210 Quantum Mechanics Assignment (25 marks)

Made available 16th Aug 2025, **due in 5pm on Tue 23rd Sept** 2025.

Hand in to chemistry reception.

In the following ***show all your working***, this means each step of the mathematics and a complete answer, remember the purpose is to show me that you understand and know what you are doing!

Your assignment should be **hand-written**, *tidy and legible.* (**5 marks**)

1. **Expand** the commutator [p_x, p_y] using the function $f(x,y) = x^2 + xy + y^2$ Do these operators commute?

(**5 marks**)

2. For an infinite square well potential of length L
   (a) **draw** and label the potential, add the first 4 energy levels, **write** the equation for E next to each energy line (do not evaluate constants)
   (b) **sketch** the wavefunction on each energy level line, **identify** the value of the maximum
   (c) on a second potential **sketch** the probability (density) P for the first 4 energy levels on each energy line, **identify** the value of the maximum

(**5 marks**)

3. **Determine** the expectation value of the position <x> for the n=2 energy level of a particle confined in a an infinite square well potential of length L. **Use the following integral**:

$$\int xsin^2(ax)dx = \frac{2a^2x^2 - 2axsin(2ax) - cos(2ax)}{8a^2}$$

(**5 marks**)

4. The wavefunction for a particle in an infinite square well is given below.

$$\psi(x) = Nsin\left(\frac{nx\pi}{L}\right) \text{ with } n = 1, 2...$$

   (a) **write** an expression for the probability (density) P of the n=2 wavefunction
   (b) **differentiate** P, set the derivate to zero and **identify** the positions (in terms of L) of the maxima and minima
   (c) what is the probability of finding the particle at the expectation value <x>? Explain your result.

(**5 marks**)

1. **Expand** the commutator [p_x, p_y] using the function $f(x,y) = x^2 + xy + y^2$ Do these operators commute?

(5 marks)

The commutator [A,B]=AB-BA where A and B are operators, if [A,B]=0 then A and B commute

$$A = p_x \text{ and } B = p_y$$
$$[p_x, p_y] = p_x p_y - p_y p_x$$
$$\text{where } p_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \text{and } p_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$$
$$\left[\frac{\hbar}{i}\frac{\partial}{\partial x}, \frac{\hbar}{i}\frac{\partial}{\partial y}\right] = (\frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial y}) - (\frac{\hbar}{i}\frac{\partial}{\partial y}\frac{\hbar}{i}\frac{\partial}{\partial x})$$
$$\text{evaluate for a function } f = x^2 + xy + y^2$$
$$\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial y} - \frac{\hbar}{i}\frac{\partial}{\partial y}\frac{\hbar}{i}\frac{\partial}{\partial x}\right](x^2 + xy + y^2)$$
$$(\frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial y})(x^2 + xy + y^2) = (\frac{\hbar^2}{i^2})\frac{\partial}{\partial x}(\frac{\partial}{\partial y}x^2 + xy + y^2)$$
$$= (\frac{\hbar^2}{i^2})\frac{\partial}{\partial x}(0 + x + 2y)$$
$$= (\frac{\hbar^2}{i^2})(1 + 0)$$
$$= (\frac{\hbar^2}{i^2})$$
$$(\frac{\hbar}{i}\frac{\partial}{\partial y}\frac{\hbar}{i}\frac{\partial}{\partial x})(x^2 + xy + y^2) = (\frac{\hbar^2}{i^2})\frac{\partial}{\partial y}(\frac{\partial}{\partial x}x^2 + xy + y^2)$$
$$= (\frac{\hbar^2}{i^2})\frac{\partial}{\partial y}(2x + y + 0)$$
$$= (\frac{\hbar^2}{i^2})(0 + 1)$$
$$= (\frac{\hbar^2}{i^2})$$
$$\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial y} - \frac{\hbar}{i}\frac{\partial}{\partial y}\frac{\hbar}{i}\frac{\partial}{\partial x}\right](x^2 + xy + y^2)$$
$$= \frac{\hbar^2}{i^2} - \frac{\hbar^2}{i^2} = 0$$
$$\text{therefore } [p_x, p_y] = 0$$

p_x and p_y do commute because the commutator is zero

statement of general commutator equation (**1 mark**)
statement of specific details to evaluate (**1 mark**)
evaluation of expression (**2 marks**)
state the result (**1 mark**)

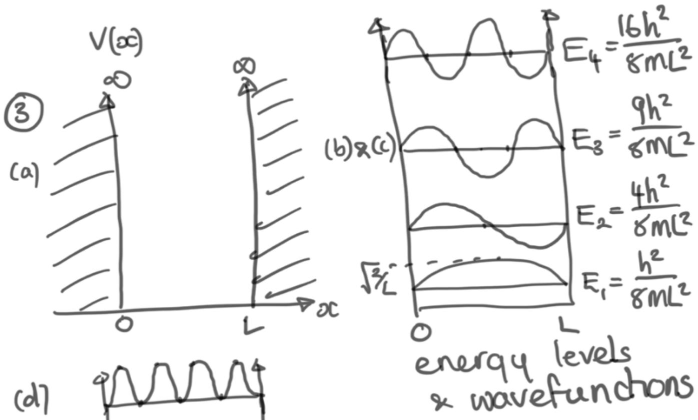
2. For an infinite square well potential of length L

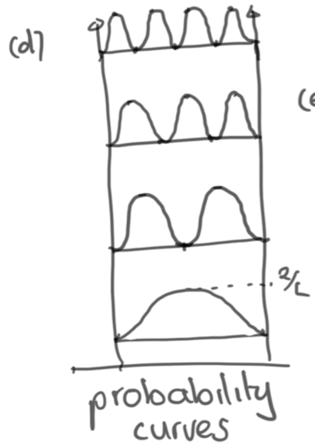
(a) **draw** and label the potential, add the first 4 energy levels, **write** the equation for E next to each energy line (do not evaluate constants)

(b) **sketch** the wavefunction on each energy level line, **identify** the value of the maximum

(c) on a second potential **sketch** the probability (density) P for the first 4 energy levels on each energy line, **identify** the value of the maximum

(**5 marks**)





(e)

$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$

will be maxima for

$\sin(\theta) = 1$

amplitude $= \sqrt{\frac{2}{L}}$

$P = \psi^* \psi = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right)$

will be maxima

for $\sin^2(\theta) = 1$

amplitude $= \frac{2}{L}$

potential and energies(**1 mark**)

wavefunctions and magnitude (**2 marks**)

probability and magnitude (**2 marks**)

3. **Determine** the expectation value of the position <x> for the n=2 energy level of a particle confined in a an infinite square well potential of length L. **Use the following integral**:

$$\int x sin^2(ax)dx = \frac{2a^2x^2 - 2axsin(2ax) - cos(2ax)}{8a^2}$$

(5 marks)

Determine the expectation value of the position for an n=2 level of a particle confined in a box of length L

expectation value of position is $\langle x \rangle$

$$\langle x \rangle = \int_{\text{limits}} \psi^* x \psi \, dx$$

limits here are $0 \to L$

we are told to use the wavefunction for the n=2 level (look this up!)

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

ψ is real $\therefore \psi^* = \psi$

$$\langle x \rangle = \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) x \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) dx$$

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

we are given

$$\int x \sin^2(ax)dx = \frac{2a^2x^2 - 2ax\sin(2ax) - \cos(2ax)}{8a^2}$$

in our case $a = \frac{2\pi}{L}$

$$\langle x \rangle = \frac{2}{L}\left[\frac{2\left(\frac{2\pi}{L}\right)^2 x^2 - 2\left(\frac{2\pi}{L}\right)x \sin\left(2\left(\frac{2\pi}{L}\right)x\right) - \cos\left(2\left(\frac{2\pi}{L}\right)x\right)}{8\left(\frac{2\pi}{L}\right)^2}\right]_0^L$$

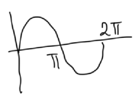
first pull out bottom line as this is independent of x, and simplify

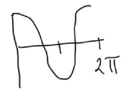
$$\langle x \rangle = \frac{\cancel{2}}{\cancel{L}} \frac{L^{\cancel{2}}}{8 \cdot 2^{\cancel{2}} \pi^2}\left[\frac{8\pi^2}{L^2}x^2 - \frac{4\pi}{L}x \sin\left(\frac{4\pi x}{L}\right) - \cos\left(\frac{4\pi x}{L}\right)\right]_0^L$$

$$= \frac{L}{16\pi^2}\left[\frac{8\pi^2}{\cancel{L^2}}\cancel{L^2} - \frac{4\pi}{\cancel{L}}\cancel{L} \sin\left(\frac{4\pi \cancel{L}}{\cancel{L}}\right) - \cos\left(\frac{4\pi \cancel{L}}{\cancel{L}}\right)\right.$$

$$\left. - \left(\underbrace{\frac{8\pi^2}{L^2}0}_{=0} - \underbrace{\frac{4\pi}{L}0 \sin\left(\frac{4\pi 0}{L}\right)}_{=0} - \cos\left(\frac{4\pi 0}{L}\right)\right)\right]$$

$$= \frac{L}{16\pi^2}\left[8\pi^2 - 4\pi \underbrace{\sin(4\pi)}_{\sin(n\pi)=0} - \underbrace{\cos(4\pi)}_{\cos(2n\pi)=+1} - 0 + 0 + \cos(0)\right]$$





$$= \frac{L}{16\pi^2}\left[8\pi^2 - 0 - \cancel{1 + 1}^{=0}\right]$$

$$= \frac{L\,\cancel{8\pi^2}}{2\,\cancel{16\pi^2}} = \frac{L}{2}$$

4. The wavefunction for a particle in an infinite square well is given below.

$$\psi(x) = N sin\left(\frac{nx\pi}{L}\right) \text{ with } n = 1, 2...$$

(a) **write** an expression for the probability (density) P of the n=2 wavefunction
(b) **differentiate** P, set the derivate to zero and **identify** the positions (in terms of L) of the maxima and minima
(c) what is the probability of finding the particle at the expectation value <x>? Explain your result.

(5 marks)

$\psi = N\sin\left(\frac{n\pi x}{L}\right)$ $n = 1, 2, 3 \ldots$

$n = 2.$

$P = \psi^* \psi$ ψ is real so $\psi^* = \psi$

$= N^2 \sin^2\left(\frac{2\pi x}{L}\right)$

max and min occur for $dP/dx = 0$

$\frac{d}{dx} N^2 \sin^2\left(\frac{2\pi x}{L}\right)$

$\frac{\partial}{\partial x} \sin^2(ax) = a\sin(2ax)$

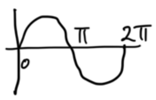
where $a = \frac{2\pi}{L}$

$= N^2 \frac{2\pi}{L} \sin\left(\frac{4\pi x}{L}\right)$

$= 0$ at max, min

$\therefore$ we evaluate when

$\sin\left(\frac{4\pi x}{L}\right) = 0$



occurs when

$\frac{4\pi x}{L} = 0, \pi, 2\pi \ldots$ ie $k\pi$
$k = 0, 1, 2$

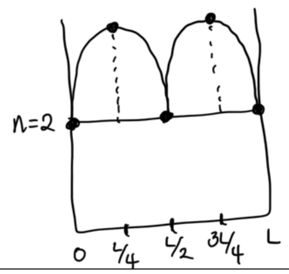
$\frac{4\cancel{\pi} x}{L} = k\cancel{\pi}$

$x = \frac{kL}{4}$

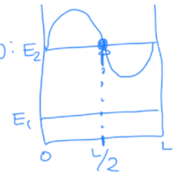
but x cannot be larger than L

so $k \leq 4$

	k=0	1	2	3	4
max, min at $x=$	0	¼	½	$\frac{3L}{4}$	L
	min	max	min	max	min



while the expectation value or "average" is to find the particle at L/2, the probability of finding the particle at L/2 is zero!



Think about this we know:

* the average position for the electron in the box is L/2, which makes sense, the e spends ½ its time on each side (the box is symmetric)
* for n=2 the measured position for the electron is NEVER L/2 as there is a node at L/2 in the wavefunction.

comments:

* it is important that the problem is set up clearly, don't start halfway in.
* each step needs to be clearly shown
* watch your clarity of symbols, these are meaning filled!