PHYS H304 Homework 8

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This is the lab report write-up of the approach and methods used for the eighth problem set in PHYS H304.

1. INTRODUCTION

This is a summary of the methods and major equations used for this problem set. In this report, we explore methods of linear algebra to solve physical systems. The major equations used are included where appropriate and a summary of the approach used to develop the code is included as well. All equations are taken from Computational Physics by Mark Newman [1].

2. METHODS

2.1. Exercise 6.9

In quantum mechanics, the behavior of the potential determines the eigenstates and corresponding eigenvalues of energy that are determined using the time indpendent Schrodinger equation. In the case where the Hamiltonian is time-independent, we can express the wave equation as the action of a linear operator, in matrix form, on a vector of eigenstates shown in Eqn 1, where H corresponds to the Hamiltonian. The Hamiltonian is dependent on the position, as shown in Eqn. 2

$$H\psi(x) = E\psi(x) \tag{1}$$

$$H = \frac{h_{bar}^2}{2M}\frac{d^2}{dx^2} + V(x) \tag{2}$$

For a Fourier synthesized wavefunction, $\psi(x)$, Newman [1] defines the wavefunction as a superposition of sine functions scaled by appropriate Fourier coefficients shown in Eqn. 3.

$$\psi(x) = \sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L}\right) \tag{3}$$

To express the wave equation in terms of the Hamiltonian and the expanded version of $\psi(x)$, we can substitute Eqns 2 and 3 into Eqn. 1. This yields the Equations 4 and 6.

$$\frac{h_{bar}^2}{2M}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{4}$$

$$\frac{h_{bar}^2}{2M}\frac{d^2}{dx^2}\sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L}\right) + V(x)\sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L}\right) = E\sum_0^\infty \psi_n \,\mathrm{s} \tag{5}$$

We can factor out the Hamiltonian such that we can simplify this expression to that shown in Eqn. ??.

$$\left(\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right)\sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L}\right) = E\sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L}\right) \tag{6}$$

Multiplying both sides by a factor of $\sin\left(\frac{m\pi x}{L}\right)$ and taking the integral from the range of x across the width of the well (0-L), we obtain Eqn. 7

$$\int_0^L \sin\left(\frac{m\pi x}{L}\right)\left(\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right)\sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L}\right) = \int_0^L \sin\left(\frac{m\pi x}{L}\right) E\sum_0^\infty \psi_n \sin\left(\frac{\pi n x}{L} \tag{7}$$

We can then factor out the sum of the Fourier coefficients, as shown in Eqn. 8. We also identify that the term in between the sine function is the action of the Hamiltonian operator, that we express as $\hat{H}$ for brevity. For all terms on the right hand side of the equation, when n differs from m, the integral evaluates to zero due to the odd/evenness of sine functions, as shown below. The first case is true when n $\neq$ m and the second case when n=m.

$$\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{\pi n x}{L}\right) = \begin{cases} 0 \\ \frac{L}{2} \end{cases}$$

The only non-zero contribution is thus the case n=m, in which case the Fourier coefficient is given by ψ_m and the expression under the integral evaluates to $L/2$.

$$\sum_0^\infty \psi_n \int_0^L \sin\left(\frac{m\pi x}{L}\right)\hat{H}\sin\left(\frac{\pi n x}{L}\right) = \sum_0^\infty \psi_n E\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{\pi n x}{L}\right) \tag{8}$$

$$\sum_{n=0}^\infty \psi_n \int_0^L \sin\left(\frac{m\pi x}{L}\right)\hat{H}\sin\left(\frac{\pi n x}{L}\right) = \psi_m E\frac{L}{2} \tag{9}$$

Hence, we can express the original wave equation in the form shown in Eqn. 9. This can be further expanded to a matrix equation if we recognize that the term containing the sum of the products of the sine functions with different m and n indices reflects an inner product of the states with the states generated by the action of the Hamiltonian upon them. From [2], this inner product of a basis state with the state generated after the action of an operator corresponds to a matrix element of that operator expressed in that basis. Therefore, we can define matrix

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elements H_{mn} of the Hamiltonian such that each superposed term in the Fourier synthesis corresponds to an element in the Hamiltonian. In this case, Eqn. 10 represents the matrix elements, defined by the inner products (integrals). The Fourier coefficients then form the set of eigenfunctions of the Hamiltonian that yield energy eigen values E when the Hamiltonian acts on them. This yields the matrix equation in Eqn. 11 shown below where $\vec{\psi}$ represents the vector of $(\psi_1, \psi_2, \psi_3 ...)$.

$$H_{mn} = \frac{2}{L}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\hat{H}\sin\left(\frac{\pi n x}{L}\right) \tag{10}$$

$$\sum_{n=0}^{\infty} H_{mn}\vec{\psi} = \hat{H}\vec{\psi} = E\vec{\psi} \tag{11}$$

In the case where the potential is well defined, we can determine the analytical solution for the elements of the Hamiltonian. We defined the potential in Eqn. 12 and show the resulting expanded Hamiltonian operation in Eqn.13.

$$V(x) = \frac{ax}{L} \tag{12}$$

$$H_{mn} = \frac{2}{L}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\left(\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \frac{ax}{L}\right)\sin\left(\frac{\pi n x}{L}\right) \tag{13}$$

Distributing the operator linearly, we can divide the integral into two smaller integrals summed together corresponding to the kinetic term and the potential term shown in Eqn. 14 and 15 respectively.

$$\frac{2}{L}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\left(\frac{\hbar^2}{2M}\frac{d^2}{dx^2}\right)\sin\left(\frac{\pi n x}{L}\right) \tag{14}$$

$$\frac{2}{L}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\left(\frac{ax}{L}\right)\sin\left(\frac{\pi n x}{L}\right) \tag{15}$$

Taking the second derivative of a sine function yields the negative of the original function; hence, applying this to Eqn. 14 and factoring out all constants from the integral, we simplify the expression to Eqn. 16.

$$\frac{\hbar^2\pi^2 n^2}{ML^3}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{\pi n x}{L}\right) \tag{16}$$

Using the solutions for the integral described earlier for different cases of n and m, this simplifies to two expressions: 0 if n differs from m and $\frac{\hbar^2\pi^2 n^2}{2ML^2}$ in the case where n is equal to m. Similarly, we can use trigonometric identities to simplify the expression in Eqn. 15 after factoring out all constants, shown in Eqns 17.

$$\frac{2a}{L}\int_0^L \sin\left(x\frac{m\pi x}{L}\right)\sin\left(\frac{\pi n x}{L}\right) \tag{17}$$

Using the relationship between oddness/evenness of sine functions shown below, we can simplify the expression.

$$\int_0^L x\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{\pi n x}{L}\right) = \begin{cases} 0 \\ \frac{L^2}{4} \\ (\frac{2L}{\pi})^2 \frac{mn}{(m^2-n^2)^2} \end{cases}$$

where the first case is true if $n \neq m$ and both are odd/even, the second alternative is true in the case that n=m, and the last case is the solution when $n \neq m$ and either n or m is odd/even.
As the sum of the Eqn 17 and 16 is a given element Hmn, we determine three possibilities for the elements of the Hamiltonian matrix. These are:

- $\frac{\hbar^2\pi^2 n^2}{2ML^2} + \frac{a}{2}$, if n=m
- $\frac{2a}{L^2} \cdot -(\frac{2L}{\pi})^2\frac{mn}{(m^2-n^2)^2}$, if $n \neq m$ and n or m is odd/even and the other is the opposite
- 0, if $n \neq m$ and both n and m are odd/even

Using these conditions, we can code the Hamiltonian matrix in Python using a series of if statements to generate an mxn matrix and the constants provided in the problem. To determine the energy eigenvalues of the system, we use the built-in function linalg.eigvalsh in the NumPy library. We do so using a 10x10 Hamiltonian, as the Fourier synthesis to infinity is not possible. However, we observe that a 10x10 approximation is accurate, as we determine the eigenvalues using a 100x100 Hamiltonian and compare the accuracy of the energy eigen values.

For the last part of the problem, we plot the superposed probability densities of the ground state, first excited state, and second excited states. To do so, we extract the corresponding eigen vectors using the eigh function in Python. Then, we use the Fourier series synthesis to determine the wavefunctions for each state shown in Eqn. 2.1 and plot the resulting wavefunction for a range of x equal to the width of the potential well.

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2.2. Exercise 6.4

Kirchoff's laws state that the current flowing into a junction must equal the current flowing out of the junction [3]. For a circuit with multiple junctions, expressing these constraints on the current flow for each flow can set up a system of linear equations. For the circuit given in Exercise 6.1, the current flow through each junction is given in Eqns 19, 20, 21, 22, where $V_+ = 5V$. We then solve for the voltages using the solve function in the NumPy library.

$$4V_1 - V_2 - V_3 - V_4 = V_+ \tag{19}$$

$$3V_2 - V_1 - V_4 = 0 \tag{20}$$

$$3V_3 - V_1 - V_4 = V_+ \tag{21}$$

$$4V_4 - V_2 - V_3 - V_1 = 0 \tag{22}$$

3. RESULTS AND CONCLUSIONS

For Exercise 6.4, we determine the solution to be:

- $V_1 = 2.99V$
- $V_2 = \frac{5}{3}V$
- $V_3 = \frac{10}{3}V$
- $V_4 = 2.0V$

We obtain the same solution using Gaussian elimination, included in our code to check the result.

For Exercise 6.9, we determine the Hamiltonian shown in our code output. Using linalg functions, we find that the ground state energy has an eigenvalue of 5.84eV given to three significant figures for a ten by ten Hamiltonian. When we increased the size of the Hamiltonian to 100x100, we find that the energy eigenvalues correspond to that of the ten by ten version, as evidenced by the ground state energy which has the same value of 5.84eV. Therefore, the ten by ten approximation of the Hamiltonian is reasonably accurate. For the probability densities, we determine the individual wavefunctions for the ground state, first excited state, and second excited state and take the magnitude squared of each of the resultant wave functions. Using Gaussian quadrature, we take the integral of each of these wavefunctions to determine the whether the normalization requirement is met (the intergal of the probability density is equal to 1). As the integral of each of the wavefunctions amounted to $2.5x10^{-10}$, we scaled the individual wavefunctions by the appropriate constant ($4x10^{9}$) to meet this requirement. The normalized superposition of the probability densities are shown in Figure 1.

4. SURVEY QUESTION

The most interesting problem was 6.9. The homework took me about 4 hours to complete coding and calculation wise, but the write up took significantly longer. I learnt how to apply concepts of linear algebra to quantum mechanics and electricity. I think the problem set length and difficulty were just right.

[1] M. Newman, *Computational Physics* ([Createspace], 2012), URL http://www-personal.umich.edu/~mejn/cp/index.html.

[2] J. S. Townsend, *Quantum Physics: A Fundamental Approach to Modern Physics* ([University Science Books], 2010).

[3] *University physics volume 2*, URL https://openstax.org/details/books/university-physics-volume-2?Book.

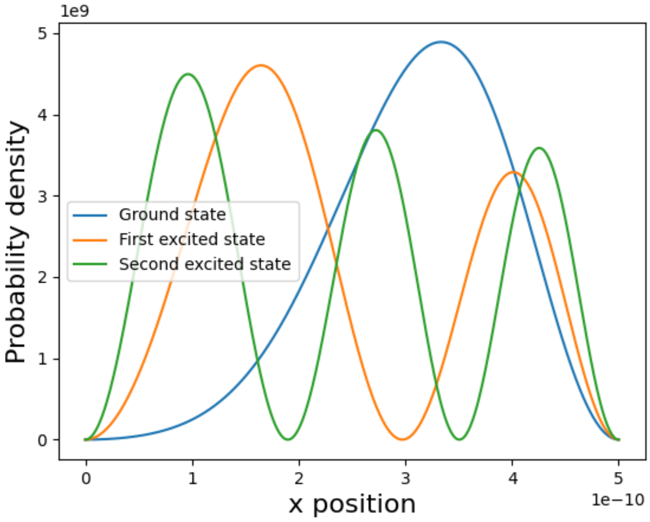

FIG. 1: A plot of the normalized probability densities for the ground state, first excited state and second excited states