Q. I

A. $$\left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\Psi(r,\theta,\varphi) = E\,\Psi(r,\theta,\varphi)$$

$$-\frac{\hbar^2}{2mr}\frac{\partial^2}{\partial r^2}(r\Psi) - \frac{\hbar^2}{2mr^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\Psi}{\partial\varphi^2}\right] + V(r)\Psi = E\Psi$$

$$\Rightarrow -\frac{\hbar^2}{2mr}\frac{\partial^2}{\partial r^2}(r\Psi) + \frac{1}{2mr^2}\hat{L}^2\Psi + V(r)\Psi = E\Psi$$

Let $\Psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$

$$\Rightarrow -Y(\theta,\varphi)\frac{\hbar^2}{2mr}\frac{d^2}{dr^2}(rR(r)) + V(r)R(r)Y(\theta,\varphi) + \frac{R(r)}{2mr^2}\hat{L}^2Y(\theta,\varphi) = E\,R(r)\,Y(\theta,\varphi)$$

$$\Rightarrow -\frac{\hbar^2}{2mr}\frac{1}{R(r)}\frac{d^2}{dr^2}(rR(r)) + (V(r)-E) + \frac{1}{2mr^2}\frac{1}{Y(\theta,\varphi)}\hat{L}^2Y(\theta,\varphi) = 0$$

$$\Rightarrow \underbrace{\left[-\hbar^2 r\frac{1}{R(r)}\frac{d^2}{dr^2}(rR(r)) + (V(r)-E)2mr^2\right]}_{=-\lambda\hbar^2} + \underbrace{\frac{1}{Y(\theta,\varphi)}\hat{L}^2Y(\theta,\varphi)}_{=\lambda\hbar^2} = 0$$

Since the first term depends only on r and the second only on (θ,φ) then each should be constant, equal to λ and $-\lambda$.

$$\Rightarrow \quad \hat{L}^2Y(\theta,\varphi) = \lambda\hbar^2 Y(\theta,\varphi) \quad \text{angular eigenvalue equation}$$

$$-\frac{\hbar^2}{2mr}\frac{d^2}{dr^2}(rR(r)) + \left(V(r) + \frac{\lambda\hbar^2}{2mr^2}\right)R(r) = E\,R(r)$$

or $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right](rR(r)) = E\,(rR(r))$$

the last equation is for the radial wavefunction $R(r)$, we see clearly the appearance of $U(r) = rR(r)$ as a natural transformation.

B. $$\hat{L}^2\,Y(\theta,\varphi) = \hbar^2\lambda Y(\theta,\varphi)$$

$$\Rightarrow -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y(\theta,\varphi) = \lambda\,Y(\theta,\varphi)$$

let $Y(\theta,\varphi) = P(\theta)\,\Phi(\varphi)$

$$\Rightarrow -\frac{\Phi(\varphi)}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}P(\theta)\right) - \frac{1}{\sin^2\theta}P(\theta)\frac{d^2\Phi(\varphi)}{d\varphi^2} = \lambda\,P(\theta)\,\Phi(\varphi)$$

(2)

$$-\frac{1}{P(\theta)}\sin\theta\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}P(\theta)-\frac{1}{\Phi(\varphi)}\frac{d^2\Phi(\varphi)}{d\varphi^2}=\lambda\sin^2\theta$$

$$\Rightarrow\underbrace{\left[+\frac{1}{P(\theta)}\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{dP(\theta)}{d\theta}\right)+\lambda\sin^2\theta\right]}_{-\mu}+\underbrace{\frac{1}{\Phi(\varphi)}\frac{d^2\Phi(\varphi)}{d\varphi^2}}_{\mu}=0$$

$$\Rightarrow\begin{cases}\dfrac{d^2\Phi}{d\varphi^2}-\mu\,\Phi(\varphi)=0\\[2mm] \sin\theta\dfrac{d}{d\theta}\left(\sin\theta\dfrac{dP(\theta)}{d\theta}\right)+\lambda\sin^2\theta\,P(\theta)=-\mu\,P(\theta)\end{cases}$$

The $\Phi(\varphi)$ is easy to solve

$$\Phi(\varphi)=e^{\pm\sqrt{\mu}\,\varphi}$$

Since $\Phi(\varphi)=\Phi(\varphi+2\pi)\Rightarrow e^{\pm\sqrt{\mu}\,(2\pi)}=1=e^{i2\pi m}$; $m\in\mathbb{Z}$

$\Rightarrow\sqrt{\mu}=im\Rightarrow\mu=-m^2$ So that

$$\Phi(\varphi)=e^{im\varphi}\quad;\quad m=-\infty,\ldots-3,-2,-1,0,1,2,3,\ldots+\infty$$

C. $L_z=xp_y-yp_x=\frac{\hbar}{i}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)$

$x=r\sin\theta\cos\varphi$; $y=r\sin\theta\sin\varphi$; $z=r\cos\theta$

$$\frac{\partial}{\partial\varphi}=\frac{\partial x}{\partial\varphi}\frac{\partial}{\partial x}+\frac{\partial y}{\partial\varphi}\frac{\partial}{\partial y}+\frac{\partial z}{\partial\varphi}\frac{\partial}{\partial z}$$

$\frac{\partial x}{\partial\varphi}=-r\sin\theta\sin\varphi$; $\frac{\partial y}{\partial\varphi}=r\sin\theta\cos\varphi$; $\frac{\partial z}{\partial\varphi}=0$

$$\Rightarrow\frac{\partial}{\partial\varphi}=-r\sin\theta\sin\varphi\frac{\partial}{\partial x}+r\sin\theta\cos\varphi\frac{\partial}{\partial y}$$

$$=x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}$$

$$\Rightarrow L_z=\frac{\hbar}{i}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)=\frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

Since $Y_\ell^m(\theta,\varphi)=e^{im\varphi}P_\ell^m(\theta)$ from previous question B

$$\Rightarrow L_zY_\ell^m(\theta,\varphi)=\frac{\hbar}{i}\frac{\partial}{\partial\varphi}\left(e^{im\varphi}P_\ell^m(\theta)\right)=\hbar m\,e^{im\varphi}P_\ell^m(\theta)$$

$$=\hbar m\,Y_\ell^m(\theta,\varphi)$$

D. Our radial differential equation in A was

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right] r R(r) = E\,(r R(r))$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right] U(r) = E\,U(r) \quad ; \quad U(r) = r R(r)$$

$$V_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2m r^2} - \frac{k e^2}{r}$$

E. $$\frac{d^2}{dr^2}U(r) - \frac{2m}{\hbar^2} V_{eff}(r)\, U(r) = -\frac{2mE}{\hbar^2} U(r)$$

$$\Rightarrow \frac{d^2 U(r)}{dr^2} + \frac{2kme^2}{\hbar^2 r} - \frac{\ell(\ell+1)}{r^2} U(r) = K^2 U(r)$$

$$\Rightarrow \frac{d^2 U(\rho)}{d\rho^2} + \left(\frac{2kme^2}{\hbar^2 K\rho} - \frac{\ell(\ell+1)}{\rho^2} - 1\right) U(\rho) = 0$$

using $K = \sqrt{\frac{-2mE}{\hbar^2}}$; $\rho = K r$ and $\rho_0 = \frac{2kme^2}{K\hbar^2}$

$$\Rightarrow \frac{d^2 U(\rho)}{d\rho^2} = \left(1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right) U(\rho)$$

(a) As $\rho \to \infty$ the dominant term in the right hand side is 1

$$\Rightarrow \frac{d^2 U(\rho)}{d\rho^2} = U(\rho) \quad \Rightarrow \quad U(\rho) \propto e^{\pm\rho}$$

Since $\rho \in [0, \infty[$ and $\int |\psi|^2 dv = 1 \Rightarrow$ only $U \propto e^{-\rho}$

(b) As $\rho \to 0$ in this case the dominant term is $1/\rho^2$, thus

$$\frac{d^2 U}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2} U(\rho)$$

which admits a power law solution $U(\rho) = \rho^{\sigma}$

$$\frac{d^2 U}{d\rho^2} = \sigma(\sigma-1)\rho^{\sigma-2} = \ell(\ell+1)\rho^{\sigma-2} \Rightarrow \sigma(\sigma-1) = \ell(\ell+1)$$

$$\Rightarrow \sigma = \begin{cases} \ell+1 \\ -\ell \end{cases}$$

again $\sigma = -\ell$ will give $U(\rho) \simeq \rho^{-\ell}$ which diverges as $\rho \to 0$

thus $$U(\rho) = A\rho^{\ell+1} \quad \text{as } \rho \to 0$$

F. (a) $E = -\dfrac{13.6\text{ eV}}{n^2}$; $n = N + (\ell+1) \geq (\ell+1)$

N is the degree of Laguerre polynomial $\Rightarrow N \geq 0$ $N = 0, 1, 2, \ldots$

thus $\ell \leq (n-1)$ or $\ell_{max} = (n-1)$

Since the eigenstates are labeled with three quantum numbers

$\Psi_{n\ell m}(r, \theta, \varphi)$

while E_n depends on n only, then for each n we have

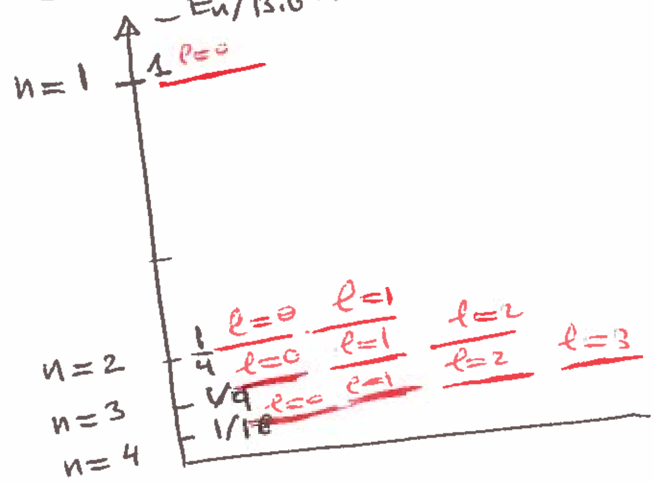
$\ell = 0, 1, 2, \ldots, (n-1)$ i.e. $\underline{n}$ values for ℓ

and for each ℓ we have

$m = -\ell, -\ell+1, \ldots, (\ell-1), \ell$ i.e. $(2\ell+1)$ value of m

Thus the degeneracy is given by

$$D = (2\cdot0+1) + (2\cdot1+1) + (2\cdot2+1) + \cdots + (2(n-1)+1)$$
$$= 2[0+1+2+\cdots+n-1] + n = 2\frac{n(n-1)}{2} + n = n^2$$



(b) $-\dfrac{E_n}{13.6\text{ eV}} = \dfrac{1}{n^2}$; $n = 1, 2, 3, 4$

The degeneracies are given by

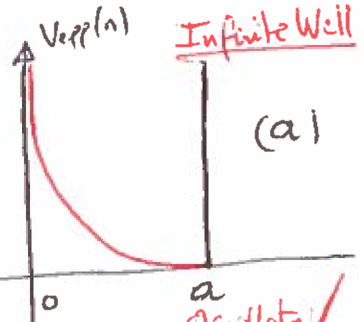
E_1	$n=1$	Degeneracy $= 1$
E_2	$n=2$	" $= 4$
E_3	$n=3$	" $= 9$
E_4	$n=4$	" $= 16$

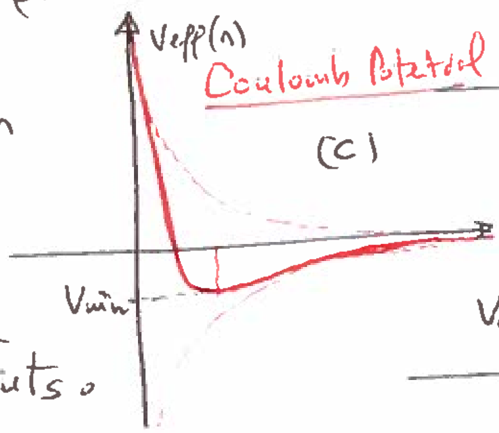
E_1: $2\cdot0+1 = 1$

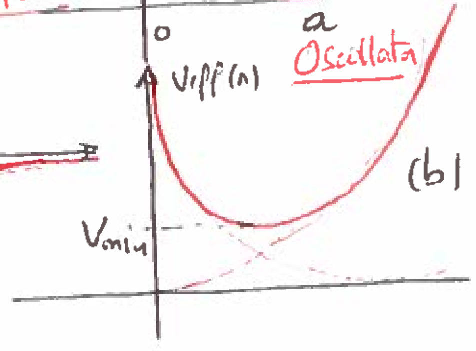
E_2: $(2\cdot0+1) + (2\cdot1+1) = 4$

E_3: $(2\cdot0+1) + (2\cdot1+1) + (2\cdot2+1) = 9$

E_4: $(2\cdot0+1) + (2\cdot1+1) + (2\cdot2+1) + (2\cdot3+1) = 16$







G. Bound states are possible for

(a) $E > 0$

(b) $E > V_{min}$

(c) $V_{min} < E < 0$

classically the particle will be confined between turning points.

Q. II

(a) $|\psi\rangle = A\begin{pmatrix}1\\2i\end{pmatrix} \Rightarrow \langle\psi| = A^*(1 \; -2i)$ row vector

$$\langle\psi|\psi\rangle = |A|^2(1 \; -2i)\begin{pmatrix}1\\2i\end{pmatrix} = |A|^2(1+4) = 5|A|^2 = 1$$

$\Rightarrow |A| = \frac{1}{\sqrt{5}}$ choose $A>0$ then $|\psi\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\2i\end{pmatrix}$

$|\langle\uparrow|\psi\rangle|^2 = |A|^2 = \frac{1}{5}$; $|\langle\downarrow|\psi\rangle|^2 = 4|A|^2 = 4/5$

(b) $\langle\frac{1}{2}\frac{1}{2}|S_z|\frac{1}{2}\frac{1}{2}\rangle = \frac{\hbar}{2}\langle\frac{1}{2}\frac{1}{2}|\frac{1}{2}\frac{1}{2}\rangle = \frac{\hbar}{2}$

$\langle\frac{1}{2}\frac{1}{2}|S_z|\frac{1}{2}-\frac{1}{2}\rangle = -\frac{\hbar}{2}\langle\frac{1}{2}\frac{1}{2}|\frac{1}{2}-\frac{1}{2}\rangle = 0$

thus S_z has only diagonal terms

$$S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$

$S_+|\frac{1}{2}\frac{1}{2}\rangle = 0$; $S_+|\frac{1}{2}-\frac{1}{2}\rangle = \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1)+\frac{1}{2}(-\frac{1}{2}+1)}\,|\frac{1}{2}\frac{1}{2}\rangle$
$= \hbar|\frac{1}{2}\frac{1}{2}\rangle$

$S_-|\frac{1}{2}+\frac{1}{2}\rangle = \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1)-\frac{1}{2}(+\frac{1}{2}-1)}\,|\frac{1}{2}\frac{1}{2}\rangle = \hbar|\frac{1}{2},-\frac{1}{2}\rangle$

$S_-|\frac{1}{2}-\frac{1}{2}\rangle = 0$

so that, $\langle\frac{1}{2}\frac{1}{2}|S_+|\frac{1}{2}\frac{1}{2}\rangle = 0$; $\langle\frac{1}{2}\frac{1}{2}|S_+|\frac{1}{2}-\frac{1}{2}\rangle = \hbar$

$\langle\frac{1}{2}-\frac{1}{2}|S_+|\frac{1}{2}\frac{1}{2}\rangle = 0$; $\langle\frac{1}{2}-\frac{1}{2}|S_+|\frac{1}{2}-\frac{1}{2}\rangle = 0$

$\Rightarrow S_+ = \hbar\begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$; $S_- = \hbar\begin{pmatrix}0 & 0\\1 & 0\end{pmatrix}$

then $S_x = \dfrac{S_+ + S_-}{2} = \dfrac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} = \dfrac{\hbar}{2}\sigma_2$

$S_y = \dfrac{S_+ - S_-}{2i} = \dfrac{\hbar}{2i}\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix} = \dfrac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix} = \dfrac{\hbar}{2}\sigma_3$

(c) $S_x = \frac{\hbar}{2}\sigma_2$, $S_y = \frac{\hbar}{2}\sigma_3$ (see previous results)
possible outcomes are given by the eigenvalues of these matrices

$|S_x - \lambda| = 0 = \begin{vmatrix}-\lambda & \hbar/2\\ \hbar/2 & -\lambda\end{vmatrix} \Rightarrow \lambda^2 = \left(\frac{\hbar}{2}\right)^2 \Rightarrow \lambda = \pm\frac{\hbar}{2}$

$|S_y - \lambda| = 0 = \begin{vmatrix}-\lambda & -i\hbar/2\\ i\hbar/2 & -\lambda\end{vmatrix} \Rightarrow \lambda^2 = \left(\frac{\hbar}{2}\right)^2 \Rightarrow \lambda = \pm\frac{\hbar}{2}$

$|S_z - \lambda| = 0 = \begin{vmatrix}\hbar/2-\lambda & 0\\ 0 & -\frac{\hbar}{2}-\lambda\end{vmatrix} \Rightarrow \lambda^2 = \left(\frac{\hbar}{2}\right)^2 \Rightarrow \lambda = \pm\frac{\hbar}{2}$

So the only possible results while measuring S_x, S_y, S_z are $\pm \hbar/2$ (6)

$$\langle S_x \rangle = \langle \psi | S_x | \psi \rangle$$
$$= \frac{1}{\sqrt{5}} (1 \quad -2i) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2i \end{pmatrix}$$
$$= \frac{\hbar}{10} (1 - 2i) \begin{pmatrix} 2i \\ 1 \end{pmatrix} = 0$$

$$\langle S_z \rangle = \frac{1}{\sqrt{5}} (1 - 2i) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 2i \end{pmatrix} \frac{1}{\sqrt{5}}$$
$$= \frac{\hbar}{10} (1 - 2i) \begin{pmatrix} 1 \\ -2i \end{pmatrix} = \frac{\hbar}{10} (1-4) = -\frac{3\hbar}{10}$$

$$\langle S_y \rangle = \frac{1}{\sqrt{5}} (1 - i2) \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2i \end{pmatrix}$$
$$= \frac{\hbar}{10} (1 - 2i) \begin{pmatrix} 2 \\ i \end{pmatrix} = \frac{\hbar}{10}(4)$$

Since $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

then $S_x^2 = S_y^2 = S_z^2 = \frac{\hbar^2}{4} \Rightarrow \langle S_x^2 \rangle = \langle S_y^2 \rangle = \langle S_z^2 \rangle = \frac{\hbar^2}{4}$

$$\sigma_{S_x}^2 = \langle S_x^2 \rangle - \langle S_x \rangle^2 = \frac{\hbar^2}{4} - 0 = \frac{\hbar^2}{4} \Rightarrow \sigma_{S_x} = \frac{\hbar}{2}$$

$$\sigma_{S_z}^2 = \langle S_z^2 \rangle - \langle S_z \rangle^2 = \frac{\hbar^2}{4} - \frac{9\hbar^2}{100} = \frac{64\hbar^2}{100} \Rightarrow \sigma_{S_z} = \frac{8\hbar}{10} = \frac{4\hbar}{5}$$

$$\sigma_{S_x} \sigma_{S_z} = \frac{4\hbar^2}{10} = \frac{2\hbar^2}{5} \geq \frac{1}{2} |\langle [S_x, S_z] \rangle| = \frac{\hbar}{2} |\langle S_y \rangle|$$

$$[S_x, S_z] = -i\hbar S_y$$

$$\sigma_{S_x} \sigma_{S_y} = \frac{2\hbar^2}{5} \geq \frac{\hbar}{2} \frac{4\hbar}{10} = \frac{4\hbar^2}{20} = \frac{\hbar^2}{5}$$