

(1) a) $\psi(r, \theta, \phi) = \Psi(r, \theta)$

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

$\hat{L} = \hat{r} \times \hat{p}$ $\hat{L}^2 |\psi\rangle = \hat{r} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\theta^2} \right) \right) |\psi\rangle$

$= 0$ since no ϕ dependence

2D with $\Psi = A \cos(\theta)$

$$\hat{L}^2 |\Psi\rangle = -A\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta x - \sin\theta) \right)$$

$$= A\hbar^2 \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin^2\theta) \quad \text{substitute}$$

$$> A\hbar^2 \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\frac{1}{2} - \frac{1}{2} \cos 2\theta \right)$$

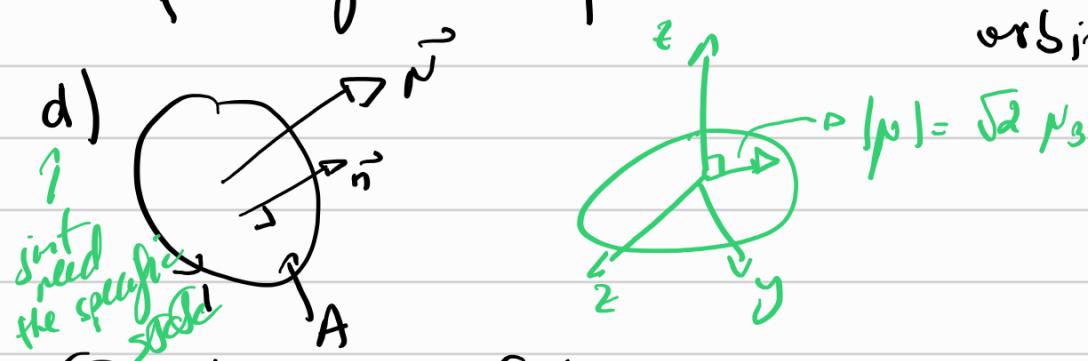
$$= \frac{A\hbar^2}{\sin\theta} 2(\sin\theta) \times \cos\theta$$

$$= 2 \quad \dots \quad \hat{L}^2 = 2\hbar^2 = 2\hbar\Psi$$

$$|\hat{L}| = \sqrt{2\hbar}$$

b) l : angular quantum number describes shape of orbital

c) m_l : magnetic "quantum number" oriented in space of orbital of a given E



(2) a) $|\Psi\rangle = S |\Psi|$ normalized

$$\langle \Psi | \Psi \rangle = \text{magnitude}^2$$

$$= \left(\frac{1}{4} - \sqrt{\frac{15}{16}} i \right) \cdot \left(\sqrt{\frac{15}{16}} i \right) = 1$$

b) $\hat{S}_z = \frac{1}{2} \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\langle \Psi | \hat{S}_z | \Psi \rangle \leq \langle S_z \rangle$$

$$|\Psi\rangle = \frac{1}{4} |1\rangle + \sqrt{\frac{15}{16}} i |2\rangle$$

$$= \left[\frac{1}{4} \langle 1 | + \sqrt{\frac{15}{16}} i \langle 2 | \right] \hat{S}_z \left[\frac{1}{4} |1\rangle + \sqrt{\frac{15}{16}} i |2\rangle \right]$$

$$\begin{aligned}
 &= \left[\frac{1}{4} |11\rangle + \sqrt{\frac{15}{16}} i |12\rangle \right] \left[\frac{1}{4} \hat{S}_z |11\rangle + \sqrt{\frac{15}{16}} i \hat{S}_z |12\rangle \right] \\
 &= \frac{1}{4} \hat{S}_z |111\rangle - \frac{15}{16} \hat{S}_z |212\rangle \\
 &\quad + \frac{\sqrt{15}}{4\sqrt{4}} i \hat{S}_z |112\rangle + \frac{\sqrt{15}}{4\sqrt{4}} i \hat{S}_z |211\rangle \\
 &= -\frac{15}{16} \hat{S}_{z=2} + \frac{15}{4\sqrt{4}} i \hat{S}_{z=1} \\
 &= -\frac{15}{16} \frac{1}{2} \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{15}{4\sqrt{4}} i \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
 &= \begin{pmatrix} -\frac{15\hbar}{32} & 0 \\ 0 & \frac{15\hbar}{32} \end{pmatrix} + \begin{pmatrix} \frac{15\hbar i}{4\sqrt{4}} & 0 \\ 0 & -\frac{15\hbar i}{4\sqrt{4}} \end{pmatrix} \\
 &= \frac{15\hbar}{4\sqrt{4}}
 \end{aligned}$$

$32 = 4 \times 4 \times 2$
 $= 4 \times 8 \times 4$

$\langle \psi | \hat{S}_z | \psi \rangle$

$$\begin{aligned}
 &= \left(\frac{1}{2} - \sqrt{\frac{15}{16}} i \right) \frac{1}{2} \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} / \sqrt{\frac{15}{16}} i \\
 &= -\frac{7}{16} \hbar
 \end{aligned}$$

$$\textcircled{3} \quad S_z = \hbar \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

x-spin

This is mostly simple 2×2 matrix maths. For y it is a touch different.

x -spin

We can write,

$$\det(\widehat{S}_x - I\lambda) = 0 \quad (11)$$

$$= \begin{vmatrix} 0 - \lambda & \frac{1}{2}\hbar \\ \frac{1}{2}\hbar & 0 - \lambda \end{vmatrix} \quad (12)$$

$$= (0 - \lambda)(0 - \lambda) - \left(\frac{1}{2}\hbar\right)\left(\frac{1}{2}\hbar\right) \quad (13)$$

$$\therefore \lambda^2 = \frac{1}{4}\hbar^2 \quad (14)$$

$$\lambda = \pm \frac{1}{2}\hbar \quad (15)$$

now that we have the eigenvalues we need to find the corresponding (normalised) eigenvectors

$$\widehat{S}_x \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \quad (16)$$

$$\frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} a \\ b \end{pmatrix} \quad (17)$$

act with the matrix on the vector to give

$$\begin{pmatrix} b \\ a \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \quad (18)$$

$\therefore a = b$

now we need to normalize the vector. First do the dot product (inner product) to find the square of the magnitude of the vector

$$(a \ a)^* \times \begin{pmatrix} a \\ a \end{pmatrix} = (a^2 + a^2) \quad (19)$$

$$= 2a^2$$

$$\approx 1$$

$$\therefore a = \frac{1}{\sqrt{2}} \quad (20)$$

$$(21)$$

$$(22)$$

By convention we take the positive root [we'll return to this for y]. For eigenvalue $\frac{1}{2}\hbar$ we have

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (23)$$

$$(24)$$

z spin \rightarrow same
 y spin (beyond what I need for atoms)

z -spin

Follow the same procedure as above (or however you solve for eigenvalues and eigenvectors). (24)

y -spin

[Beyond examinable material, but interesting.] Here we need to watch our complex conjugates and we need to introduce an arbitrary phase factor. We follow the same analysis again to get the eigenvalues of $\pm \frac{1}{2}\hbar$. Then we can tackle the eigenvectors. Say we take the $+$ eigenvalue then,

$$\widehat{S}_y \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \quad (25)$$

$$\frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} a \\ b \end{pmatrix} \quad (26)$$

if you do the maths ...

if you do the matrix multiplication you get

$$\begin{pmatrix} -ib \\ ia \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\therefore -ib = a$$

and

$$ia = b$$

Let's say $a = Ae^{i\alpha}$

$$\therefore b = ie^{i\alpha} = Ae^{i(\alpha + \pi/2)}$$

recall your Argand diagrams. Therefore we have the eigenvector

$$\begin{pmatrix} Ae^{i\alpha} \\ Ae^{i(\alpha+\pi/2)} \end{pmatrix} \quad (32)$$

we need to normalize the vector. First do the dot product (inner product) to find the square of the magnitude of the vector

$$\begin{pmatrix} Ae^{-i\alpha} & Ae^{-i(\alpha+\pi/2)} \end{pmatrix} \times \begin{pmatrix} Ae^{i\alpha} \\ Ae^{i(\alpha+\pi/2)} \end{pmatrix} = 2A^2 \quad (33)$$

$$= 1 \quad (34)$$

$$\therefore A = \frac{1}{\sqrt{2}} \quad (35)$$

for eigenvalue $\frac{1}{2}i$ we have eigenvector

$$\frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\alpha} \\ e^{i(\alpha+\pi/2)} \end{pmatrix} \quad (37)$$

a similar analysis for the $-i/2$ eigenvalue gives

$$\frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\alpha'} \\ e^{i(\alpha'-\pi/2)} \end{pmatrix} \quad (38)$$

We can choose any value for the angles since these 'phase' factors never survive measurement, they always die out in any expectation measurement or any normalization. Therefore it doesn't matter what values we choose. We choose to match convention by picking $\alpha = 0$ and $\alpha' = 0$. Hence we have

$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad \left. \begin{array}{l} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \end{array} \right\} \text{2 eigenvectors}$

