run your program and demonstrate that it gives the same answers as the original program when applied to previous exercise.

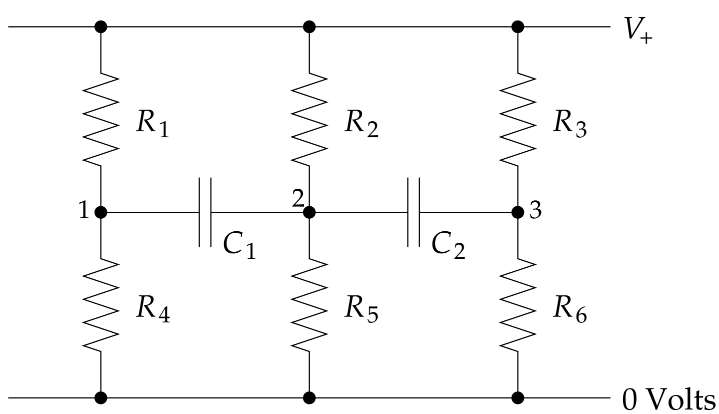
b) Modify the program to solve the equations:

$$\begin{pmatrix} 0 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

and show that it can find the solution to these as well, even though Gaussian elimination without pivoting fails.

Exercise 12: Write a program to solve the resistor network problem of Exercise 10 using the function `solve` from `numpy.linalg`. You should check that you get the same answer both times.

Exercise 13: Here's a more complicated circuit problem:



The voltage V_+ is time-varying and sinusoidal of the form $V_+ = x_+ e^{i\omega t}$ with x_+ a constant. The resistors in the circuit can be treated using Ohm's law as usual. For the capacitors the charge Q and voltage V across them are related by the capacitor law $Q = CV$, where C is the capacitance. Differentiating both sides of this expression gives the current I flowing in on one side of the capacitor and out on the other:

$$I = \frac{dQ}{dt} = C\frac{dV}{dt}.$$

a) Assuming the voltages at the points labeled 1, 2, and 3 are of the form $V_1 = x_1 e^{i\omega t}$, $V_2 = x_2 e^{i\omega t}$, and $V_3 = x_3 e^{i\omega t}$, apply Kirchhoff's law at each of the three points, along with Ohm's law and the capacitor law, to show that the constants x_1, x_2, and x_3 satisfy the equations

$$\begin{aligned}
\left(\frac{1}{R_1} + \frac{1}{R_4} + i\omega C_1\right) x_1 - i\omega C_1 x_2 &= \frac{x_+}{R_1}, \\
-i\omega C_1 x_1 + \left(\frac{1}{R_2} + \frac{1}{R_5} + i\omega C_1 + i\omega C_2\right) x_2 - i\omega C_2 x_3 &= \frac{x_+}{R_2}, \\
-i\omega C_2 x_2 + \left(\frac{1}{R_3} + \frac{1}{R_6} + i\omega C_2\right) x_3 &= \frac{x_+}{R_3}.
\end{aligned}$$

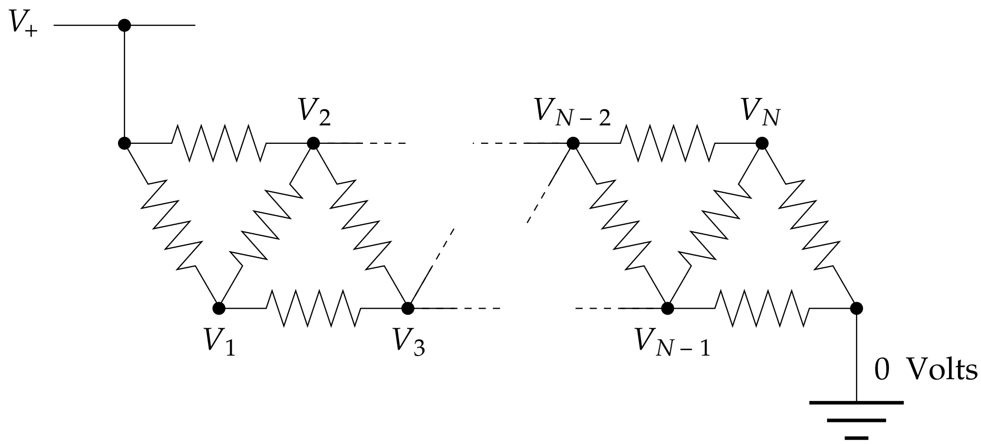
b) Write a program to solve for x_1, x_2, and x_3 when

$$\begin{aligned}
&R_1 = R_3 = R_5 = 1\,\mathrm{k}\Omega, \\
&R_2 = R_4 = R_6 = 2\,\mathrm{k}\Omega, \\
&C_1 = 1\,\mu\mathrm{F}, \qquad C_2 = 0.5\,\mu\mathrm{F}, \\
&x_+ = 3\,\mathrm{V}, \qquad \omega = 1000\,\mathrm{s}^{-1}.
\end{aligned}$$

Notice that the matrix for this problem has complex elements. You will need to define a complex array to hold it, but you can still use the `solve` function just as before to solve the equations—it works with either real or complex arguments. Using your solution have your program calculate and print the amplitudes of the three voltages V_1, V_2, and V_3 and their phases in degrees. (Hint: You may find the functions `polar` or `phase` in the `cmath` package useful. If `z` is a complex number then "`r,theta = polar(z)`" will return the modulus and phase (in radians) of `z` and "`theta = phase(z)`" will return the phase alone.)

Exercise 14: A chain of resistors

Consider a long chain of resistors wired up like this:



All the resistors have the same resistance R. The power rail at the top is at voltage $V_+ = 5$V. The problem is to find the voltages $V_1 \dots V_N$ at the internal points in the circuit.

a) Using Ohm's law and the Kirchhoff current law, which says that the total net current flow out of (or into) any junction in a circuit must be zero, show that the voltages $V_1 \dots V_N$ satisfy the equations

$$\begin{aligned}
3V_1 - V_2 - V_3 &= V_+, \\
-V_1 + 4V_2 - V_3 - V_4 &= V_+, \\
&\vdots \\
-V_{i-2} - V_{i-1} + 4V_i - V_{i+1} - V_{i+2} &= 0, \\
&\vdots \\
-V_{N-3} - V_{N-2} + 4V_{N-1} - V_N &= 0, \\
-V_{N-2} - V_{N-1} + 3V_N &= 0.
\end{aligned}$$

Express these equations in vector form $\mathbf{Av} = \mathbf{w}$ and find the values of the matrix $\mathbf{A}$ and the vector $\mathbf{w}$.

b) Write a program to solve for the values of the V_i when there are $N = 6$ internal junctions with unknown voltages. (Hint: All the values of V_i should lie between zero and 5V. If they don't, something is wrong.)

c) Now repeat your calculation for the case where there are $N = 10\,000$ internal junctions. Notice that you have a banded matrix and brute force Gaussian elimination is much more expensive than a banded Gaussian elimination. Write a program that solves a banded matrix equation and solve for the potential at junctions. Save the potential in order $(V_1, V_2, \dots)$ in a text file `potentials.txt`.

Exercise 15: The QR algorithm

In this exercise you'll write a program to calculate the eigenvalues and eigenvectors of a real symmetric matrix using the QR algorithm. The first challenge is to write a program that finds the QR decomposition of a matrix. Then we'll use that decomposition to find the eigenvalues.

b) Write a Python function that takes as its argument a real square matrix $\mathbf{A}$ and returns the two matrices $\mathbf{Q}$ and $\mathbf{R}$ that form its QR decomposition. As a test case, try out your function on the matrix

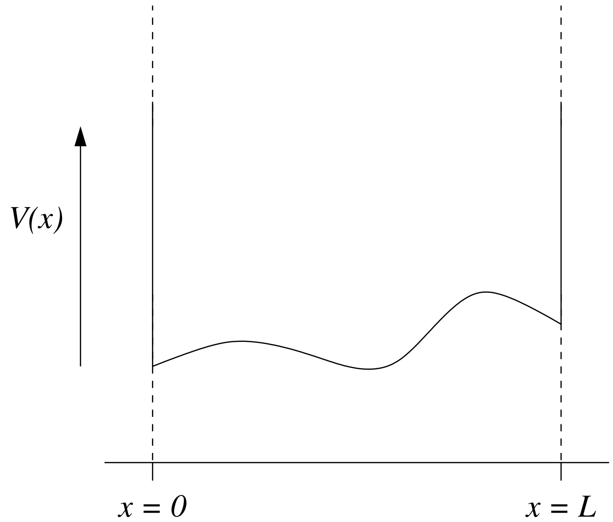
$$\mathbf{A} = \begin{pmatrix} 1 & 4 & 8 & 4 \\ 4 & 2 & 3 & 7 \\ 8 & 3 & 6 & 9 \\ 4 & 7 & 9 & 2 \end{pmatrix}.$$

Check the results by multiplying $\mathbf{Q}$ and $\mathbf{R}$ together to recover the original matrix $\mathbf{A}$ again. You can use any of the methods that were covered in class (Gram-Schmidt orthogonalization or Householder triangulation).

c) Using your function, write a complete program to calculate the eigenvalues and eigenvectors of a real symmetric matrix using the QR algorithm (see section 6.2 of Newman's book). Continue the calculation until the magnitude of every off-diagonal element of the matrix is smaller than 10^{-6}. Test your program on the example matrix above. You should find that the eigenvalues are $1, 21, -3$, and -8.

Exercise 16: Asymmetric quantum well

Quantum mechanics can be formulated as a matrix problem and solved on a computer using linear algebra methods. Suppose, for example, we have a particle of mass M in a one-dimensional quantum well of width L, but not a square well like the examples you've probably seen before. Suppose instead that the potential $V(x)$ varies somehow inside the well:



We cannot solve such problems analytically in general, but we can solve them on the computer.

In a pure state of energy E, the spatial part of the wavefunction obeys the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$, where the Hamiltonian operator $\hat{H}$ is given by

$$\hat{H} = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x).$$

For simplicity, let's assume that the walls of the well are infinitely high, so that the wavefunction is zero outside the well, which means it must *go to* zero at $x = 0$ and $x = L$. In that case, the wavefunction can be expressed as a Fourier sine series thus:

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin\frac{\pi n x}{L},$$

where $\psi_1, \psi_2, \ldots$ are the Fourier coefficients.

a) Noting that, for m, n positive integers

$$\int_0^L \sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \begin{cases} L/2 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases}$$

show that the Schrödinger equation $\hat{H}\psi = E\psi$ implies that

$$\sum_{n=1}^{\infty} \psi_n \int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \tfrac{1}{2}LE\psi_m.$$

Hence, defining a matrix $\mathbf{H}$ with elements

$$
\begin{aligned}
H_{mn} &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\,\hat{H}\sin\frac{\pi n x}{L}\,\mathrm{d}x \\
&= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\left[-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\sin\frac{\pi n x}{L}\,\mathrm{d}x,
\end{aligned}
$$

show that Schrödinger's equation can be written in matrix form as $\mathbf{H}\boldsymbol{\psi} = E\boldsymbol{\psi}$, where $\boldsymbol{\psi}$ is the vector $(\psi_1, \psi_2, \ldots)$. Thus $\boldsymbol{\psi}$ is an eigenvector of the *Hamiltonian matrix* $\mathbf{H}$ with eigenvalue E. If we can calculate the eigenvalues of this matrix, then we know the allowed energies of the particle in the well.

b) For the case $V(x) = ax/L$, evaluate the integral in H_{mn} analytically and so find a general expression for the matrix element H_{mn}. Show that the matrix is real and symmetric. You'll probably find it useful to know that

$$
\int_0^L x\sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \begin{cases} 0 & \text{if } m \neq n \text{ and both even or both odd,} \\ -\left(\dfrac{2L}{\pi}\right)^2 \dfrac{mn}{(m^2-n^2)^2} & \text{if } m \neq n \text{ and one is even, one is odd,} \\ L^2/4 & \text{if } m = n. \end{cases}
$$

Write a Python program to evaluate your expression for H_{mn} for arbitrary m and n when the particle in the well is an electron, the well has width 5 Å, and $a = 10\,\text{eV}$. (The mass and charge of an electron are $9.1094 \times 10^{-31}\,\text{kg}$ and $1.6022 \times 10^{-19}\,\text{C}$ respectively.)

c) The matrix $\mathbf{H}$ is in theory infinitely large, so we cannot calculate all its eigenvalues. But we can get a pretty accurate solution for the first few of them by cutting off the matrix after the first few elements. Modify the program you wrote for part (b) above to create a 10×10 array of the elements of $\mathbf{H}$ up to $m, n = 10$. Calculate the eigenvalues of this matrix using the appropriate function from `numpy.linalg` and hence print out, in units of electron volts, the first ten energy levels of the quantum well, within this approximation. You should find, for example, that the ground-state energy of the system is around 5.84 eV. (Hint: Bear in mind that matrix indices in Python start at zero, while the indices in standard algebraic expressions, like those above, start at one. You will need to make allowances for this in your program.)

d) Modify your program to use a 100×100 array instead and again calculate the first ten energy eigenvalues. Comparing with the values you calculated in part (c), what do you conclude about the accuracy of the calculation?

e) Now modify your program once more to calculate the wavefunction $\psi(x)$ for the ground state and the first two excited states of the well. Use your results to make a graph with three curves showing the probability density $|\psi(x)|^2$ as a function of x in each of these three states. Pay special attention to the normalization of the wavefunction—it should satisfy the condition $\int_0^L |\psi(x)|^2 \, dx = 1$. Is this true of your wavefunction?