PHYS304 HW8

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(Dated: June 23, 2023)

1. EXERCISE 6.16: COMETARY ORBITS

In this problem, we are asked to calculate the Lagrange point, L_1 which is a point between the Earth and the Moon at which a satellite will orbit the Earth in perfect synchrony with the Moon, staying always in between the two. This works because the inward pull of the Earth and the outward pull of the Moon combine to create exactly the needed centripetal force that keeps the satellite in its orbit as shown in the graphic below (Newman, p.274).

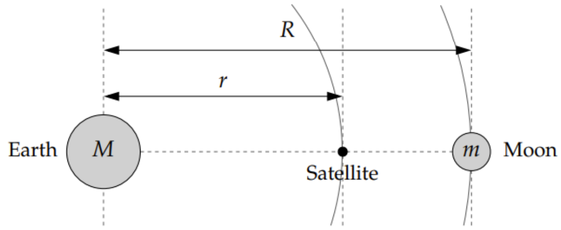

FIG. 1: The diagram showing the arrangement of the Earth, the Moon, and the satellite with the distances indicates L_1.

a) Assuming circular orbits, and assuming that the Earth is much more massive than either the Moon or the satellite, according to Newton's laws, the gravitational force from the Earth acting on the satellite is

$$\frac{GMs}{r^2} \tag{1}$$

where r is the distance from the L_1 point to earth, G is the gravitational constant, s is the mass of the satellite and M is the mass of the earth. And, the gravitational force from the Moon acting on the satellite is

$$-\frac{Gms}{(R-r)^2} \tag{2}$$

where $R-r$ is the distance from the Moon to the satellite, m is the mass of the Moon. The negative sign indicates that the Moon and the Earth are on opposite sides of the satellite, and their forces acting on the satellite on the opposite direction. Then, the centripetal force can be described as

$$s \times \omega^2 \times r \tag{3}$$

where ω is the centripetal acceleration. Then we can combine equation 1 and equation 2 for the total gravitational force which is equal to the centripetal force in 3. After removing the common factors, the equation results in 4 which shows that the distance r from the center of the Earth to the L_1 point satisfies the equation.

$$\frac{GM}{r^2} - \frac{Gm}{(R-r)^2} = \omega^2 r \tag{4}$$

where M and m are the Earth and Moon masses, G is Newton's gravitational constant, and ω is the angular velocity of both the Moon and the satellite.

b) The equation above (4) is a fifth-order polynomial equation in r which we can solve for the distance r from the Earth to the L_1 point using the secant method. According to the values of the parameters given in the problem, and the chosen suitable two starting values of $r_1 = 3.0 \times 10^4$ and $r_2 = 3.0 \times 10^6$. The program results in the distance r from the Earth to L_1 of 325606860.5717274 meters, which is accurate to at least four significant figures according to the online source.

2. EXERCISE 6.9: ASYMMETRIC QUANTUM WELL

Quantum mechanics can be formulated as a matrix problem and solved on a computer using linear algebra methods. Suppose, for example, we have a particle of mass M in a one dimensional quantum well of width L, but not a square well, instead that the potential $V(x)$ varies inside the well as shown below in figure 2 (Newman, p. 248)

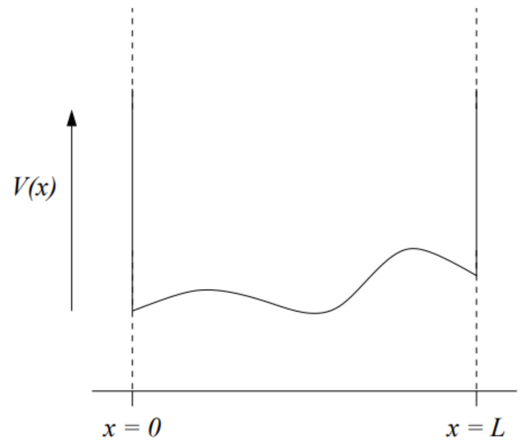

FIG. 2: The varied potential $V(x)$ in a one dimensional quantum well.

In a pure state of energy E, the spatial part of the wavefunction obeys the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$, where the Hamiltonian operator $\hat{H}$ is given by

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

For simplicity, let's assume that the walls of the well are infinitely high, so that the wavefunction is zero outside the well, which means it must go to zero at $x = 0$ and $x = L$. In that case, the wavefunction can be expressed as a Fourier sine series thus:

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

where $\psi_1, \psi_2, \ldots$ are the Fourier coefficients.

a) Noting that, for m, n positive integers

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

show that the Schrödinger equation $\hat{H}\psi = E\psi$ implies that

$$\sum_{n=1}^{\infty} \psi_n \int_0^L \sin\frac{\pi m x}{L} \hat{H} \sin\frac{\pi n x}{L}\, dx = \frac{1}{2} L E \psi_m.$$

Hence, defining a matrix H with elements

$$\begin{aligned} H_{mn} &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L} \hat{H} \sin\frac{\pi n x}{L}\, dx \\ &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right] \sin\frac{\pi n x}{L}\, dx, \end{aligned}$$

The problem asks us to show that Schrödinger's equation can be written in matrix form as $H\boldsymbol{\psi} = E\boldsymbol{\psi}$, where $\boldsymbol{\psi}$ is the vector $(\psi_1, \psi_2, \ldots)$. Thus $\boldsymbol{\psi}$ is an eigenvector of the Hamiltonian matrix H with eigenvalue E. If we can calculate the eigenvalues of this matrix, then we know the allowed energies of the particle in the well.

Starting from the given equations,

$$\int_0^L \sin\frac{\pi m x}{L} \sin\frac{\pi n x}{L}\, dx = \begin{cases} L/2 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases} \tag{5}$$

and

$$\psi(x) = \sum_{n=1}^{\infty} \psi_{m,n} \sin\frac{\pi(m,n)x}{L}, \tag{6}$$

We can combine equation 5 into equation 6, resulting in

$$\int_0^L \sin\frac{\pi m x}{L} \sin\frac{\pi n x}{L}\, dx = \int_0^L \psi_m \psi_n dx \tag{7}$$

Then according to,

$$\sum_{n=1}^{\infty} \psi_n \int_0^L \sin\frac{\pi m x}{L} \hat{H} \sin\frac{\pi n x}{L}\, dx = \frac{1}{2} L E \psi_m \tag{8}$$

we need to prove that this is true, which can be done by applying $\hat{H}\psi(x) = E\psi(x)$ to the left hand side of the equation, resulting in,

$$\sum_{n=1}^{\infty} \psi_n E \int_0^L \psi_m \psi_n dx \tag{9}$$

then

$$\sum_{n=1}^{\infty} \psi_n E \frac{L}{2} \begin{cases} 1 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases} \tag{10}$$

Now, we can find $H_{m,n}$ from the given matrix H with elements

$$H_{mn} = \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(m)\right] \sin\frac{\pi n x}{L}\, dx, \tag{11}$$

equal to

$$H_{mn} = \frac{-2}{L}\frac{\hbar^2}{2m}\int (sin(\frac{\pi m x}{L}))(\frac{-\hbar^2 n^2}{L^2})(sin(\frac{\pi n x}{L}))dx \tag{12}$$

solving the integral and simplifying, we have

$$H_{mn} = \frac{n^2\pi^2\hbar^2}{gmL^2} \tag{13}$$

Thus,

$$H_{mn} = \frac{n^2\pi^2\hbar^2}{gmL^2} = \begin{cases} 1 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases} \tag{14}$$

where $E_1 = \frac{\pi^2\hbar^2}{gmL^2}$,

$$H_{mn} = n^2 E_1 = \begin{cases} 1 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases} \tag{15}$$

For m = n, Hamiltonian matrix H can be written as matrix m × n, results in

$$H = \begin{pmatrix} H_{11} & H_{12} & H_{13} & \ldots \\ H_{21} & H_{22} & H_{23} & \ldots \\ H_{31} & H_{32} & H_{33} & \ldots \end{pmatrix} (m \times n) \tag{16}$$

equal to

$$H = \begin{pmatrix} E_1 & 0 & 0 & \ldots \\ 0 & \psi E_1 & 0 & \ldots \\ 0 & 0 & gE_1 & \ldots \end{pmatrix} \tag{17}$$

where $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \ldots \end{pmatrix}$

Therefore, we can conclude that that Schrödinger's equation can be written in matrix form as $H\boldsymbol{\psi} = E\boldsymbol{\psi}$, where $\boldsymbol{\psi}$ is the vector $(\psi_1, \psi_2, \ldots)$. Thus $\boldsymbol{\psi}$ is an eigenvector of the Hamiltonian matrix H with eigenvalue E.

b) With the evaluated the integral in H_{mn} for the case $V(x) = ax/L$, I wrote a program which take the input of m and n values to evaluate the expression for H_{mn} for arbitrary m and n when the particle in the well is an electron. According to the problem, the well has width 5 Å, and $a = 10\,\mathrm{eV}$ which I use as the parameters for the taken integral defined in the program.

c) I modify the program for part b) above to create an 10 × 10 array of the elements of H up to m, n = 10. Then we can calculate the eigenvalues of this matrix using the function from numpy.linalg and hence print out, in units of electron volts, the first ten energy levels of the quantum well. The ground state energy of the system is at 5.83640353 eV which is as expected approximation, show that the matrix is real and symmetric.

d) Again, I modify the program to use an 100 × 100 array and calculate the first ten energy eigenvalues. The result is identical to part c) which is accurate as expected.

e) In the last part of the question, I modify the program once more to calculate the wavefunction $\psi(x)$ for the ground state and the first two excited states of the well. Then use the results to make a graph with three curves showing the probability density $|\psi(x)|^2$ as a function of x in each of these three states. The resulting plot is shown below (3), and according to the graph the normalization of the wavefunction satisfies the condition $\int_0^L |\psi(x)|^2\, dx = 1$.

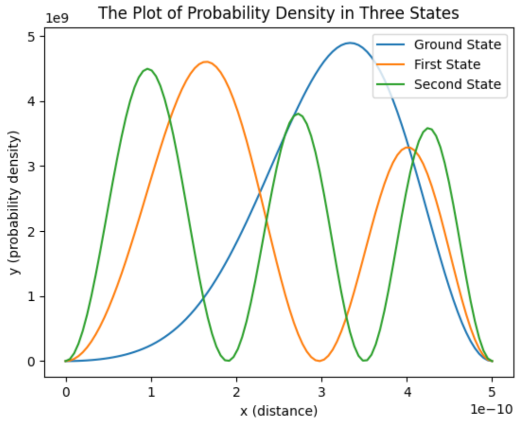

FIG. 3: The plot with three curves showing the probability density for the ground state and the first two excited states of the well

3. FEEDBACK

I spent about 20 hours on this homework including meeting with classmates and attending office hours outside of classes. I and all of my peers whom I talked to did not enjoy this problem set. We found Exercise 6.9: Asymmetric Quantum Well to be unnecessary time-consuming. We didn't think that showing Schrödinger's equation in matrix forms in 6.9 a) was a good use of our time as we have to report the derivation of the equations in Latex, consuming most of our time spent just writing mathematical equations in the write up. It was not helpful in terms of improving our computational skill. Additionally, 6.9 e) required complicated planning and discussing which caused additional time taken, yet was fun and challenging in a good way. I found the use of np.linalg to be very helpful. If part a) is not required, I think this problem would be more appropriate. All things considered, the problem set caught us at the end of the semester, making it more challenging than usual as we were finishing the semester, and by all means 6.9 is not a bad problem. I do appreciate the various options for another problem which I found 6.16 to be fun and interesting.

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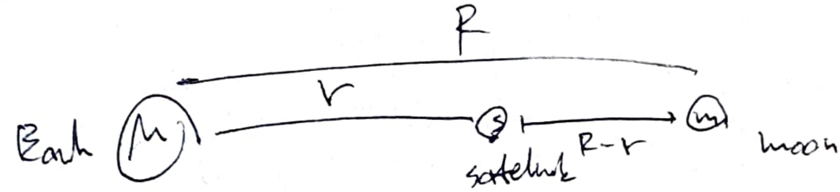
6.16

a) 

→ $F_{E\,on\,s} = \frac{GMs}{r^2}$ → $F_{m\,on\,s} = -\frac{Gms}{(R-r)^2}$

→ $F_{E\,on\,s} + F_{m\,on\,s} = s \times w^2 \times r$

→ $\frac{GM\cancel{s}}{\cancel{s}r^2} - \frac{Gm\cancel{s}}{\cancel{s}(R-r)^2} = w^2 r$

→ $\frac{GM}{r^2} - \frac{Gm}{(R-r)^2} = w^2 r$ ✓

b) → def secant

r_1 = ______

r_2 = ______

for x in

return r

→ print secant ()

b) For, $V(x) = ax/L$ → $L = 5\text{Å} = 5\times10^{-10}$ m

→ $a = 10$ eV

→ def Hmn (m, n)

condition in def

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

input m, n

c) $H = (10, 10)$ np. zeros

energy = np. linalg. eigvalsh

check

d) $H = (100, 100)$

e) → Define matrix first

for i in range

for j in range

$H[i, j] = Hmn(i+1, j+1)$

→ Define psi in eigenstate

look up np. linalg. eigh

→ Solve psi for wavefunction

def solve psi

→ E_0 solve psi 0

E_1 solve psi 1

E_2 solve psi 2

in function

6.9)

a) Show that $\hat{H}\psi = E\psi$ implies $\sum_{n=1}^{\infty} \psi_n \int_0^L \sin\frac{\pi m x}{L} \hat{H} \sin\frac{\pi n x}{L}\, dx = \frac{1}{2} L E \psi_m$ and $H\psi = E\psi$ can be written in matrix form, when ψ is a vector $(\psi_1, \psi_2, \dots)$

Ans → According to

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

and $\psi(x) = \sum_{n=1}^{\infty} \psi_{(n,m)} \sin \pi (n,m) x/L$

→ Then $\int_0^L \sin\frac{\pi m x}{L} \sin\frac{\pi n x}{L}\, dx = \int_0^L \psi_m \psi_n\, dx$

→ According to $\sum_{n=1}^{\infty} \psi_n \int_0^L \sin\frac{\pi m x}{L} \hat{H} \sin\frac{\pi n x}{L}\, dx = \frac{1}{2} L E \psi_m$

→ We can start from $\sum_{n=1} \psi_n \int_0^L \psi_m \hat{H} \psi_n\, dx$ to see if this is true

$$= \sum_{n=1}^{\infty} \psi_n \int_0^L \psi_m E \psi_n\, dx \text{, where } \hat{H}\psi = E\psi$$

$$= \sum_{n=1}^{\infty} \psi_n E \int_0^L \psi_m \psi_n\, dx$$

$$= \sum_{n=1}^{\infty} \psi_n E \frac{L}{2} \begin{cases} 1 & m = n \\ 0 & \text{else} \end{cases}$$

$$= \frac{1}{2} L E \psi_m \checkmark$$

→ Then we can find H_{mn}

$$\to H_{mn} = \frac{2}{L} \int_0^L \left[\sin\left(\frac{\pi m x}{L}\right)\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(m)\right)\right] \sin\left(\frac{\pi n x}{L}\right) dx$$

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

$$= \left(\frac{-2}{L}\right)\left(\frac{\hbar^2}{2m}\right) \int_0^L \sin\left(\frac{\pi m x}{L}\right) \left(\frac{-\hbar^2 n^2}{L^2}\right) \sin\left(\frac{\pi n x}{L}\right) dx$$

$$= \left(\frac{2}{L}\right)\left(\frac{L}{2}\right) \frac{n^2 \pi^2 \hbar^2}{2 m L^2}$$

$$H_{mn} = \frac{n^2\pi^2\hbar^2}{8mL^2} \cdot \begin{cases} 1 & m=n \\ 0 & \text{else} \end{cases}$$

$$= n^2 E_1 = \begin{cases} 1 & n=m \\ 0, & \text{else} \end{cases} \quad \text{, where } E_1 = \frac{\pi^2\hbar^2}{8mL^2}$$

→ Thus,

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \end{pmatrix} \quad (n \times n)$$

$$= \begin{pmatrix} E_1 & 0 & 0 & \cdots \\ 0 & 4E_1 & 0 & \cdots \\ 0 & 0 & 9E_1 & \cdots \end{pmatrix}$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix}$$

→ Therefore, $\hat{H}\psi = E\psi$