PHYS 304 HW 8

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1. EXERCISE 6.9

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1.1. Part A

In an asymmetric quantum well, a particle of mass M is placed in a one-dimensional quantum well of width L that has a varying potential. The wavefunction obeys the time-independent Schrodinger equation (1), where the Hamiltonian, $\hat{H}$, is given by equation 2, and $\psi(x)$ is a Fourier sine series (3).

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

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

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin\frac{\pi n x}{L} \tag{3}$$

The following is known for m, n positive integers (4)

$$\int_0^L \sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}dx = \begin{cases} L/2, & \text{if m=n.} \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Using all of the above equations, it is possible to prove that the Schrodinger equation (1) implies the following (5)

$$\sum_{n=1}^{\infty}\psi_n\int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}dx = \frac{1}{2}LE\psi_m \tag{5}$$

The first step is to plug the Fourier sine expansion of $\psi(x)$ (3) into the Schrodinger equation (1), and then multiply both sides of the resulting equation by $\sin\frac{\pi m x}{L}$. This results in the following (6) after some rearranging

$$\sum_{n=1}^{\infty}\psi_n \sin\frac{\pi n x}{L}\hat{H}\sin\frac{\pi m x}{L} = \sin\frac{\pi n x}{L}\sin\frac{\pi m x}{L}E\sum_{n=1}^{\infty}\psi_n \tag{6}$$

Both sides of this equation (6) are then integrated from 0 to L. All terms within the sum go to zero except for when m=n. Taking the integral of the terms before E on the right hand side of the equation yields L/2, as given in equation 4. Since m=n, the ψ_n on the right can be replaced with ψ_m. These actions yield equation 5.

Defining a matrix **H** with elements given by equation 7, where $\hat{H}$ is given by equation 2, we show that the Schrodinger equation can be written in matrix form (8), where ψ is an eigenvector.

$$H_{mn} = \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}dx \tag{7}$$

$$\mathbf{H}\psi = E\psi \tag{8}$$

1.2. Part B

Evaluating the integral in H_{mn} first involves plugging the case $V(x) = ax/L$ into the equation for the hamiltonian (2). Multiplying this factor out yields the following equation (9)

$$H_{mn} = \frac{\pi^2 n^2\hbar^2}{ML^3}\int_0^L \sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}dx + \frac{2a}{L}\int_0^L x\sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}dx \tag{9}$$

The following is given (10)

$$\int_0^L x\sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}dx = \begin{cases} 0, & \text{if } m \neq n \text{ and both even/odd.} \\ -(\frac{2L}{\pi})^2\frac{mn}{(m^2-n^2)^2}, & \text{if } m \neq n \text{ and one even/odd.} \\ L^2/4, & \text{if m=n} \end{cases} \tag{10}$$

Using both of these equations, as well as equation 4, H_{mn} can be evaluated for each scenario. It yields the following results (11)

$$H_{mn} = \begin{cases} \frac{-8a}{\pi^2}\frac{mn}{(m^2-n^2)^2}, & \text{if } m \neq n. \\ \frac{\pi^2 n^2\hbar^2}{2ML^2} + \frac{a}{2}, & \text{if m=n.} \end{cases} \tag{11}$$

I have created a python program that evaluates H_{mn} for user inputted values of m and n, given constants of

$$M = 9.1094 \times 10^{-31} kg$$
$$e = 1.6022 \times 10^{-19} C$$
$$L = 5 \times 10^{-10} m$$
$$a = 10 eV$$

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These are not the bottom 3 states. The ground state should have 1 peak, the first excited 2, and the 2nd excited 3.

Where M and e are the mass and charge of the particle (an electron in this case), respectively, L is the width of the well (originally measured in angstroms but converted to meters for simplicity), and a is the variable in the potential function.

1.3. Part C

Modifying the program I wrote for part b, I created a 10 x 10 array of **H** up to m, n = 10. I calculated the eigenvalues of this matrix using the numpy "eigvalsh" command, which yielded the energies of the first ten states of the asymmetrical quantum well. They are as follows:

$$\text{Ground state} = 5.84eV$$
$$\text{First excited state} = 11.18eV$$
$$\text{Second excited state} = 18.66eV$$
$$\text{and so on...}$$

All ten of the values can be seen by running the code.

1.4. Part D

I modified the program yet again, this time creating a **H** matrix that is 100 x 100. Calculating the first ten energy eigenvalues yields identical values to those calculated in part C. The calculation is very accurate.

1.5. Part E

Finally, I modified the program a final time to calculate the wave functions for the ground state, first excited state, and second excited state. I used a similar technique to when I solved a similar problem of the non-asymmetrical quantum well. I calculated the wavefunctions and then plotted the probability density of each (the absolute value of the wavefunction squared) against x, seen in figure 1.

2. EXERCISE 6.16

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The Lagrange point is a point in between the Earth and the Moon at which a satellite will orbit the Earth in synchrony with the Moon. To find the distance to this point, we first assume the following (12)

$$F_{Earth} + F_{Moon} = F_{centripetal} \tag{12}$$

The force exerted by the Earth plus the force exerted by the Moon add to the total centripetal force needed to keep the satellite in its orbit. Substituting in the formulas for these values yields equation 13.

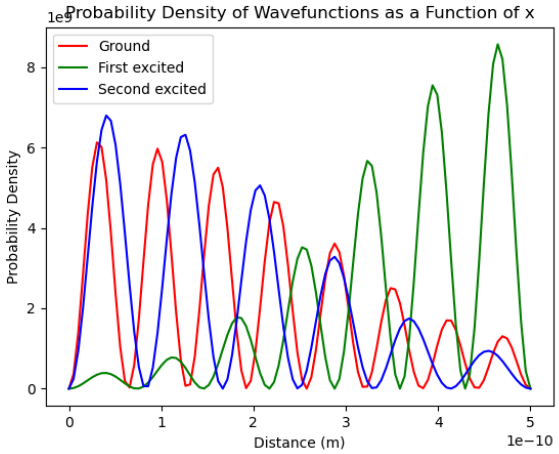

FIG. 1: Probability density of the first three wavefunctions vs x.

$$\frac{GMm_{satellite}}{r^2} - \frac{Gmm_{satellite}}{(R-r)^2} = \frac{m_{satellite}v^2}{r} \tag{13}$$

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

Where G is the gravitational constant, M is Earth's mass, m is the Moon's mass, R is the distance between the Earth and Moon, and ω is the angular velocity produced by the Moon and satellite combined. We are solving for r, the distance between Earth and the Lagrange point.

In this equation, the mass of the satellite is so much smaller than the mass of the Earth and Moon that it is insignificant, and can be ignored. The expression $\omega^2 r$ can be substituted in for the expression on the right hand side of the equation, yielding a final equation of (14)

Very clear work!

$$\frac{GM}{r^2} - \frac{Gm}{(R-r)^2} = \omega^2 r \tag{14}$$

I created a python program to calculate the distance between the Earth and the Lagrange point utilizing the secant method. I used the constants previously mentioned. To conduct the secant method, I needed to choose two suitable starting values of r. I chose my first r value to be $3 \times 10^4 m$, approximately halfway between the Earth and the Moon. I chose my second r value to be $3 \times 10^6 m$, as in the provided diagram, the satellite appears to be closer to the Moon than Earth. I set a range of 20, around the highest value I could use without the program producing an error of a zero in the denominator.

My program produced a value of $3.2561 \times 10^8 m$, which aligns with the diagram showing the point as closer to the Moon than the Earth.

3. SURVEY +5

Out of all the homework LaTeX write ups, this was the one I spent the most time on, by far. I believe I spent around 5 hours doing the actual calculations and code for this assignment, and then around 3 hours typesetting everything in LaTeX. This is mostly due to the math/calculation heavy parts a and b of problem 6.9. I am very confident in my LaTeX skills, however, I am definitely not the fastest when it comes to typesetting equations. There were several instances where I had to play around with the formatting of long equations that couldn't fit on a single line. Besides this, the homework actually went very smoothly, especially problem 6.16. I am much more confident with the secant method, and found the topic of the question very interesting!

Problem 6.16

Lanava +25

Computational Physics/Astrophysics, Winter 2023: Grading Rubrics [1]

Haverford College, Prof. Daniel Grin

For coding assignments, roughly 25 points will be available per problem.

+3 1. Does the program complete without crashing in a reasonable time frame? If yes, up to +3 points.

+1 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? If yes, +1 points

3. Does the code follow the problem specifications (i.e +2 numerical method; output requested etc.) Up to +2 points

+4 4. Is the answer correct? Up to+4points

+2 5. Is the code readable? Up to+2points

. 5.1. Are variables named reasonably?

. 5.2. Are the user-functions and imports used?

. 5.3. Are units explained (if necessary)?

. 5.4. Are algorithms found on the internet/book/etc. properly attributed?

[1] Inspired by rubric of D. Narayanan, U. Florida, and C. Cooksey, U. Hawaii

+3

6. Is the code well documented? +3points

. 6.1. Is the code author named?

. 6.2. Are the functions described and ambiguous variables defined?

. 6.3. Is the code functionality (i.e. can I run it easily enough?) documented?

7. LaTeX writeup (up to 10 points)

+10

- Are key figures and numbers from the problem given? (3 points)
- Is a brief explanation of physical context given? (2 points)
- If relevant, are helpful analytic scalings or known solutions given? (1 point)
- Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (2 points)
- Are collaborators clearly acknowledged? (1 point)
- Are any outside references appropriately cited? (1 point)

Note, even if (1), (2), (3), or (4) are not correct, one can still obtain many points via (5), (6), and (7).

Problem 6.9

Lanava +23

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+2 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) Up to +2 points

+2 4. Is the answer correct? Up to+4points

I think that the first 3 eigenvalues that your eigensystem solver find are not necessarily the lowest 3 values and so when you went to plot you plotted some higher energy states.

5. Is the code readable? Up to+2points

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