$$\psi_{210} = \sqrt{\left(\frac{2}{2a}\right)^3 \frac{(2-1-1)!}{2\cdot 2[(2+1)!]}} \cdot e^{-r/2a} \cdot \left(\frac{2r}{2a}\right)^1 \cdot L^{2\cdot 1+1}_{2-1-1}\left(\frac{2r}{2a}\right) \cdot Y_1^0(\theta,\varphi)$$

$$= \frac{1}{2}\sqrt{\frac{1}{6a^3}} \cdot e^{-\frac{r}{2a}} \cdot \left(\frac{r}{a}\right) \cdot L_0^3\left(\frac{r}{a}\right) \cdot Y_1^0(\theta,\varphi)$$

L_0^3: associated Laguerre polynomials

Y_1^0: sherical harmonics (Kugelflächenfunktionen)

There are different ways of finding the polynomials (see also 2
lecture). For example

$$L_n^\alpha(x) = \sum_{k=0}^{n} \binom{n+\alpha}{n-k} \frac{(-x)^k}{k!}$$

(Bronstein, p 531, eq. 9.626. There you also find recursion formulas, ...)

$$\Rightarrow L_0^3 = \binom{3}{0} \cdot \frac{(-x)^0}{0!} = 1$$

spherical harmonics: $Y_{\ell m}(\theta,\varphi) = \frac{1}{\sqrt{2\pi}} N_{\ell m} \cdot P_{\ell m}(\cos\theta) \cdot e^{im\varphi}$

with normalization $N_{\ell m} = \sqrt{\frac{2\ell+1}{2} \cdot \frac{(\ell-|m|)!}{(\ell+|m|)!}}$

$P_{\ell m}$: associated Legendre polynomials:

$$P_{\ell m}(x) = (1-x^2)^{\frac{|m|}{2}} \left(\frac{\partial}{\partial x}\right)^{|m|} P_\ell(x)$$

$P_\ell(x)$: Legendre polynomial

integer part only $\rightarrow [\ell/2]$

$$P_\ell(x) = \frac{1}{2^\ell} \cdot \sum_{k=0}^{[\ell/2]} (-1)^k \frac{(2\ell-2k)!}{k!(\ell-k)!(\ell-2k)!} \cdot x^{\ell-2k}$$

$\Rightarrow$ For Y_1^0: $\quad N_{1,0} = \sqrt{\frac{3}{2} \cdot \frac{1}{1}} = \sqrt{\frac{3}{2}}$

$$P_1 = \frac{1}{2} \cdot (-1)^0 \cdot \frac{2}{1} \cdot x^1 = x$$

only $k=0$

$$P_{1,0} = (1-x)^0 \left(\frac{\partial}{\partial x}\right)^0 x = x$$

$$\Rightarrow Y_1^0 = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3}{2}} \cdot \underbrace{\cos(\theta)}_{x} \cdot \underbrace{e^{im\varphi}}_{m=0} = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos(\theta)$$

$$\Rightarrow \psi_{210} = \frac{1}{4}\sqrt{\frac{1}{2\pi a^3}} \cdot \frac{r}{a} \cdot e^{-\frac{r}{2a}} \cdot \cos(\theta)$$

ii) $\Psi_{211} = \sqrt{\left(\frac{2}{2a}\right)^3 \frac{(2-1-1)!}{2\cdot 2\cdot (2+1)!}} \cdot e^{-r/2a}\cdot \frac{r}{a}\cdot \underbrace{L_0^3\left(\frac{r}{a}\right)}_{=1}\cdot Y_1^1(\theta,\varphi)$

$= \frac{1}{2}\sqrt{\frac{1}{6a^3}}\cdot e^{-r/2a}\cdot \frac{r}{a}\cdot Y_1^1(\theta,\varphi)$

~~Next~~ $N_{1,1} = \sqrt{\frac{3}{2}\cdot\frac{1}{2}} = \sqrt{\frac{3}{4}}$; $P_1 = x$, $P_{1,1} = (1-x^2)^{1/2}\overbrace{\frac{\partial}{\partial x}(x)}^{=1} = (1-x^2)^{1/2} \overset{x=\cos\theta}{=} \sqrt{1-\cos^2\theta} = \sin\theta$

$\Rightarrow \underline{\Psi_{211}} = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{3}{4}}\cdot\frac{1}{2}\sqrt{\frac{1}{6a^3}}\cdot\frac{r}{a}\cdot e^{-r/2a}\cdot\sin(\theta)\cdot e^{i\varphi}$ ← $m=1$

$= \frac{1}{8}\sqrt{\frac{1}{\pi a^3}}\cdot\frac{r}{a}\cdot e^{-r/2a}\cdot\sin(\theta)\cdot e^{i\varphi}$

The energy of each eigenstate is determined by the quantum number n: $E_n = \frac{E_1}{n^2}$, E_1 given in problem.

$\Rightarrow E_2 = E(\Psi_{210}) = E(\Psi_{211}) = \frac{E_1}{2^2} = \frac{E_1}{4}$

$E_3 = E(\Psi_{32-1}) = \frac{E_1}{3^2} = \frac{E_1}{9}$

} possible outcomes of an energy measurement (i.e. projection on eigenstates)

The probability of E_2 is $P(E=E_2) = \frac{a^2+b^2}{a^2+b^2+c^2}$

of E_3 : $P(E=E_3) = \frac{c^2}{a^2+b^2+c^2}$

The expectation value of the energy is

$\langle E\rangle = E_2\cdot P(E_2) + E_3\cdot P(E_3) = \frac{E_1}{4}\cdot\frac{a^2+b^2}{a^2+b^2+c^2} + \frac{E_1}{9}\cdot\frac{c^2}{a^2+b^2+c^2} = \frac{E_1}{a^2+b^2+c^2}\cdot\left(\frac{a^2+b^2}{4}+\frac{c^2}{9}\right)$

2 Groundstate: $\Psi_{100} = R_{10}(r)\cdot Y_0^0(\theta,\varphi) = \underbrace{\sqrt{\left(\frac{2}{a}\right)^3\cdot\frac{1}{2}}}_{=\frac{2}{a^{3/2}}}\cdot e^{-r/a}\underbrace{\left(\frac{2r}{a}\right)^0}_{=1}\cdot\underbrace{L_0^1\left(\frac{2r}{a}\right)}_{=1}\underbrace{Y_0^0(\theta,\varphi)}_{\frac{1}{\sqrt{2\pi}}\cdot\frac{1}{\sqrt{2}}}$

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

The probability to find r is

$P(r) = \int_0^{2\pi}\int_0^{\pi}\Psi^*(r)\Psi(r)\cdot\underbrace{r^2\cdot\sin(\theta)\,d\varphi\,d\theta}_{\text{volume elements}} = \underbrace{\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta}_{4\pi}\cdot r^2 e^{-2r/a}\cdot\frac{1}{a^3}\cdot\frac{1}{\pi} = \frac{4}{a^3}r^2 e^{-2r/a}$

for a constant r, but for all angles

Find maximum: $\frac{d}{dr}(P(r)) = \frac{4}{a^3}\left(2r e^{-2r/a} - \frac{2}{a}r^2 e^{-2r/a}\right) \overset{!}{=} 0$

$\Rightarrow r/a \overset{!}{=} 1$ or $\underline{r_m = a}$ is the most probable radius to find an electron.

b) $\underline{\langle r\rangle} = \int_0^\infty\int_0^\pi\int_0^{2\pi} \psi^*\cdot r\,\psi\,\underbrace{\cancel{d}r^2\cdot\sin(\theta)\,d\varphi\,d\theta\,dr}_{\text{volume element}}$

$$= \underbrace{\int_0^{2\pi} d\varphi\cdot\int_0^\pi \sin\theta\,d\theta}_{4\pi}\cdot\int_0^\infty \psi^* r^3\psi\,dr = 4\cancel{\pi}\cdot\frac{1}{\cancel{\pi}a^3}\int_0^\infty e^{-2r/a}\cdot r^3\,dr$$

Bronstein p. 1077, eq. 450

$$= \underbrace{-\frac{4a}{a^3 2} r^3 e^{-2r/a}\Big|_0^\infty}_{=0} + \frac{4}{a^3}\cdot\frac{a}{2}\int_0^\infty r^2 e^{-2r/a}\,dr \underset{\uparrow}{=} \frac{6}{a^2}\left[e^{-\frac{2r}{a}}\left(\frac{ar^2}{2}+\underbrace{\frac{2a^2 r}{4}}_{=0}+\frac{2a^3}{8}\right)\right]_{r=0}^\infty = \underline{\underline{\frac{3}{2}a}}$$

Bronstein p. 1077 eq. 449

$\Rightarrow$ The expectation value of a measurement of the distance between the electron and the nucleus is 50% larger than the most probable value.

3

ii) $$1 \overset{!}{=} \int\int\int_{-\infty}^{\infty} \overbrace{|\psi|^2}^{\psi^*\psi} dx\,dy\,dz = A^2 e^{-2\alpha(x^2+y^2+z^2)}\cdot\left(\frac{\overbrace{(x+iy)(x-iy)}^{x^2+y^2}}{x^2+y^2}\right)^m dx\,dy\,dz$$

$$= A^2\cdot\int_{-\infty}^{\infty} e^{-2\alpha x^2}dx\cdot\int_{-\infty}^{\infty} e^{-2\alpha y^2}dy\cdot\int_{-\infty}^{\infty} e^{-2\alpha z^2}dz \underset{\uparrow}{=} A^2\left(\left(\frac{\pi}{2\alpha}\right)^{1/2}\right)^3 = A^2\left(\frac{\pi}{2\alpha}\right)^{3/2}$$

given formula

$$\Rightarrow \underline{\underline{A = \left(\frac{2\alpha}{\pi}\right)^{3/4}}}$$

(ii) Goal: $\langle L_z\rangle \left(= \langle\psi|L_z|\psi\rangle\right) = \int \psi^*(L_z\psi)\,dx$

$$\underline{\underline{L_z|\psi\rangle}} \overset{\text{real space}}{=} \underbrace{-i\hbar\,(x\partial_y - y\partial_x)}_{L_z}\underbrace{\left\{Ae^{-\alpha(x^2+y^2+z^2)}\cdot(x+iy)^m\cdot(x^2+y^2)^{-m/2}\right\}}_{\psi}$$

$$= -i\hbar A e^{-\alpha z^2}\cdot\left\{x\cdot e^{-\alpha x^2}\frac{\partial}{\partial y}\left[e^{-\alpha y^2}(x+iy)^m(x^2+y^2)^{-m/2}\right] - y e^{-\alpha y^2}\frac{\partial}{\partial x}\left[e^{-\alpha x^2}(x+iy)^m(x^2+y^2)^{-m/2}\right]\right\}$$

$$= -i\hbar A e^{-\alpha z^2}\Big\{x e^{-\alpha x^2}\Big[-2\alpha y e^{-\alpha y^2}(x+iy)^m(x^2+y^2)^{-m/2} + (im)\cdot e^{-\alpha y^2}(x+iy)^{m-1}(x^2+y^2)^{-m/2}$$
$$- (m/2)2y e^{-\alpha y^2}(x+iy)^m(x^2+y^2)^{-m/2-1}\Big]$$
$$- y e^{-\alpha y^2}\Big[-2\alpha x e^{-\alpha x^2}(x+iy)^m(x^2+y^2)^{-m/2} + m e^{-\alpha x^2}(x+iy)^{m-1}(x^2+y^2)^{-m/2}$$
$$-(m/2)2x e^{-\alpha x^2}(x+iy)^m(x^2+y^2)^{-m/2-1}\Big]$$

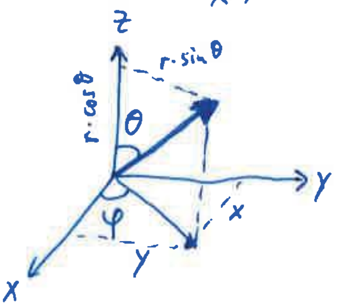
$$= -i\hbar A e^{-\alpha(x^2+y^2+z^2)}(x+iy)^m(x^2+y^2)^{-m/2}\cdot\left[\cancel{-2\alpha xy} + \frac{imx}{x+iy} - \cancel{\frac{mxy}{x^2+y^2}} + \cancel{2\alpha xy} - \frac{my}{x+iy} + \cancel{\frac{mxy}{x^2+y^2}}\right]$$

$$= -i\hbar A e^{-\alpha(x^2+y^2+z^2)}(x+iy)^m(x^2+y^2)^{-m/2}\cdot im$$

$$\underline{\underline{= m\hbar|\psi\rangle}}$$

<u>Alternatively</u>: use spherical coordinates! $r = \sqrt{x^2+y^2+z^2}$, $\varphi = \arctan\left(\frac{y}{x}\right)$

$\theta = \arctan\left(\frac{z}{\sqrt{x^2+y^2}}\right)$



⇒ use (x,y) plane as complex plane

→ $x+iy = r\cdot\sin(\theta)\cdot e^{i\varphi}$

$x^2+y^2 = z^2\cdot\tan^2(\theta)$

$$\Rightarrow \psi = A\cdot e^{-\alpha r^2}\cdot\underbrace{e^{im\varphi}\cdot r^m\cdot\sin^m\theta}_{(x+iy)^m}\cdot\underbrace{[z\cdot\tan(\theta)]^{-m}}_{(x^2+y^2)^{-m/2}} = A\cdot e^{-\alpha r^2}e^{im\varphi}r^m\cdot\sin^m(\theta)\cdot\underbrace{\cancel{r^{-m}\cos^{-m}(\theta)}}_{z^{-m}}\cdot\left(\frac{\sin\theta}{\cancel{\cos\theta}}\right)^{-m}$$

$$= A\cdot e^{-\alpha r^2}\cdot e^{im\varphi}$$

The z-component of the angular momentum operator reads

$L_z = -i\hbar\frac{\partial}{\partial\varphi}$ (from any text book or by direct calculation)

$\Rightarrow \underline{\underline{L_z|\psi\rangle}} = -i\hbar\frac{\partial}{\partial\varphi}\left[A e^{-\alpha r^2}e^{im\varphi}\right] = -i\hbar A e^{-\alpha r^2}\cdot(im)\cdot e^{im\varphi} = \underline{\underline{\hbar m\cdot|\psi\rangle}}$ (as above)

Expectation value: $\underline{\underline{\langle\psi|L_z|\psi\rangle}} = \langle\psi|\underset{\substack{\uparrow\\ \text{number!}}}{m\hbar}|\psi\rangle = m\hbar\underbrace{\langle\psi|\psi\rangle}_{\text{normalized}} \underline{\underline{= m\hbar}}$

(iii) From (ii) we have $L_z|\psi\rangle = m\hbar|\psi\rangle$, so $|\psi\rangle$ is an eigenstate of L_z with eigenv. $m\hbar$.

Physics III

4 We want to show that $[\hat{p}^2, \hat{L}_z] = 0$, i.e. that $\hat{p}^2$ and $\hat{L}_z$ commute. This could be done easily by looking up some algebraic relations, but we calculate this explicitly here in real space:

$$\hat{L}_z = -i\hbar\,(x\partial_y - y\partial_x) \quad ; \quad \hat{p}^2 = \left[-i\hbar\begin{pmatrix}\partial_x\\ \partial_y\\ \partial_z\end{pmatrix}\right]^*\left[-i\hbar\begin{pmatrix}\partial_x\\ \partial_y\\ \partial_z\end{pmatrix}\right] = \hbar^2(\partial_x^2+\partial_y^2+\partial_z^2)$$

$$\Longrightarrow \underline{\underline{[\hat{p}^2, \hat{L}_z]}} = -i\hbar^3\left[\partial_x^2+\partial_y^2+\partial_z^2,\ x\partial_y - y\partial_x\right]$$

$$+\partial_z^2(x\partial_y - y\partial_x)$$

$$= -i\hbar^3\{\partial_x^2(x\partial_y) - \partial_x^2(y\partial_x) + \partial_y^2(x\partial_y) - \partial_y^2(y\partial_x) - x\partial_y(\partial_x^2) - x\partial_y(\partial_y^2) - x\partial_y(\partial_z^2) + y\partial_x(\partial_x^2) + y\partial_x(\partial_y^2) + y\partial_x(\partial_z^2)\}$$

$$= -i\hbar^3\{\partial_x(\partial_y + x\partial_x\partial_y) - y\partial_x^3 \cancel{+ x\partial_x^3} - \partial_y(\partial_x + y\partial_y\partial_x) - x\partial_x^2\partial_y \cancel{- x\partial_x^3} \cancel{- x\partial_y\partial_z^2} + y\partial_x^3 + y\partial_x\partial_y^2 \cancel{+ y\partial_x\partial_z^2} \cancel{+ x\partial_y\partial_z^2} \cancel{- y\partial_x\partial_z^2}\}$$

$$= -i\hbar^3\{\cancel{\partial_x\partial_y} \cancel{+ \partial_x\partial_y} \cancel{+ x\partial_x^2\partial_y} - y\partial_x^3 \cancel{+ x\partial_y^3} \cancel{- \partial_x\partial_y} \cancel{- \partial_x\partial_y} - y\partial_x\partial_y^2 \cancel{- x\partial_x^2\partial_y} + y\partial_x^3 + y\partial_x\partial_y^2\}$$

$$\underline{\underline{= 0}}$$