Name : ______________________________

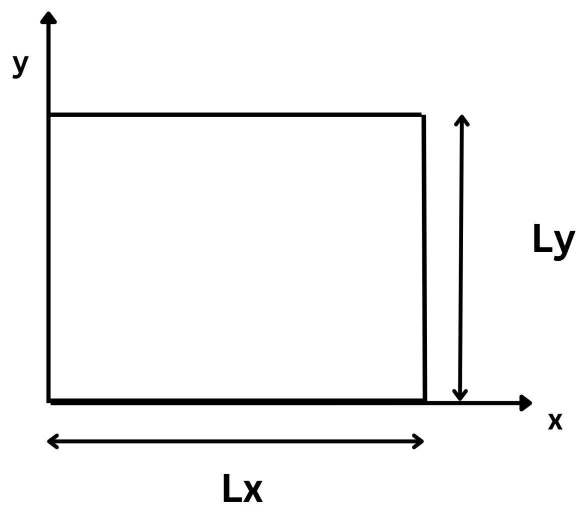
Roll Number: ______________________________

Question 1

A hydrogen atom is in the state
$$\frac{1}{\sqrt{2}}(\psi_{100} - \psi_{200}).$$
Write the integral that, when computed, will give the probability of finding the electron between the radii $r = 0$ and $r = a_0$ (the Bohr radius). You do not have to compute this integral.

Question 2

Consider a particle in a 2-d potential well. The potential V(x,y) is infinite at the boundary and everywhere outside the well and zero inside the well. The length of the 2-d well is L_x and L_y as shown in the diagram.



The two dimensional Schrodinger equation for the particle is the following:
$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y).$$

(a) Find a general expression for the possible energies of the given system. Also find the general expression for the corresponding wavefunctions.

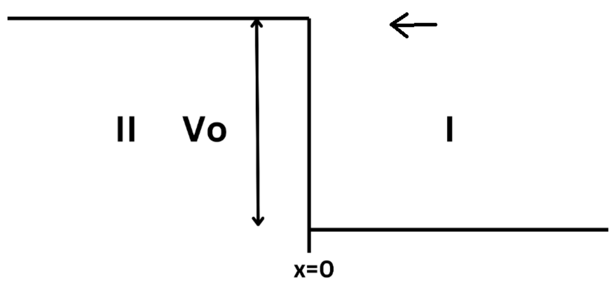
It is possible that $L_x = L_y$ or $L_x \neq L_y$. Do parts b,c twice: once with the assumption that $L_x = L_y$ and once with the assumption that $L_x < L_y$.

(b) Are energy levels degenerate for the first excited state ? Justify your answer.

(c) Write down the wavefunctions for the first excited state for each case you mentioned above.

Question 3

Consider the potential step shown below.



(a) If a particle comes in from the right (as shown with the arrow) with $E > V_O > 0$, find its wavefunction in region I and II.

(b) Use boundary conditions to write down all the possible coefficients of the wavefunctions we found in part (a).

(c) What is the probability density of position in region I?

①

$$\psi_{100} \rightarrow \begin{array}{l} n=1 \\ \ell=0 \\ m_\ell=0 \end{array} \qquad \psi_{100} = Y_0^0 R_{10}$$

$$= 2\sqrt{\frac{1}{a_0^3}}\, e^{-r/a_0} \cdot \frac{1}{\sqrt{4\pi}}$$

$$\psi_{200} = Y_0^0 R_{20} = \frac{1}{\sqrt{4\pi}} \cdot \frac{1}{2}\sqrt{\frac{1}{2a_0^3}} \left[\frac{-r}{a_0} + 2\right] e^{-r/2a_0}$$

$$= \frac{1}{\sqrt{4\pi}} \frac{1}{2} \sqrt{\frac{1}{2a_0^3}} \left(\frac{-r}{a_0} e^{-r/2a_0} + 2e^{-r/2a_0}\right)$$

Let's define
$$A = 2\sqrt{\frac{1}{a_0^3}} \cdot \frac{1}{4\pi}$$

$$B = \frac{+1}{2a_0\sqrt{8a_0^3\pi}}$$

$$C = \frac{1}{\sqrt{8\pi a_0^3}}$$

$$\frac{1}{\sqrt{2}}\left(\psi_{100} - \psi_{200}\right) = \frac{1}{\sqrt{2}}\left(A e^{-r/a_0} + B r e^{-r/2a_0} - C e^{-r/2a_0}\right)$$

$$\left|\frac{1}{\sqrt{2}}\left(\psi_{100} - \psi_{200}\right)\right|^2 = \frac{1}{2}\left(A^2 e^{-2r/a_0} + A r B^* e^{-3r/2a_0} - A C^* e^{-3r/2a_0}\right.$$

$$+ r B A^* e^{-3/2a_0} + B^2 r^2 e^{-r/a_0} - r B C e^{-r/a_0}$$

$$\left. + C^2 e^{-r/a_0} - C B e^{-r/a_0} - C A^* e^{-3r/2a_0}\right|$$

②

$$= \frac{1}{2}\left(A^2 e^{-2r/a_0} + B^2 r^2 e^{-r/a_0} + C^2 e^{-r/a_0} \ldots \right)$$

$$= \frac{1}{2}\Big\{ e^{-3r/2a_0}\left(ABr + AC + BA - CA\right)$$

$$+ e^{-2r/a_0}\left(A^2\right) + e^{-r/a_0}\left(B^2 r^2 - rBC + C^2 - CB\right)\Big\}$$

each term can be integrated individually.

We need to compute integrals of the form $\Rightarrow$

① $\lambda e^{-\alpha r} r \,(r^2) = \lambda e^{-\alpha r} r^3$

② $\lambda e^{-\alpha r} (r^2) = \lambda e^{-\alpha r} r^2$

③ $\lambda e^{-\alpha r} r^2 (r^2) = \lambda e^{-\alpha r} r^4$

$\longleftrightarrow$

Let's compute

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\Psi(x,y)+V(x,y)\Psi(x,y)=E\Psi(x,y)$$

$\Psi(x,y) = XY$ (separation of variables

$$-\frac{\hbar^2}{2m}\left[Y\frac{\partial X}{\partial x^2}+X\frac{\partial Y}{\partial y^2}\right]+VXY=EXY$$

divide both sides of equation by XY

$$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial X}{\partial x^2}+\frac{1}{Y}\frac{\partial Y}{\partial y^2}=(E-V).$$

$$\rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial X}{\partial x^2}=E_x \quad \text{and} \quad \frac{1}{Y}\frac{\partial}{\partial y^2}Y=E_y.$$

For a 2-D potential $V_x=0$ and $V_y=0$ inside the box.

Solving $-\frac{\hbar^2}{2m}\frac{d^2X}{dX^2}=XE_x \rightarrow \cancel{X6}\frac{d^2X}{dx^2}=\frac{-2m}{\hbar^2}E_xX$

~~Ansatz X(x)~~ = $\quad$ $\cancel{X(x)=}\ K_x^2=\frac{2m}{\hbar^2}E_x$

$$X(x)=A\sin(k_x x)+B\cos(k_x x)$$

Similarly, we can solve for y, $k_y^2=\frac{2m}{\hbar^2}E_y$

$$Y(y)=C\sin(k_y x)+D\cos(k_y x).$$

Boundary Conditions

$X(0) = A\sin(0) + B\cos(0) = 0$

$= B = 0$

$X(L_x) = A\sin(L_x k_x) = 0$

For a non-trivial solution

$k_x L_x = n\pi$ where $n = 1, 2, 3 \ldots$

$\frac{\sqrt{2mE_x}}{\hbar} L_x = n\pi$ $\Rightarrow$ $X(x) = A\sin\left(\frac{n\pi}{L_x}x\right)$

$\frac{2mE_x L_x^2}{\hbar^2} = n^2\pi^2$

To find $A \Rightarrow$

$\int_0^{L_x} |A|^2 \sin^2\left(\frac{n\pi x}{L_x}\right) = 1$

$|A|^2 \frac{L_x}{2} = 1$ $A = \sqrt{\frac{2}{L_x}}$

$$E_x = \frac{n_x^2\pi^2\hbar^2}{L_x^2 2m}$$

Similarly we can write

$$Y(y) = \sqrt{\frac{2}{L_y}} \sin\left(\frac{n\pi y}{L_y}\right)$$

$$E_y = \frac{n_y^2\pi^2\hbar^2}{L_y^2 2m}$$

b(i) $L_x = L_y = L$

$$E = \frac{n_x^2\pi^2\hbar^2}{L^2 2m} + \frac{n_y^2\pi^2\hbar^2}{L^2 2m} = \frac{\pi^2\hbar^2}{L^2 2m}\left(n_x^2 + n_y^2\right)$$

For the 1st excited state $n_x = 1$ and $n_y = 2$ OR
$n_x = 2$ and $n_y = 1$ $\Leftarrow$ Degeneracy = 2

b(ii) $L_x < L_y$.

$$E = \frac{n_x^2 \pi^2 \hbar^2}{L_x^2 2m} + \frac{n_y^2 \pi^2 \hbar^2}{L_y^2 2m}$$

1st Excited state $\rightarrow$ $n_x = 1$ $n_y = 2$

degeneracy = 0

(c)(i) $\Psi = X(x)\, Y(y) \rightarrow L_x = L_y$

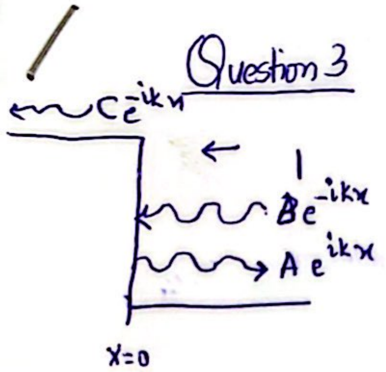
$$\Rightarrow \sqrt{\frac{2}{L_x}} \sqrt{\frac{2}{L_y}} = \frac{2}{L}$$

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

d(ii) $= \frac{2}{\sqrt{2 x L_y}} \sin\left(\frac{n\pi y}{L_y}\right) \sin\left(\frac{n\pi x}{L_x}\right)$

Question 3

(a)



Wave function in region I

$\psi(x) = Ae^{ikx} + Be^{-ikx}$ where $k \equiv \frac{\sqrt{2mE}}{\hbar}$

Wave function in region II

$\chi(x) = Ce^{-ik_1x}$ where $k_1 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

(b) Wavefunction is continous and its derivative is also constant

~~$\psi(0)$ Ae^{ikx}~~ $\psi(0) = \lambda(0)$

$A + B = C$ $\qquad B = C - A$ — (1)

$\psi'(0) = \lambda'(0)$

$ikA - Bik = -ik_1C$ — (2)

Plug (1) in (2)

$ikA - Cik + Aik = -ik_1C$

$2ikA = Cik - ik_1C$

$$\boxed{A = C\frac{(ik - ik_1)}{2ik}}$$

$$\boxed{A = \frac{B\lambda}{1-\lambda}}$$

~~$B = C - C\frac{(ik - ik_1)}{2ik}$~~ $A = C\lambda$

$B = C - C\lambda$

$C = \frac{B}{1-\lambda}$

- we have expressed C and A, both in terms of incoming particles