

PHYS304 HW8

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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).

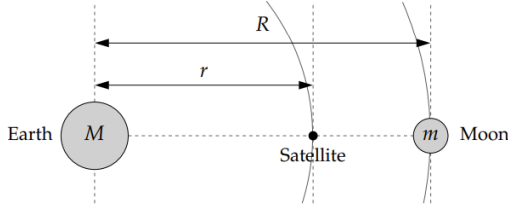


FIG. 1: The diagram showing the arrangement of the Earth, the Moon, and the satellite with the distances indicates L_1 .

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

$$\frac{GMs}{r^2} \quad (1)$$

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

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

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

$$s \times \omega^2 \times r \quad (3)$$

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.

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

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)

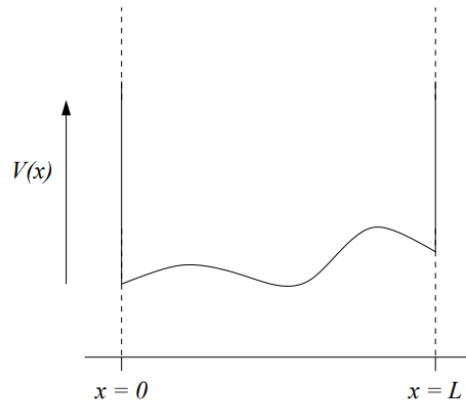


FIG. 2: The varied potential $V(x)$ in a one dimensional quantum well.

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 ψ_1, ψ_2, \dots 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 $H\psi = E\psi$, where ψ is the vector (ψ_1, ψ_2, \dots) . Thus ψ 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,

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

and

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

We can combine equation 5 into equation 6, resulting in

$$\int_0^L \sin \frac{\pi m x}{L} \sin \frac{\pi n x}{L} dx = \int_0^L \psi_m \psi_n dx \quad (7)$$

Then according to,

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

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,

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

then

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

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

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

equal to

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

solving the integral and simplifying, we have

$$H_{mn} = \frac{n^2 \pi^2 \hbar^2}{gmL^2} \quad (13)$$

Thus,

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

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

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

For $m = n$, Hamiltonian matrix H can be written as matrix $m \times n$, results in

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

equal to

$$H = \begin{pmatrix} E_1 & 0 & 0 & \dots \\ 0 & \psi E_1 & 0 & \dots \\ 0 & 0 & g E_1 & \dots \end{pmatrix} \quad (17)$$

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

Therefore, we can conclude that that Schrödinger's equation can be written in matrix form as $H\psi = E\psi$, where ψ is the vector (ψ_1, ψ_2, \dots) . Thus ψ 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 \AA , and $a = 10 \text{ eV}$ 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 $\int_0^L |\psi(x)|^2 dx = 1$.

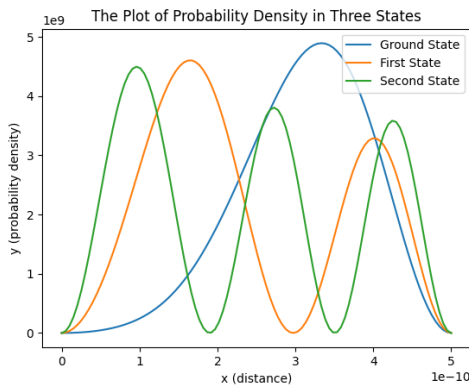


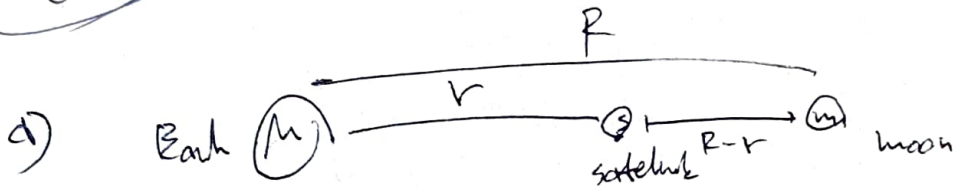
FIG. 3: The plot with three curves showing the probability density for the ground state and the first two excited states of the well

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



$$\rightarrow F_{\text{Earth}} = \frac{GM_s}{r^2} \quad \rightarrow F_{\text{Moon}} = -\frac{GM_s}{(R-r)^2}$$

$$\rightarrow F_{\text{Earth}} + F_{\text{Moon}} = s \times \omega^2 \times r$$

$$\rightarrow \frac{GM_s}{r^2} - \frac{GM_s}{(R-r)^2} = \omega^2 r$$

$$\rightarrow \frac{GM}{r^2} - \frac{Gm}{(R-r)^2} = \omega^2 r \quad \checkmark$$

b)

\rightarrow if secant

$r_1 = \underline{\hspace{2cm}}$

$r_2 = \underline{\hspace{2cm}}$

for α in $\underline{\hspace{2cm}}$ return r

\rightarrow print secant ()

b) $\psi(x, y) = \alpha x / L$ $\xrightarrow{\text{def}} H_{mn}(u, v)$ $\xrightarrow{L = 5 \text{ \AA} = 5 \times 10^{-10} \text{ m}}$ $d = 10 \text{ eV}$

condition in def

$$\int_a^b x \sin \frac{\pi u x}{L} \sin \frac{\pi v y}{L} dx = \begin{cases} -\left(\frac{2L}{\pi}\right)^2 \frac{uv}{(u^2 - v^2)^2} & u \neq v \\ L^2/4 & u = v \end{cases}$$

input u, v

c) $H = \begin{pmatrix} 10 & 10 \end{pmatrix}$ up. 2000

energy = up. lindg. eigvalsch check

d) $H = \begin{pmatrix} 100 & 100 \end{pmatrix}$

e) \rightarrow Defining matrix link

for i in u
for j in v
 $H[i, j] = H_{mn}(i+1, j+1)$

\rightarrow Defn ψ_i in eigustern

look up up. lindg. eigh

\rightarrow solve ψ_i der vordurch

def solve ψ_i

\rightarrow E_0 solve ψ_0
 B_1 solve ψ_1
 E_2 solve ψ_2

$\begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}$ in ψ_i

6.9) a) Show that $\hat{H}\psi = E\psi$ implies $\sum_{n=1}^{\infty} U_n \int_0^L \sin \frac{\pi n x}{L} \hat{H} \sin \frac{\pi n x}{L} dx = \frac{1}{2} L E \psi_m$
and $\hat{H}\psi = E\psi$ can be written in matrix form, where ψ is a vector (ψ_1, ψ_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 $\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin \frac{\pi n x}{L}$

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

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

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

$= \sum_{n=1}^{\infty} U_n E \int_0^L U_n U_n dx$

$= \sum_{n=1}^{\infty} U_n E \frac{1}{2} \int_0^L 1^{m=n} dx$

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

→ Then we can find H_{mn}

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

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

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

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

$$U_{nn} = \frac{n^2 \pi^2 \hbar^2}{8mL^2} = \begin{cases} n^2 E_1 & n=1 \\ 0 & \text{else} \end{cases}$$

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

→ Thus,

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

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

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

→ Therefore, $\hat{H}\psi = E\psi$ ~~✗~~

Overall score = 22.5 + 20.5 + 5 for feedback = 48/55

Computational Physics/Astrophysics, Winter 2023:

Grading Rubrics ¹

Lagrange point problem 22.5

Haverford College, Prof. Daniel Grin

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

1. Does the program complete without crashing in a reasonable time frame? If yes, up to +3 points.
+3
2. Does the program use the exact program files given (if given), and produce an answer in the specified format? If yes, +1 points
+1
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 +4 points
+4
5. Is the code readable? Up to +2 points
+2
 - 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

+1.5 — mentions secant method
but doesn't explain how or why form of equations in code

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? +8 — generally very good, but an outside source is mentioned
7. LaTeX writeup (up to 10 points) without a proper citation
 - . 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).

Computational Physics/Astrophysics, Winter 2023:

Grading Rubrics ¹

QM Problem 20.5/25

Haverford College, Prof. Daniel Grin

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

1. Does the program complete without crashing in a reasonable time frame? If yes, up to +3 points. 3
2. Does the program use the exact program files given (if given), and produce an answer in the specified format? If yes, +1 points +1
3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) Up to +2 points +2
+2 — your kinetic function has some units problems, and this leads to incorrect answers down the line
4. Is the answer correct? Up to +4 points
5. Is the code readable? Up to +2 points +1.5 — good, sum over eigenfunctions not clearly documented internally
 - . 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

6. Is the code well documented? +3points +3
 - . 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?
+8/10, but no explanation of high separation preferred in ground state
7. LaTeX writeup (up to 10 points) I think this is an error 10 points
 - . 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)

Feedback to feedback - I realize this was a hard set late in term, but it is important to make the connection between linear algebraic and functional representations of QM - builds on our understanding and important for future classes.

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