PHYS304 Assignment5

Shufan Xia
(Dated: March 3rd, 2020)

Collaborated with Linda Yuan

1. 6.4 RESISTOR NETWORK

From Ohm's law and Kirchhoff current law on four of the junctions in this configuration, we have:

$$\frac{V_1 - V_2}{R} + \frac{V_1 - V_3}{R} + \frac{V_1 - V_4}{R} + \frac{V_1 - V_+}{R} = 0 \quad (1)$$

$$\frac{V_2 - V_1}{R} + \frac{V_2 - V_4}{R} + \frac{V_2 - V_-}{R} = 0 \quad (2)$$

$$\frac{V_4 - V_-}{R} + \frac{V_4 - V_2}{R} + \frac{V4 - V1}{R} + \frac{V_4 - V_3}{R} = 0 \quad (3)$$

$$\frac{V_3 - V_4}{R} + \frac{V_3 - V_1}{R} + \frac{V_3 - V_+}{R} = 0 \quad (4)$$

Given $V_+ = 5V$ and $V_- = 0V$, this system of equations is equivalent to solving the matrix function:

$$\begin{pmatrix} 4 & -1 & -1 & -1 \\ -1 & 3 & 0 & -1 \\ -1 & -1 & -1 & 4 \\ -1 & 0 & 3 & -1 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{pmatrix} = \begin{pmatrix} 5 \\ 0 \\ 0 \\ 5 \end{pmatrix} \quad (5)$$

Using **numpy.linalg.solve()**, I got:

$$V_1 = 3.0V, V2 = 1.667V, V3 = 3.33V \ and \ V4 = 2.0V \quad (6)$$

2. 6.6 ASYMMETRIC QUANTUM WELL

a)

$$I = \sum_{n=1}^{\infty} \psi_n \int_0^L sin\frac{m\pi x}{L} \hat{H} sin\frac{n\pi x}{L} dx \quad (7)$$

$$= \int_0^L \sum_{n=1}^{\infty} \psi_n sin\frac{m\pi x}{L} \hat{H} sin\frac{n\pi x}{L} dx \quad (8)$$

$$= \int_0^L sin\frac{m\pi x}{L} \hat{H}(\sum_{n=1}^{\infty} \psi_n sin\frac{n\pi x}{L})dx \quad (9)$$

Given $\hat{H}\Psi = E\Psi$ and $\Psi = \sum_{n=1}^{\infty} \psi_n sin\frac{n\pi x}{L}$, we have:

$$\hat{H}(\sum_{n=1}^{\infty} \psi_n sin\frac{n\pi x}{L}) = E\sum_{n=1}^{\infty} \psi_n sin\frac{n\pi x}{L} \quad (10)$$

and

$$I = \int_0^L E\sum_{n=1}^{\infty} \psi_n sin\frac{n\pi x}{L} sin\frac{m\pi x}{L} dx \quad (11)$$

$$= E\sum_{n=1}^{\infty} \psi_n \int_0^L sin\frac{n\pi x}{L} sin\frac{m\pi x}{L} dx \quad (12)$$

$$(13)$$

Since:

$$\int_0^L sin\frac{n\pi x}{L} sin\frac{m\pi x}{L} dx = \begin{cases} \frac{L}{2} & m = n, \\ 0 & m \neq n. \end{cases} \quad (14)$$

we have:

$$\sum_{n=1}^{\infty} \psi_n \int_0^L sin\frac{n\pi x}{L} sin\frac{m\pi x}{L} dx = \frac{L}{2}\psi_m \quad (15)$$

Plugging in the result of Eq.16 to Eq.9, we have:

$$I = \sum_{n=1}^{\infty} \psi_n \int_0^L sin\frac{m\pi x}{L} \hat{H} sin\frac{n\pi x}{L} dx = \frac{1}{2} LE\psi_m \quad (16)$$

b) **H** is defined as a matrix of :

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & \dots & H_{1n} \\ H_{21} & H_{22} & \dots & & H_{2n} \\ \vdots & \ddots & & & \vdots \\ H_{m1} & H_{m2} & \dots & & H_{mn} \end{pmatrix} \quad (17)$$

Then we have $\mathbf{H}\vec{\psi} =$:

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & \dots & H_{1n} \\ H_{21} & H_{22} & \dots & & H_{2n} \\ \vdots & \ddots & & & \vdots \\ H_{m1} & H_{m2} & \dots & & H_{mn} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \quad (18)$$

The result of this matrix multiplication is:

$$\begin{pmatrix} H_{11}\psi_1 + H_{12}\psi_2 \cdots + H_{1n}\psi_n \\ H_{11}\psi_1 + H_{22}\psi_2 \cdots + H_{2n}\psi_n \\ \vdots \\ H_{m1}\psi_1 + H_{m2}\psi_2 \cdots + H_{mn}\psi_n \end{pmatrix} = \begin{pmatrix} \sum_{n=1}^{\infty} H_{1n}\psi_n \\ \sum_{n=1}^{\infty} H_{2n}\psi_n \\ \vdots \\ \sum_{n=1}^{\infty} H_{mn}\psi_n \end{pmatrix} \quad (19)$$

For the entry of each row m :

$$\sum_{n=1}^{\infty} H_{mn}\psi_n = \sum_{n=1}^{\infty} \psi_n \frac{2}{L} \int_0^L sin\frac{m\pi x}{L} \hat{H} sin\frac{n\pi x}{L} dx \quad (20)$$

$$= \frac{2}{L}\frac{1}{2} LE\psi_m = E\psi_m \quad (21)$$

Thus, $\mathbf{H}\vec{\psi} =$

$$\begin{pmatrix} E\psi_1 \\ \vdots \\ E\psi_n \end{pmatrix} = E\vec{\psi} \tag{22}$$

Therefore, the Schrödinger's equation can be written as $\mathbf{H}\vec{\psi} = E\vec{\psi}$

b)

$$H_{mn} = \frac{2}{L}\int_0^L sin\frac{m\pi x}{L}[-\frac{h^2}{2M}\frac{d^2}{dx^2} + V(x)]sin\frac{n\pi x}{L}dx \tag{23}$$

$$= \frac{2}{L}[\int_0^L -\frac{h^2}{2M}\frac{d^2}{dx^2}(sin\frac{n\pi x}{L})sin\frac{m\pi x}{L}dx \tag{24}$$

$$+ \int_0^L sin\frac{m\pi x}{L}V(x)sin\frac{n\pi x}{L}dx] \tag{25}$$

For the first integral in Eq.25:

$$\int_0^L -\frac{\hbar^2}{2M}\frac{d^2}{dx^2}(sin\frac{n\pi x}{L})sin\frac{m\pi x}{L}dx \tag{26}$$

$$= \frac{\hbar^2}{2M}(\frac{\pi n}{L})^2\int_0^L sin\frac{n\pi x}{L}sin\frac{m\pi x}{L}dx \tag{27}$$

$$= \begin{cases} \frac{\hbar^2 n^2\pi^2}{4ML} & m = n, \\ 0 & m \neq n. \end{cases} \tag{28}$$

$V(x) = ax/L$, for the second integral in Eq.25 :

$$\int_0^L sin\frac{m\pi x}{L}(\frac{ax}{L})sin\frac{n\pi x}{L}dx \tag{29}$$

$$= \frac{a}{L}\int_0^L xsin\frac{n\pi x}{L}sin\frac{m\pi x}{L}dx \tag{30}$$

$$= \begin{cases} 0 & \text{if } m \neq n \text{ and both are even or both odd,} \\ -\frac{4aL}{\pi^2}\frac{mn}{(m^2-n^2)^2} & \text{if } m \neq n \text{ and one is odd, one is even} \\ \frac{aL}{4} & \text{if m=n.} \end{cases} \tag{31}$$

Then, we have:

$$H_{mn} = \begin{cases} 0 & \text{if } m \neq n \text{ and both are even or odd} \\ -\frac{8amn}{\pi^2(m^2-n^2)^2} & \text{if } m \neq n\text{, one is odd, one is even} \\ \frac{\hbar^2 n^2\pi^2}{2ML^2} + \frac{a}{2} & \text{if m=n} \end{cases} \tag{32}$$

I used **meshgrid()** to create a 10 by 10 matrix of **H**. Each entry of **H** is H_{mn}, where m represents row indices and n stands for column indices. Using **np.linalg.eigh(H)**, I found eigenvalues and their corresponding eigenvectors, $(\psi_1, \psi_2, ...\psi_n)$. The ground state energy or the lowest eigenvalue is $5.836eV$ with precision to 10^{-15}.

Using a 100 by 100 matrix of **H**, I found the ground state energy is also $5.836eV$ and with precision to 10^{-15} as well. Therefore, the accuracy of this calculation does not improve significantly with more elements in the matrix **H** after $m, n = 10$.

With the conclusion about the accuracy of this calculation, I used only a 10×10 matrix to find the eigenvectors $\vec{\psi}$ that satisfy the Schrödinger's equation. For each eigenvalue or energy state N, each entry of $\vec{\psi}$, $\psi_1, \psi_2, ..., \psi_1 0$, are the coefficients of the orthogonal bases $sin\frac{n\pi x}{L}$ of the wave function $\Psi_N(x)$:

$$\Psi_N(x) = \sum_{n=1}^{10}\psi_n sin\frac{n\pi x}{L} \tag{33}$$

To normalize the probability density function, I used Gaussian quadrature integration method with N=100 from x=0 to L (the length of the potential well) to integrate $\Psi_N(x)$, and divided the result by 1 to find the normalization constant C_N:

$$1 = C_N\int_0^L (\sum_{n=1}^{10}\psi_n sin\frac{n\pi x}{L})^2 dx \tag{34}$$

After normalizing the wave functions for $N = 1, 2$ and 3, I plotted the probability density function for the ground state and the first two excited states:

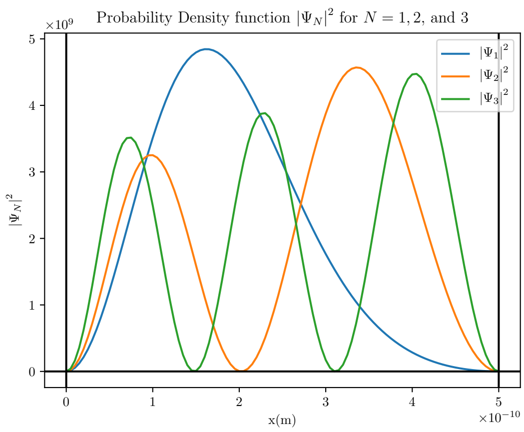

FIG. 1: Probability density function for the ground state and the first two excited states: $\Psi_1(x)$, $\Psi_2(x)$ and $\Psi_3(x)$

3. SURVEY QUESTION

This homework took me about 9 to 10 hours. I learned how to use **numpy** library to solve linear equations, find eigenvalues and vectors. The most interesting problem and also the one from which I learned the most is Asymmetric quantum well problem. It provided an example of turning a DEQ problem into a linear algebra problem. I used the identity of orthogonal bases and eigenvectors. It was also a really great practice to typeset matrices and piece wise functions in LaTeX. This problem set was just right.