Physics 371, Fall 2022

Project 2: One-dimensional Waves and Eigenvalue Problems

Due Monday, October 31st

I. INTRODUCTION

In this project, we apply computational methods for boundary value problems to solving one-dimensional linear differential equations involving eigenvalues. Along the way, we will explore applications to both classical and quantum mechanics. We begin with problems that have known analytical solutions and then move onto more complicated cases where numerical approaches are necessary. Finally, we will illustrate and highlight the underlying mathematical structure (namely linear algebra) that govern wave equations.

II. ONE-DIMENSIONAL WAVES ON A STRING

1) Recall that the one-dimensional wave equation can be separated into two ordinary differential equations in x and t, respectively. The x-equation is

$$\frac{d^2y}{dx^2} = -k^2 y. \tag{1}$$

Consider a horizontal string of length L tied down at both ends so that

$$y(x=0) = y(x=L) = 0. \tag{2}$$

Rewrite equation (1) in terms of appropriate dimensionless variables. Along the way, please clearly indicate the physical scales you used.

2) Rewrite your dimensionless equation (1) as two first-order differential equations, and create functions that capture the right-hand side of these equations.

3) Write a program that uses 4th order the Runge-Kutta method to solve the system of first-order equation with initial conditions $y(x=0) = 0$ and $dy/dx|_{x=0} = a$. Here you will explain what are the potential values of the constant a. Your code should also allow you to vary (in other words, accept as input) the wavelength $\lambda = 2\pi/k$.

4) Extend your code for 3) to solve the first-order equations with a starting wavelength (or wavenumber) where the solution has no nodes within the computational domain ($0 \leq x \leq L$).

Change to a new wavelength that moves $y(x = L)$ towards the right direction. Iterate the process until you arrive at a solution where $y(x = L)$ changes sign.

5) Now that you have two solutions that bracket the true solution that satisfies the boundary condition, complete your code to obtain an answer within tolerance $\delta y = L/1000$ at $x = L$. Along the way, extract the wave number k of the fundamental mode on the string.

6) Continue the process to obtain numerical estimates for the wave numbers and frequencies of the first two higher harmonics ($n = 2$ and $n = 3$). What is the fractional discrepancy between your numerical results and the 'true' analytic answers?

7) Possible physical wave forms on the string are of course not limited to sines and cosines. Problem 3 in Problem Set 3 is an example where a string is initially plucked into a clearly non-sinusoidal shape. Write a code to numerically evaluate (using your favorite method) the integrals that gives the first ten non-vanishing Fourier coefficients (c_n's). **For this and subsequent questions, please use the exact analytic solutions for the allowed standing wave modes on the bounded string**.

8) Numerically compute and plot successive partial sums of the Fourier series representing the initial shape $\xi(x, t = 0)$ up to the first ten non-vanishing terms. Does your final plot (that includes all ten terms) resemble the exact $\xi(x, t = 0)$?

9) Numerically evaluate the full time-dependent $\xi(x, t)$ using the first ten Fourier terms. Plot spatial snapshots of the solution at several (maybe five?) representative times. You are welcome to instead make a movie that shows the string's motion if you like!

III. SCHRODINGER EQUATION WITH MORSE POTENTIAL

The Morse potential is a popular and useful model for describing the vibrational modes of a diatomic molecule. This (more or less phenomenological) potential energy function is

$$V(x) = D[e^{-2a(x-x_0)} - 2e^{-a(x-x_0)}], \tag{3}$$

where D, a and x_0 are constants determined (in principle) via experiments.

1) What are the dimensions of D, a and x_0?

2) Find the minima $V_{\min}$ of $V(x)$ and the corresponding position.

3) At low-energies near $V_{\min}$, compute the effective spring constant k.

4) Combine the above results to sketch the full potential. Please label your graph in way that demonstrates the physical interpretation of D, a and x_0.

5) Imagine a classical particle that begins with some energy $E < 0$ trapped inside the potential well. What do you expect this particle to do?

6) Next, we proceed to solving the time-independent Schrodinger equation

$$\frac{-\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{4}$$

where μ is the reduced mass of the diatomic molecule. We have in fact reduced a two particle problem into a single effective particle with mass μ, and $V(x)$ is the interaction potential between the atoms. **Without solving the Schrodinger equation either analytically or numerically**, estimate the ground state energy and justify your answer.

7) What is the allowed energy range for bound states (corresponding to particles that would be trapped classically)? Your answer should be an inequality in terms of D, a and x_0.

8) Rewrite the Schrodinger equation in dimensionless form by scaling x, ψ and E to appropriate characteristic values. You should find that the dimensionless equation is parametrized by only two parameters, which you will determine in terms of D, a and x_0.

9) Next, we impose boundary conditions on the differential equation. First, the atoms cannot literally touch at $\bar{x} = 0$. The solution must also be normalizable. Write down the mathematical boundary conditions on $\bar{\psi}$ that these physical constraints imply.

10) Finally, to use Runge-Kutta, we need an initial condition (at $\bar{x} = 0$) on the derivative of $\bar{\psi}$, which we will set to 1. Is this the only possible choice of $d\bar{\psi}/d\bar{x}|_{x=0}$?

11) Write a program that uses 4th order Runge-Kutta method to calculate $\bar{\psi}(\bar{x})$. Please specify the parameters that your solver needs as input.

12) Before proceeding, we first need to address an additional complication compared to Part I. For the Morse potential, the wave function vanishes as $\bar{x}$ goes to ∞ instead of at a finite value. How will you get around this difficulty numerically?

13) Extend your program so that it can systematically obtain the lowest eight energy eigenvalues and associated solutions. The general approach is similar to what you did in Part I. For this part, please use the following parameters:

$$D = 100\left(\frac{\hbar^2}{2\mu x_0^2}\right) \quad \textit{and} \quad \bar{x}_0 = ax_0 = 0.7. \tag{5}$$

14) Compute and plot the wave functions (energy eigenfunctions) corresponding to the energies you obtained. Please over plot the potential on the same graph(s).