

Graduate QM

HW # 1 - solution

Dr. Gassem Alzoubi

① show that $[H, L_z] = 0$; where $H = \frac{p^2}{2m} + V(r)$ central

$$\vec{L} = L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

$$\text{and } L_z = x p_y - y p_x$$

$$[H, L_z] = \left[\frac{p^2}{2m} + V(r), x p_y - y p_x \right] = \left[\frac{p^2}{2m}, x p_y - y p_x \right] + [V(r), x p_y - y p_x]$$

$$= \frac{1}{2m} [p^2, x p_y] - \frac{1}{2m} [p^2, y p_x] + \underbrace{[V(r), x p_y] - [V(r), y p_x]}_0$$

$$= \frac{1}{2m} \left([p_x^2, x p_y] + [p_y^2, x p_y] + [p_z^2, x p_y] \right) \left. \begin{array}{l} \text{as } [V(r), x_j] = 0 ; j=1,2,3 \\ \text{and } [V(r), p_j] = 0 ; j=1,2,3 \end{array} \right\}$$

$$- \frac{1}{2m} \left([p_x^2, y p_x] + [p_y^2, y p_x] + [p_z^2, y p_x] \right)$$

$$= \frac{1}{2m} \left(x [p_x^2, p_y] + [p_x^2, x] p_y + x [p_y^2, p_y] + [p_y^2, x] p_y + x [p_z^2, p_y] + [p_z^2, x] p_y \right)$$

$$- \frac{1}{2m} \left(y [p_x^2, p_x] + [p_x^2, y] p_x + y [p_y^2, p_x] + [p_y^2, y] p_x + y [p_z^2, p_x] + [p_z^2, y] p_x \right)$$

$$= \frac{1}{2m} \left[\begin{array}{l} p_x [p_x, x] p_y + [p_x, x] p_x p_y \\ - p_y [p_y, y] p_x - [p_y, y] p_y p_x \end{array} \right]$$

$$= \frac{1}{2m} \left(-i \hbar p_x p_y - i \hbar p_x p_y + i \hbar p_y p_x + i \hbar p_y p_x \right) ;$$

$$= 0 \quad , \quad \text{as } p_x p_y = p_y p_x$$

similarly $[H, L_y] = [H, L_x] = 0$

now $\vec{L} = L_x^2 + L_y^2 + L_z^2$

$$[H, L^2] = [H, L_x^2 + L_y^2 + L_z^2]$$

$$= [H, L_x^2] + [H, L_y^2] + [H, L_z^2]$$

$$= L_x [H, L_x] + [H, L_x] L_x$$

$$+ L_y [H, L_y] + [H, L_y] L_y$$

$$+ L_z [H, L_z] + [H, L_z] L_z$$

$$= 0$$

Q. E. D

(2) $\psi(r, \theta, \phi) = -B(x+iy) e^{-r/2a_0}$; a_0 is Bohr radius

(a) in spherical $= -B(r \sin \theta \cos \phi + i r \sin \theta \sin \phi) e^{-r/2a_0}$
 $= -Br (\sin \theta \cos \phi + i \sin \theta \sin \phi) e^{-r/2a_0}$

now using $Y_{11} = -\left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{i\phi} = -\left(\frac{3}{8\pi}\right)^{1/2} \sin \theta (\cos \phi + i \sin \phi)$
 $= -\left(\frac{3}{8\pi}\right)^{1/2} (\sin \theta \cos \phi + i \sin \theta \sin \phi)$

$\Rightarrow \sin \theta \cos \phi + i \sin \theta \sin \phi = -Y_{11} \left(\frac{8\pi}{3}\right)^{1/2}$

$\Rightarrow \psi = Br \left(\frac{8\pi}{3}\right)^{1/2} Y_{11} e^{-r/2a_0}$

now using $R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{1}{2a_0}\right)^{3/2} \frac{1}{a_0} r e^{-r/2a_0}$

$\Rightarrow r e^{-r/2a_0} = R_{21} \sqrt{3} a_0 (2a_0)^{3/2}$

$\Rightarrow \psi(r, \theta, \phi) = B \frac{\sqrt{8\pi}}{\sqrt{3}} Y_{11} R_{21} \sqrt{3} a_0 (2a_0)^{3/2}$

$= B \sqrt{8\pi} a_0^{5/2} (2)^{3/2} Y_{11} R_{21} = 8B\sqrt{\pi} a_0^{5/2} Y_{11} R_{21}$

$\Rightarrow n=2, l=1, m=1$

(b) $\int |\psi|^2 d^3r = 1 \Rightarrow 64B^2 \pi a_0^5 \int_0^\infty r^2 |R_{21}|^2 dr \int d\Omega |Y_{11}|^2 = 1$

$\Rightarrow B^2 = \frac{1}{64\pi a_0^5}$

$B = \frac{1}{8\sqrt{\pi} a_0^{5/2}} \Rightarrow \psi = 8 \frac{1\sqrt{\pi}}{8\sqrt{\pi} a_0^{5/2}} a_0^{5/2} Y_{11} R_{21} = R_{21}(r) Y_{11}(\theta, \phi)$

$$\textcircled{c} \therefore \psi(r, \theta, \phi) = R_{21}(r) Y_{11}(\theta, \phi)$$

$$\Rightarrow \langle r \rangle = \int_0^{\infty} r^3 |R_{21}|^2 dr \quad \text{where } R_{21}(r) = \frac{1}{\sqrt{24}} a_0^{-3/2} \frac{r}{a_0} e^{-r/2a_0}$$

$$= \frac{1}{24} \frac{1}{a_0^5} \int_0^{\infty} r^5 e^{-r/a_0} dr = \frac{1}{24} \frac{1}{a_0^5} \frac{5!}{(1/a_0)^6}$$

$$= \frac{5!}{24} \frac{a_0^6}{a_0^5} = 5a_0$$

$$\textcircled{d} P_{21}(r) = r^2 |R_{21}(r)|^2 = r^2 \frac{1}{24} \frac{1}{a_0^5} r^2 e^{-r/a_0}$$

$$\frac{dP_{21}}{dr} = 0 = \frac{1}{24} a_0^5 \left[r^4 \left(-\frac{1}{a_0} \right) e^{-r/a_0} + 4r^3 e^{-r/a_0} \right]$$

$$\Rightarrow 4r^3 e^{-r/a_0} = \frac{r^4}{a_0} e^{-r/a_0}$$

$$\Rightarrow 4 = \frac{r}{a_0}$$

$$\Rightarrow r = 4a_0$$

$$(3) \Psi(r, \theta, \phi) = 2\psi_{100} + \psi_{210} \quad ; \quad \Psi^*(r, \theta, \phi) = 2\psi_{100}^* + \psi_{210}^*$$

a) normalize $\Psi(r, \theta, \phi) = A [2\psi_{100} + \psi_{210}]$

$$\int_{-\infty}^{\infty} |\Psi(r, \theta, \phi)|^2 d^3r = 1 = \int d^3r (2\psi_{100}^* + \psi_{210}^*) (2\psi_{100} + \psi_{210})$$

$$\Rightarrow \underbrace{4A^2 \int_{-\infty}^{\infty} |\psi_{100}|^2 d^3r}_1 + \underbrace{A^2 \int_{-\infty}^{\infty} |\psi_{210}|^2 d^3r}_1 = 1 \quad \Rightarrow 5A^2 = 1$$

$$\Rightarrow A = \frac{1}{\sqrt{5}}$$

b) $P(n=3) = 0$, electron exists only in either $n=1$ or $n=2$

c) $n=1 \Rightarrow E_1 = \frac{-13.6}{1^2} = -13.6 \text{ eV}$; $E_2(n=2) = \frac{-13.6}{4} = -3.4 \text{ eV}$

\Downarrow $l=0$; \Downarrow $l=0, 1$

$$\Rightarrow L = \sqrt{l(l+1)} \hbar = \begin{cases} 0, & l=0 \\ \sqrt{2} \hbar, & l=1 \end{cases}$$

Possible values of L_z is $m_l \hbar$; where $m_l = 0$ only as show in the wave function $2\psi_{100} + \psi_{210} \rightarrow m=0$

$\therefore L_z = 0 \hbar$

d) $P(E_1) = P(l=0) = \left| \langle \psi_{100} | \frac{2}{5} \psi_{100} + \frac{1}{\sqrt{5}} \psi_{210} \rangle \right|^2 = \left| \frac{2}{\sqrt{5}} \right|^2 = \frac{4}{5}$

$$P(E_2) = P(l=\sqrt{2} \hbar) = \left| \langle \psi_{210} | \frac{2}{\sqrt{5}} \psi_{100} + \frac{1}{\sqrt{5}} \psi_{210} \rangle \right|^2 = \left| \frac{1}{\sqrt{5}} \right|^2 = \frac{1}{5}$$

now $P(L_z=0) = 1$ as $L_z = 0$ is the only possible m value

4) $V(r) = -g \delta(r-a)$; $g > 0$

the radial eqⁿ reads

$$-\frac{\hbar^2}{2m r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2m r^2} \right] R(r) = E R(r)$$

let $R(r) = \frac{\psi(r)}{r}$

$$\Rightarrow -\frac{\hbar^2}{2m r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \left(\frac{\psi}{r} \right) \right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2m r^2} \right] \frac{\psi}{r} = E \frac{\psi}{r}$$

$$= \frac{d}{dr} \left(r^2 \left(\frac{1}{r} \frac{d\psi}{dr} - \frac{1}{r^2} \psi \right) \right) = \frac{d}{dr} \left(r \frac{d\psi}{dr} - \psi \right)$$

$$= r \frac{d^2\psi}{dr^2} + \cancel{\frac{d\psi}{dr}} - \cancel{\frac{d\psi}{dr}} = r \frac{d^2\psi}{dr^2}$$

$$-\frac{\hbar^2}{2m r^2} r \frac{d^2\psi}{dr^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2m r^2} \right] \frac{\psi}{r} = E \frac{\psi}{r}$$

multiply by $r \Rightarrow -\frac{\hbar^2}{2m} \psi'' + \left[V(r) + \frac{\hbar^2 l(l+1)}{2m r^2} \right] \psi = E \psi$

now for ground state $l=0$ and $E < 0$, where $V(r) = 0$ for $r \neq a$

so for $r \neq a \Rightarrow$ the equation reads

$$-\frac{\hbar^2}{2m} \psi'' - E \psi = 0 \Rightarrow \psi'' + \frac{2mE}{\hbar^2} \psi = 0 ; \text{ where } E = -\frac{\hbar^2 k^2}{2m}$$

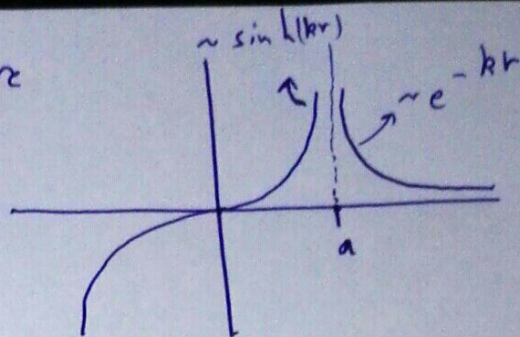
$\Rightarrow \psi'' - k^2 \psi = 0$, with the boundary conditions that $\psi(r) \rightarrow 0$ as $r \rightarrow 0$ and as $r \rightarrow \infty$

the wavefunctions that satisfy these B.C.s are

$$\psi(r) = \begin{cases} A \sinh(kr) ; & 0 < r \leq a \\ B e^{-kr} ; & r > a \end{cases}$$

Now at $r=a$, the wave functions are continuous

$$A \sinh(ka) = B e^{-ka} \quad \text{--- (1)}$$



and the discontinuity of the first derivative at $r=a$ gives

$$\psi'_+(a+\epsilon) - \psi'_+(a-\epsilon) = -\frac{2mg}{\hbar^2} \psi_+(a)$$

$$-k B e^{-ka} - k A \cosh(ka) = -\frac{2mg}{\hbar^2} B e^{-ka}$$

$$\Rightarrow B \left(\frac{2mg}{\hbar^2} - 1 \right) e^{-ka} = A \cosh(ka) \quad \text{--- (2)}$$

divide 2 by 1 yields

$$\coth(ka) = \frac{2mg}{\hbar^2} - 1$$

multiply by $ka \Rightarrow ka \coth(ka) = \frac{2mag}{\hbar^2} - ka$

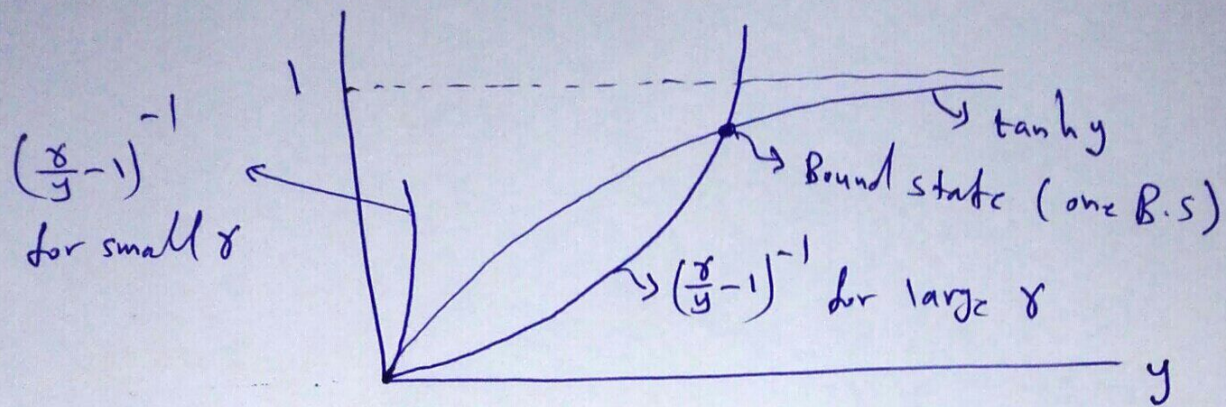
let $y=ka \Rightarrow y \coth y = \frac{2mag}{\hbar^2} - y$;

$y \coth y = \delta - y$; where $\delta = \frac{2mg}{\hbar^2}$

$$\coth y = \frac{\delta}{y} - 1$$

$$\tanh y = \left(\frac{\delta}{y} - 1 \right)^{-1}$$

let us solve this eqⁿ Graphically



the intersection occurs only if the slope of $(\frac{x}{y}-1)^{-1}$ at $y=0$ is smaller than the slope of $\tanh y$

$$\text{i.e. } \left. \frac{d}{dy} \left(\frac{x}{y}-1 \right)^{-1} \right|_{y=0} < \left. \frac{d}{dy} \tanh y \right|_{y=0}$$

$$\left. \frac{(\delta-y)(-1) - y(-1)}{(\delta-y)^2} \right|_{y=0} < \left. 1 - \tanh^2 y \right|_{y=0}$$

$$\left. \frac{\delta}{(\delta-y)^2} \right|_{y=0} < \left. 1 - \tanh^2 y \right|_{y=0}$$

$$\frac{1}{\delta} < 1 \quad \text{or} \quad \delta > 1$$

$$\frac{2mag}{\hbar^2} > 1$$

$$g > \frac{\hbar^2}{2ma}$$

this is the range of g that supports one bound state

(5) in polar coordinates $x = \rho \cos \phi$; $y = \rho \sin \phi$

$$\text{and } \rho^2 = x^2 + y^2$$

$$\nabla^2 = \frac{1}{\rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \quad \text{or } \nabla^2 = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2}$$

the schrodinger eqⁿ reads

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\rho) \psi = E \psi$$

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right] \psi + V(\rho) \psi = E \psi \quad \dots (1)$$

let $\Psi(\rho, \phi) = R(\rho) \Phi(\phi)$; substitute this in (1)

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\rho} \Phi \frac{\partial}{\partial \rho} \left(\rho \frac{\partial R}{\partial \rho} \right) + \frac{1}{\rho^2} R \frac{\partial^2 \Phi}{\partial \phi^2} \right] + V(\rho) R \Phi = E R \Phi$$

multiply by ρ^2 and divide by $\Psi = R \Phi$

$$\frac{\rho}{R} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial R}{\partial \rho} \right) + \frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} - \frac{2m}{\hbar^2} V(\rho) \rho^2 + \frac{2m}{\hbar^2} E \rho^2 = 0$$

$$\frac{\rho}{R} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial R}{\partial \rho} \right) + \frac{2m}{\hbar^2} (E - V(\rho)) \rho^2 = -\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} \quad \dots (2)$$

the L.H.S is a function of ρ and the R.H.S is a function of ϕ , so they are equal if and only if they both equal the same constant. let us call this constant

$$m^2 \Rightarrow -\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} = m^2 \Rightarrow \frac{d^2 \Phi}{d\phi^2} + m^2 \Phi = 0$$

$$\Rightarrow \Phi(\phi) = A e^{im\phi}; \text{ normalize } \int_0^{2\pi} |\Phi|^2 d\phi = 1 \Rightarrow A = \frac{1}{\sqrt{2\pi}}$$

$$\therefore \Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

but Φ is periodic and single-valued

$$\Rightarrow \Phi(2\pi + \phi) = \Phi(\phi) \Rightarrow e^{im(2\pi + \phi)} = e^{im\phi}$$

$$\Rightarrow e^{im2\pi} = 1 \Rightarrow \cos(2\pi m) = 1 \Rightarrow 2\pi m = 0, \pm 2\pi, \pm 4\pi, \dots$$

$$m = 0, \pm 1, \pm 2, \pm 3, \dots$$

now the radial eqⁿ reads

$$\frac{p}{R} \frac{\partial}{\partial p} \left(p \frac{\partial R}{\partial p} \right) + \frac{2m}{\hbar^2} (E - V(p)) p^2 = m^2$$

$$\frac{p}{R} \left[\frac{dR}{dp} + p \frac{d^2 R}{dp^2} \right] + \frac{2m}{\hbar^2} (E - V(p)) p^2 = m^2$$

multiply by R/p^2

$$\frac{d^2 R}{dp^2} + \frac{1}{p} \frac{dR}{dp} + \frac{2m}{\hbar^2} (E - V(p)) R = \frac{m^2 R}{p^2}$$

$$\frac{d^2 R}{dp^2} + \frac{1}{p} \frac{dR}{dp} - \frac{m^2 R}{p^2} + \frac{2m}{\hbar^2} (E - V(p)) R = 0$$