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$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|Y_0^0\rangle + |Y_1^0\rangle\right), \quad \langle L^2\rangle, \quad \langle L_z\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{4\pi}} + \sqrt{\frac{3}{4\pi}}\cos\theta\right) = \frac{1}{\sqrt{8\pi}}\left(1 + \sqrt{3}\cos\theta\right)$$

$$\langle L^2\rangle = \frac{1}{\sqrt{2}}\left(\langle Y_0^0| + \langle Y_1^0|\right) L^2 \frac{1}{\sqrt{2}}\left(|Y_0^0\rangle + |Y_1^0\rangle\right)$$

$$L^2 |Y_l^m\rangle = \hbar^2 l(l+1) |Y_l^m\rangle$$

$$= \frac{1}{2}\left(\langle Y_0^0| + \langle Y_1^0|\right)\left(0 \, |Y_0^0\rangle + 2\hbar^2 |Y_1^0\rangle\right)$$

$$= \frac{1}{2} 2\hbar^2 = \hbar^2 \quad \text{(average of eigenvals)}$$

$$\langle L_z\rangle = \frac{1}{\sqrt{2}}\left(\langle Y_0^0| + \langle Y_1^0|\right) L_z \frac{1}{\sqrt{2}}\left(|Y_0^0\rangle + |Y_1^0\rangle\right)$$

$$L_z |Y_l^m\rangle = \hbar m |Y_l^m\rangle$$

using θ, ϕ

$$L_z = -i\hbar \frac{\partial}{\partial\phi} \qquad L^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$-i\hbar\frac{\partial}{\partial\phi} \cdot \frac{1}{\sqrt{8\pi}}\left(1 + \sqrt{3}\cos\theta\right) = 0$$

$$-\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\frac{1}{\sqrt{8\pi}}\left(1 + \sqrt{3}\cos\theta\right)$$

$$= -\hbar^2\frac{\sqrt{3}}{\sqrt{8\pi}}\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}\right)(\cos\theta)$$

$$= -\hbar^2\frac{\sqrt{3}}{\sqrt{8\pi}}\left(-\cos^2\theta + \frac{\cos\theta}{\sin\theta}(-\sin\theta)\right) = \hbar^2\sqrt{\frac{3}{8\pi}}\left(2\cos\theta + \cancel{\cos^2\theta}\right)$$

$$\langle L^2\rangle = \frac{1}{\sqrt{8\pi}}\hbar^2\sqrt{\frac{3}{8\pi}}\int_0^\pi d\theta \sin\theta \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \left[1 + \sqrt{3}\cos\theta\right]\left[2\cos\theta + \cancel{\cos^2\theta}\right]$$

$$= \frac{\sqrt{3}}{8\pi}\hbar^2 \, 2\pi \int_0^\pi d\theta \, \sin\theta\left[\cos\theta + \cancel{\cos^2\theta} + 2\sqrt{3}\cos^2\theta + \cancel{\sqrt{3}\cos^3\theta}\right]$$

$$= \cancel{\frac{\sqrt{3}}{8\pi}\hbar^2} \; \frac{\sqrt{3}}{4}\hbar^2 \int_{-1}^{1} dt \left[\underbrace{t}_{\to 0} + 2t^2(\cancel{1}\sqrt{3}) + \underbrace{\cancel{\sqrt{3}t^3}}_{\to 0}\right]$$

$$= \frac{\sqrt{3}}{4}\hbar^2\left[\frac{t^3}{3}\Big|_{-1}^{1}(2\sqrt{3})\right] = \frac{\sqrt{3}}{4}\hbar^2 \, \frac{2}{3}\,(2\sqrt{3}) = \frac{\hbar^2}{2}\frac{(2\sqrt{3})}{\sqrt{3}} = \hbar^2 \quad \text{OK}$$

$$L_+ = L_x + i L_y$$
$$L_- = L_x - i L_y$$
$$L_x = \frac{1}{2}(L_+ + L_-)$$
$$L_y = \frac{1}{2i}(L_+ - L_-)$$

$$\to L_x = \frac{\hbar}{2}\left[\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}\right] = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$$L_y = \frac{\hbar}{2i}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}$$

$$L_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 2 & 0 & 2 \\ 0 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix} = \hbar^2\begin{pmatrix} 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix}$$

$$L_y^2 = -\frac{\hbar^2}{4}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} = -\frac{\hbar^2}{4}\begin{pmatrix} -2 & 0 & 2 \\ 0 & -4 & 0 \\ 2 & 0 & -2 \end{pmatrix} = \hbar^2\begin{pmatrix} 1/2 & 0 & -1/2 \\ 0 & 1 & 0 \\ -1/2 & 0 & 1/2 \end{pmatrix}$$

$$L_z^2 = \hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}^2 = \hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$L_x^2 + L_y^2 + L_z^2 = \hbar^2\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{OK}$$

stav $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ v bázi Y_0^0, Y_1^1, Y_1^0, Y_1^{-1}

$$\mathbb{L}^2 = \hbar^2\begin{pmatrix} 0 & & & \\ & 2 & & \\ & & 2 & \\ & & & 2 \end{pmatrix} \qquad \mathbb{L}_z = \hbar\begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 0 & \\ & & & -1 \end{pmatrix}$$

& $v^T \mathbb{L}^2 v = \frac{1}{2}(1\ 0\ 1\ 0)\,\hbar^2\begin{pmatrix} 0 & & & \\ & 2 & & \\ & & 2 & \\ & & & 2 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \hbar^2$ $\qquad L_z = 0$

$$L_x L_y = \frac{\hbar^2}{4i}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} = \frac{\hbar^2}{4i}\begin{pmatrix} -2 & 0 & 2 \\ 0 & 4 & 0 \\ -2 & 0 & 2 \end{pmatrix}$$

$$L_y L_x = \frac{\hbar^2}{4i}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} = \frac{\hbar^2}{4i}\begin{pmatrix} 2 & 0 & -2 \\ 0 & 4 & 0 \\ -2 & 0 & -2 \end{pmatrix}$$

$$L_x L_y - L_y L_x = \frac{\hbar^2}{4i}\begin{pmatrix} -4 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix} = i\hbar\left[\hbar\begin{pmatrix} 1 & & 0 \\ & 0 & \\ 0 & & -1 \end{pmatrix}\right] = i\hbar L_x$$

- matice + operátory z 11
- vodík + výběrová pravidla
- vodík – základní stav (vodíku-podobný iont

$$a_0 = \frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2}$$

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r) Y_l^m(\theta,\phi)$$

$$R_{10} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \qquad Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$\to \psi_{nlm}(r,\theta,\phi) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \frac{1}{\sqrt{4\pi}} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

- Normalizovaná?

$$\underbrace{\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi}_{4\pi} \int_0^\infty dr\, r^2 \frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3 e^{-2Zr/a_0}$$

$$= 4\left(\frac{Z}{a_0}\right)^3 \int_0^\infty dr\, r^2 e^{-2Zr/a_0} \quad (*)$$

$$\int_0^\infty r^2 e^{-\alpha r} dr = \underbrace{\left[-\frac{r^2 e^{-\alpha r}}{\alpha}\right]_0^\infty}_{\to 0} + \int_0^\infty 2r \frac{e^{-\alpha r}}{\alpha} dr = \underbrace{\left[-\frac{2r e^{-\alpha r}}{\alpha^2}\right]_0^\infty}_{\to 0} + \int_0^\infty \frac{2 e^{-\alpha r}}{\alpha^2} dr$$

$$= -\frac{2e^{-\alpha r}}{\alpha^3}\Big|_0^\infty = -\left[0 - \frac{2}{\alpha^3}\right] = \frac{2}{\alpha^3} \qquad \alpha = \frac{2Z}{a_0} \quad \to \frac{2 a_0^3}{8Z^3} = \frac{a_0^3}{4Z^3}$$

$$(*) \Rightarrow 4\left(\frac{Z}{a_0}\right)^3 \cdot \frac{a_0^3}{4Z^3} = \underline{1} \qquad \text{OK}$$

Obecně $\int_0^\infty r^n e^{-\alpha r} dr = \frac{1}{\alpha^{n+1}} n!$ $\rightsquigarrow$ Γ - funkce

- střední hodnota $\langle r \rangle$

$$\to \underbrace{\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi}_{4\pi} \int_0^\infty dr\, r^3 \frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3 e^{-2Zr/a_0}$$

$$\to 4\left(\frac{Z}{a_0}\right)^3 \underbrace{\int_0^\infty dr\, r^3 e^{-2Zr/a_0}}_{} \to \frac{1}{\alpha^4} 3! = \frac{a_0^4}{16Z^4} 6$$

$$\Rightarrow 4\left(\frac{Z}{a_0}\right)^3 \frac{a_0^4}{8Z^4} \cdot 3 = \frac{3}{2}\frac{a_0}{Z}$$

- maximum p.p. $\Leftrightarrow \max |\psi_{100}|^2 \cdot r^2 = \max \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} r^2 e^{-2Zr/a_0}$

$$\frac{d}{dr}\left(e^{-2Zr/a_0} \cdot r^2\right) = \underbrace{\left(-\frac{2Z}{a_0} r^2 + 2r\right)}_{=0} e^{-Zr/a_0}$$

$$2 = \frac{2Z}{a_0} r \Rightarrow \underline{\underline{r = \frac{a_0}{Z}}}$$

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· interakce se zářením
→ operátory $\vec{r}$ (el. pole)
$x = r\sin\theta\cos\phi$
$y = r\sin\theta\sin\phi$
$z = r\cos\theta$

jaké jsou nenulové maticové elementy mezi zákl. stavem a excitovanými?

· víme $\langle n'l'm'|nlm\rangle = 0$
· tvar $l \sim (\sin\theta)^{l}$ $\sin\theta, \cos\theta \rightsquigarrow$ změna l o ± 1
· tvar $m \sim e^{im\phi}$ $\cos\phi, \sin\phi \sim e^{i\phi} \pm e^{-i\phi}$ → změna m o ± 1
· r ?

$Y_0^0 = \frac{1}{\sqrt{4\pi}}$ $Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$ | $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$

inverzně:
$x \sim \sin\theta\cos\phi = \frac{1}{2}\sin\theta\left(e^{i\phi} + e^{-i\phi}\right) =$
$= \frac{1}{2}\sqrt{\frac{8\pi}{3}} \cdot \underbrace{\sqrt{\frac{3}{8\pi}}\left[\sin\theta e^{i\phi}\right.}_{-Y_1^1} + \underbrace{\left.\sin\theta e^{-i\phi}\right]}_{Y_1^{-1}}$

$\psi_{100} = \frac{1}{\sqrt{4\pi}}\frac{2}{a_0^{3/2}}e^{-r/a_0}$

$\psi_{211} = Y_1^1 \frac{1}{2\sqrt{6}\, a_0^{3/2}}\frac{r}{a_0}e^{-r/(2a_0)}$

$= \frac{1}{2}\sqrt{\frac{2\pi}{3}}\left[-Y_1^1 + Y_1^{-1}\right]$

→ $\langle 100|x|210\rangle = 0$, $\langle 100|x|200\rangle = 0$

$\langle 100|x|211\rangle = \int_0^\infty dr\, r^2 \frac{2}{a_0^{3/2}}e^{-r/a_0}\, r\, \frac{1}{2\sqrt{6}\, a_0^{3/2}}\frac{r}{a_0}e^{-r/(2a_0)}$

r část

$= \frac{1}{\sqrt{6}a_0^4}\int_0^\infty dr\, r^4 e^{-\frac{3r}{2a_0}}$ $\alpha = \frac{3}{2a_0}$, $n = 4$ → $n!\frac{1}{\alpha^5} = 24 \cdot \frac{(2a_0)^5}{3^5}$

$= \frac{2^8 a_0}{\sqrt{6}\, 9} \neq 0$ převodní Y_0^0

úhlová část: $\sqrt{\frac{2\pi}{3}}\left[-\langle Y_1^1| + \langle Y_1^{-1}|\right]\frac{1}{\sqrt{4\pi}}|Y_1^1\rangle = -\frac{1}{\sqrt{6}} \neq 0$

→ celkem $-\frac{2^8 a_0}{\sqrt{6}\, 9}\cdot\frac{1}{\sqrt{6}} = -\frac{2^7 a_0}{27}$

→ pro $\langle\ |Y_1^{-1}\rangle = \frac{2^7 a_0}{27}$ $\langle\ |Y_1^0\rangle = 0$ → $\Delta l = 1$, $\Delta m = \pm 1$

$z = r\cdot\cos\theta = r\sqrt{\frac{4\pi}{3}}\, Y_1^0$

→ $\Delta l \pm 1$, $\Delta m = 0$