PHYS6350 (Computational Physics)

Problem Set 3

Due:

Mon, Apr 3, 2023, end of the day

Instructions:

Send via Teams (preferably) or email. Should include code (or, where applicable, note) which solves the problems and, where applicable, plots and/or annotations. The preferred languages are Python/Jupyter notebook/C++ while other choices may be accepted on an individual basis.

Problem 3.1: The Lorenz equations (4 points)

Adapted from Exercise 8.3 from M. Newman "Computational Physics''

One of the most celebrated sets of differential equations in physics is the Lorenz equations:

$$\frac{dx}{dt} = \sigma(y - x), \qquad \frac{dy}{dt} = rx - y - xz, \qquad \frac{dz}{dt} = xy - bz,$$

where σ, r, and b are constants. (The names σ, r, and b are odd, but traditional---they are always used in these equations for historical reasons.)

These equations were first studied by Edward Lorenz in 1963, who derived them from a simplified model of weather patterns. The reason for their fame is that they were one of the first incontrovertible examples of *deterministic chaos*, the occurrence of apparently random motion even though there is no randomness built into the equations. We encountered a different example of chaos in the logistic map of Exercise 3.6.

a) Write a program to solve the Lorenz equations for the case $\sigma = 10$, $r = 28$, and $b = \frac{8}{3}$ in the range from $t = 0$ to $t = 50$ with initial conditions $(x, y, z) = (0, 1, 0)$. Have your program make a plot of y as a function of time. Note the unpredictable nature of the motion.

b) Modify your program to produce a plot of z against x. You should see a picture of the famous ``strange attractor'' of the Lorenz equations, a lop-sided butterfly-shaped plot that never repeats itself.

Problem 3.2: Quantum oscillators (6 points)

Adapted from Exercise 8.14 from M. Newman "Computational Physics''

Consider the one-dimensional, time-independent Schroedinger equation in a harmonic (i.e., quadratic) potential $V(x) = V_0 x^2/a^2$, where V_0 and a are constants.

a) Write down the Schroedinger equation for this problem and convert it from a second-order equation to two first-order ones.

b) Write a program to find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50$ eV, and $a = 10^{-11}$ m. Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Try using $x = -10a$ to $+10a$, with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic oscillator in a box with impenetrable walls.) The wavefunction is real everywhere, so you don't need to use complex variables, and you can use evenly spaced points for the solution --- there is no need to use an adaptive method for this problem.

You may want to use the shooting method to solve this boundary value problem.

The quantum harmonic oscillator is known to have energy states that are equally spaced. Check that this is true, to the precision of your calculation, for your answers. (Hint: The ground state has energy in the range 100 to 200 eV.)

c) Now modify your program to calculate the same three energies for the anharmonic oscillator with $V(x) = V_0 x^4/a^4$, with the same parameter values.

d) Modify your program further to calculate the properly normalized wavefunctions of either the harmonic and anharmonic oscillator for the three states and make a plot of them, all on the same axes, as a function of x.

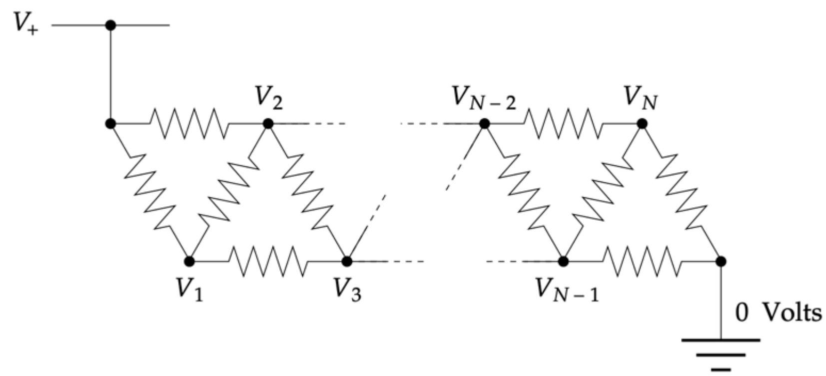
To normalize the wavefunctions you will have to evaluate the integral $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx$ and then rescale ψ appropriately to ensure that the area under the square of each of the wavefunctions is 1. Either the trapezoidal rule or Simpson's rule will give you a reasonable value for the integral. Note, however, that you may find a few very large values at the end of the array holding the wavefunction. Where do these large values come from? Are they real, or spurious?

One simple way to deal with the large values is to make use of the fact that the system is symmetric about its midpoint ($|\psi(x)|^2$ is an even function of x) and calculate the integral of the wavefunction over only the left-hand half of the system, then double the result. This neatly misses out the large values.

Problem 3.3: A chain of resistors (4 points)

Adapted from Exercise 6.7 from M. Newman "Computational Physics"

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 $\mathbf{A}\mathbf{v} = \mathbf{w}$ 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 5 V. If they don't, something is wrong.)

c) Now repeat your calculation for the case where there are $N = 10\,000$ internal junctions. This part is unfeasible using a generic solver.
You need to make use of the fact that the matrix $\mathbf{A}$ is banded and use the appropriate method.