$\cdot\ L_z = -i\hbar \frac{d}{d\varphi}$

$$\langle L_z\rangle = \frac{-i\hbar\, 3}{8\pi}\int_{-1}^{1}\int_{0}^{2\pi}\Big(\overset{0}{c_\theta} - \frac{1}{\sqrt{2}}\, s_\theta e^{-i\varphi}\Big)\frac{-i}{\sqrt{2}}\, s_\theta e^{i\varphi}\, d\varphi\, dc_\theta$$

$$= \frac{3\hbar\cdot \cancel{2\pi}}{8\cancel{\pi}\cdot \cancel{2}}\cdot\int_{-1}^{1}(1-c_\theta^2)\,dc_\theta = \frac{3\hbar}{8}\Big(\underbrace{2-\frac{2}{3}}_{4/3}\Big) = \frac{\hbar}{2}.$$

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Do enakih rezultatov lahko pridemo z uporabo relacij za lastna stanja. Velja:

$$\int_\Omega Y^*_{l'm'}\,\hat{L}_x\,Y_{lm} = \frac{\hbar}{2}\sqrt{l(l+1)-m(m\pm 1)}\;\delta_{l'l}\,\delta_{m'm\pm 1}$$

$$\int_\Omega Y^*_{l'm'}\,\hat{L}_y\,Y_{lm} = \mp\frac{i\hbar}{2}\sqrt{l(l+1)-m(m\pm 1)}\;\delta_{l'l}\,\delta_{m'm\pm 1}$$

Ti integrali so neničelni le kadar se $m$ spremeni za $\pm 1$. Za operatorja $L_z$ in $L^2$ dobimo nazaj $Y_{lm}$ ker so to lastne funkcije, torej velja:

$$\int Y^*_{l'm'}\,\hat{L}_z\,Y_{lm} = \hbar m\;\delta_{l'l}\,\delta_{m'm}$$

$$\int Y^*_{l'm'}\,\hat{L}^2\,Y_{lm} = \hbar^2 l(l+1)\;\delta_{l'l}\,\delta_{m'm}.$$

· sedaj lahko vstavimo $\psi = \frac{1}{\sqrt{2}}(Y_{10} + Y_{11})$ in dobimo

$$\langle L_x \rangle = \frac{1}{2} \int_\Omega (Y_{10}^* + Y_{11}^*) \hat{L}_x (Y_{10} + Y_{11})$$

$$= \frac{1}{2} \Big( \int_\Omega \underset{m'}{Y_{10}^*} \hat{L}_x \underset{m}{Y_{11}} + Y_{11}^* \hat{L}_x Y_{10} \Big)$$

$$= \frac{1}{2} \Big( \frac{\hbar}{2}\sqrt{1(2) - 1\cdot 0} + \frac{\hbar}{2}\sqrt{2 - 0\cdot 1} \Big) = \frac{\hbar}{\sqrt{2}}.$$

$$\langle L_y \rangle = \frac{1}{2} \Big( \int_\Omega Y_{10}^* L_y Y_{11} + Y_{11}^* L_y Y_{10} \Big)$$

$$= \frac{1}{2} \frac{i\hbar}{2} \Big( +\sqrt{2 - 1\cdot 0} - \sqrt{2 - 0\cdot 1} \Big) = 0.$$

· Za $L_z$ in $L^2$ so neničelni členi le med $l = l'$ in $m = m'$

$$\langle L_z \rangle = \frac{1}{2} \int_\Omega Y_{10}^* \hat{L}_z Y_{10} + Y_{11}^* \hat{L}_z Y_{11}$$

$$= \frac{1}{2} \hbar (0 + 1) = \frac{\hbar}{2}.$$

$$\langle L^2 \rangle = \frac{1}{2} \int_\Omega Y_{10}^* \hat{L}^2 Y_{10} + Y_{11}^* \hat{L}^2 Y_{11}$$

$$= \frac{\hbar^2}{2} \Big( 1\cdot(1+1) + 1\cdot(1+1) \Big) = 2\hbar^2.$$

(55) Atom vodika v osnovnem stanju

$$\psi_{nlm}(r,\theta,\varphi) = \psi_{100}(r,\theta,\varphi) = \frac{1}{\sqrt{4\pi}}\, e^{-r/r_B}\, \frac{2}{r_B^{3/2}}$$

Povprečni radij dobimo iz:

$$\langle r\rangle = \int_V \psi^* r\, \psi\, dV = \frac{1}{4\pi} \underbrace{\int d\Omega}_{\int_{-1}^{1} d(\cos\theta)\int_0^{2\pi} d\varphi = 4\pi} \cdot \int_0^\infty r^3 dr\, e^{\overbrace{-2r/r_B}^{t}} \frac{4r}{r_B^3}$$

$$\frac{2r}{r_B} = t$$

$$dr = \frac{r_B}{2} dt$$

$$= \frac{4}{r_B^3} \int_0^\infty \left(\frac{r_B}{2}\right)^4 e^{-t}\, t^3\, dt$$

$$= \frac{r_B}{4} \underbrace{\Gamma(3+1)}_{3!} = \frac{3}{2} r_B .$$

Verjetnost, da se $e^-$ nahaja izven $\langle r\rangle$ pa je

$$P(r > \langle r\rangle) = \int_{\langle r\rangle}^{\infty} |\psi|^2 dV = \int_{\frac{3}{2}r_B}^{\infty} e^{-t}\, \frac{4}{r_B^3} \cdot r^2 dr$$

$$= \frac{1}{2}\int_3^\infty e^{-t}\, t^2 dt = \frac{1}{2}\int_0^\infty e^{-(x+3)} (x+3)^2 dx$$

spravimo na 0 z $x = t-3$

$$= \frac{e^{-3}}{2}\left(\int x^2 e^{-x} + 6x e^{-x} + 9 e^{-x} dx\right) = \frac{e^{-3}}{2}\left(2! + 6 + 9\right)$$

$$= \frac{17}{2} e^{-3} = 0{,}42.$$

57 $n=2$, $l=1$, $m=0$ $\qquad r_B = \frac{\hbar c}{\alpha m c^2}$

$$\psi_{210} = \frac{1}{\sqrt{32\pi r_B^3}} \left(\frac{r}{r_B}\right) e^{-r/2r_B} \cos\Theta$$

$\langle V \rangle = ?$ Primerjaj z Bohrovim modelom.

$$\hat{V} = -\frac{\alpha}{\hbar c} \frac{\hat{1}}{r}$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{16\cancel{32}\pi r_B^3} \cdot \cancel{2\pi} \int_0^\infty \left(\frac{r}{r_B}\right)^2 e^{-\overbrace{r/r_B}^{=t}} \frac{1}{\cancel{r}} r^{\cancel{2}} dr \underbrace{\int_{-1}^{1} c_\Theta^2 \, dc_\Theta}_{2/3}$$

$$= \frac{1}{8\cancel{16} r_B^{\cancel{3}}} \cancel{r_B^2} \underbrace{\int_0^\infty t^3 e^{-t} dt}_{} \cdot \frac{\cancel{2}}{3}$$

$$= \frac{1}{24 r_B} \cdot 3! = \frac{1}{4 r_B} \Rightarrow \langle V \rangle = -\frac{\alpha \hbar c}{4 r_B} = -\left(\frac{\alpha}{2}\right)^2 mc^2$$

<u>Bohrov</u> model predpostavi da je $2\pi r = n\lambda$ in

$\lambda = \frac{h}{p}$ oziroma $p = \frac{h}{\lambda} = \frac{nh}{2\pi r} = \frac{n\hbar}{r}$

potem predpostavi da je $F_c = F_e$

$$\frac{mv^2}{r} = \frac{p^2}{m\cancel{r}} = \frac{\alpha \hbar c}{r^2} \quad (F = -\nabla V) \quad \text{oz.:} \quad \frac{(n\hbar)^2}{m r^{\cancel{3}}} = \frac{\alpha \hbar c}{\cancel{r^2}}$$

in $\langle V \rangle_{Bohr} = -\frac{\alpha \hbar c}{r} \simeq -\frac{\alpha \hbar c}{n^2 r_B}$ $\Rightarrow r = n^2 \frac{\hbar c}{\alpha m c^2} = n^2 r_B$

$\xrightarrow{n=2} -\frac{\alpha^2}{4} mc^2$ SE SKLADA!

# Virialni teorem za osnovno stanje atoma H

$n=1$, $l=0$

$$2\langle T\rangle = a\langle V\rangle \quad , \quad V = \alpha r^a$$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} - \frac{\alpha\hbar c}{r} \quad , \quad \hat{p}^2 = -\hbar^2\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{\hat{l}^2}{2mr} \xrightarrow{l=0} 0$$

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

$$\langle T\rangle = \int_0^\infty \psi^* \left(-\frac{\hbar^2}{2m}\right)\left(\psi'' + \frac{2}{r}\psi'\right) 4\pi r^2 dr$$

$$= -\frac{\hbar^2}{\cancel{2}m}\frac{\cancel{4}2}{r_B^3}\int_0^\infty e^{-r/r_B}\left(\frac{(-1)^2}{r_B} + \frac{2}{r}\left(-\frac{1}{r_B}\right)\right)e^{-r/r_B} r^2 dr$$

$$= -\frac{2\hbar^2}{m r_B^5}\int_0^\infty e^{-\overbrace{2r/r_B}^{=t}}\left(1 - 2\frac{r_B}{r}\right) r^2 dr$$

$$= \frac{2\hbar^2}{m r_B^5}\int_0^\infty e^{-t}\left(\frac{4}{t} - 1\right)\left(\frac{r_B}{2}\right)^3 t^2 dt \quad , \quad r_B = \frac{\hbar c}{\alpha mc^2}$$

$$= \frac{\hbar^2}{4mr_B^2}\int_0^\infty \underbrace{(4t - t^2)e^{-t}dt}_{4-2=2} = \frac{\hbar^2 c^2}{2mc^2 r_B^2} = \frac{\alpha^2 mc^2}{2}$$

$$\langle V\rangle = -\alpha\hbar c\int \psi^* \frac{1}{r}\psi\, dV = -\alpha\hbar c\frac{4}{r_B^3}\int_0^\infty e^{-2r/r_B}\cancel{\frac{1}{r}} r^{\cancel{2}} dr$$

$$= -\alpha\hbar c\frac{\cancel{4}}{r_B^{\cancel{3}}}\int_0^\infty e^{-t} t\, dt \left(\frac{r_B}{\cancel{2}}\right)^{\cancel{2}} = -\alpha\hbar c\frac{1}{r_B} = -\alpha^2 mc^2$$

$$a = -1 \; : \; 2\langle T\rangle = -\langle V\rangle \quad \text{in} \quad \cancel{2}\frac{\alpha^2 mc^2}{\cancel{2}} = +(+\alpha^2 mc^2) \checkmark$$

Določi nedoločenost $\delta r\, \delta p$ za atom - H v $\psi_{100}$.

$$\langle p \rangle = 0 \quad , \quad \langle p^2 \rangle = 2m \langle T \rangle = \cancel{2m} \frac{\hbar^2}{\cancel{2m} r_B^2} = \left(\frac{\hbar}{r_B}\right)^2$$

$$\langle r^a \rangle = \frac{4}{r_B^3} \int_0^\infty e^{-2r/r_B} \, r^a \, r^2 dr$$

$$= \frac{4}{r_B^3} \int_0^\infty e^{-t} \left(\frac{r_B}{2}\right)^{a+3} t^{a+2} dt$$

$$= \frac{r_B^{\,a}}{2^{a+1}} (a+2)!$$

$$\langle r \rangle = \frac{r_B}{2^2} 3! = \frac{3 r_B}{2} \quad , \quad \langle r^2 \rangle = \frac{r_B^2}{2^3} 4! = \frac{3 r_B^2}{1}$$

$$\delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} = r_B \sqrt{3 - \frac{9}{4}} = \frac{\sqrt{3}}{2} r_B$$

$$\delta r\, \delta p = \frac{\sqrt{3}}{2} \cancel{r_B} \frac{\hbar}{\cancel{r_B}} = \frac{\hbar}{2} \cdot \sqrt{3}$$