b) Uporabimo zveze med lastnimi stanji:

$$\int_\Omega Y^*_{l'm'} \hat{L}_x Y_{lm} = \frac{\hbar}{2} \sqrt{l(l+1) - m(m \pm 1)}\, \delta_{l'l}\, \delta_{m'm\pm1},$$

$$\int_\Omega Y^*_{l'm'} \hat{L}_y Y_{lm} = \mp \frac{i\hbar}{2} \sqrt{l(l+1) - m(m \pm 1)}\, \delta_{l'l}\, \delta_{m'm\pm1},$$

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

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

$$\psi = \frac{1}{\sqrt{2}} (Y_{10} + Y_{11})$$

$$\langle L_z \rangle = \frac{1}{2} \left( \int_\Omega Y_{10}^* \hat{L}_z Y_{10} + Y_{11}^* \hat{L}_z Y_{11} \right) = \frac{\hbar}{2} (0+1) = \frac{\hbar}{2},$$

$$\langle L^2 \rangle = \frac{1}{2} \left( \int_\Omega Y_{10}^* \hat{L}^2 Y_{10} + Y_{11} \hat{L}^2 Y_{11} \right) = \frac{\hbar^2}{2} (1 \cdot 2 + 1 \cdot 2) = 2\hbar^2.$$

V obeh primerih smo izpustili mešane člene, ker $\delta_{l'l} = \delta_{10} = 0$.

Pri $\langle L_{x,y} \rangle$ so ravno ti mešani členi različni od nič; dobimo:

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

$$= \frac{1}{2} \frac{\hbar}{2} \Big( \underbrace{\sqrt{2 - 1(1-1)}}_{m'=0,\ m=1,\ \ominus} + \underbrace{\sqrt{2 - 0\cdot(0+1)}}_{m'=1,\ m=0,\ \oplus} \Big) = \frac{\hbar}{\sqrt{2}},$$

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

$$= \frac{i\hbar}{4} \left( +\sqrt{2} - \sqrt{2} \right) = 0.$$

# Atom vodika – radialni del

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \quad , \quad \hat{V} = -\frac{\alpha \hbar c}{r} = -\alpha \hbar c \, \hat{\frac{1}{r}}$$

kjer je: $$\hat{p}^2 = -\hbar^2 \left( \frac{d}{dr^2} + \frac{2}{r}\frac{d}{dr} \right) + \frac{\hat{l}^2}{2mr^2}$$

lastne energije: $$E_n = -\frac{\alpha^2 mc^2}{2}\frac{1}{n^2}$$

lastne funkcije: $$\psi_{nlm} = R_{nl}(r)\, Y_{lm}(\theta, \varphi)$$

$$R_{nl} = \sqrt{\left(\frac{2}{n r_B}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}}\; e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \, , \quad \rho = \frac{2r}{n r_B}$$

kjer: $r_B = \dfrac{\hbar c}{\alpha mc^2}$ ... Bohrov radij.

Seveda: $$\int_0^\infty R_{n'l'}(r)\, R_{nl}(r)\, r^2 \, dr = \delta_{n'n} .$$

Par funkcij:
$$R_{10} = \frac{1}{2\sqrt{2}\, r_B^{3/2}} \left(2 - \frac{r}{r_B}\right) e^{-\frac{r}{2r_B}} ,$$
$$R_{20} = \frac{1}{2\sqrt{6}\, r_B^{3/2}} \left(2 - \frac{r}{r_B}\right) e^{-\frac{r}{2r_B}} ,$$
$$R_{21} = \frac{1}{2\sqrt{6}\, r_B^{3/2}} \frac{r}{r_B} e^{-\frac{r}{2r_B}} .$$

55 Osnovno stanje : $\psi_{00} = \underbrace{\frac{1}{\sqrt{4\pi}}}_{Y_{00}} \underbrace{\frac{2}{r_B^{3/2}} e^{-r/r_B}}_{R_{10}}$

Zanima nas povprečni radij

$$\langle r \rangle = \int \psi_{100}^* \, r \, \psi_{100} \, dV$$

$$= \frac{1}{\cancel{4\pi}} \underbrace{\int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\varphi}_{\cancel{4\pi}} \int_0^\infty dr \, r^2 \frac{4}{r_B^3} e^{-\overbrace{2r/r_B}^{t}} \cdot r$$

$$= \frac{r_B}{4} \underbrace{\int_0^\infty dt \, t^3 e^{-t}}_{\Gamma(4) = 3!} = \frac{3 \cdot \cancel{2} \, r_B}{\cancel{4}2} = \frac{3}{2} r_B .$$

Sedaj, ko imamo povprečni radij, lahko dobimo verjetnost, da se $e^-$ nahaja izven $\langle r \rangle$ :

$$P(r > \langle r \rangle) = \int_{\langle r \rangle}^{\infty} |\psi|^2 dV = \int_{3/2 r_B}^{\infty} \int \overbrace{\cancel{d\Omega}}^{4\pi} \, r^2 dr \, \frac{1}{\cancel{4\pi}} \frac{4}{r_B^3} e^{-\overbrace{2r/r_B}^{t}}$$

$$= \frac{1}{2} \int_3^\infty dt \, t^2 e^{-t} \quad , \; x = t - 3$$

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

$r = \frac{3}{2} r_B , \; t = 3$

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

$$= \frac{e^{-3}}{2} \left( \int_0^\infty dx \, (x^2 + 6x + 9) e^{-x} \right)$$

$$= \frac{e^{-3}}{2} (2! + 6 + 9) = \frac{17}{2} e^{-3} = \underline{0{,}42} .$$

57) Poglejmo si prvo vzbujeno stanje:

$$n=2,\quad l=1,\quad m=0,\quad \psi_{210} = \frac{1}{\sqrt{32\pi r_B^3}}\left(\frac{r}{r_B}\right)e^{-\frac{r}{2r_B}}\cos\theta,$$

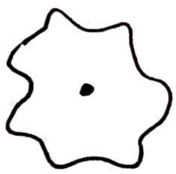
$$V = -\frac{\alpha\hbar c}{r},\quad \alpha = \frac{1}{137},\quad \hbar c = 200\ \mathrm{eV\,nm}$$

* Kvantnomehanski račun:

$$\left\langle \frac{1}{r}\right\rangle = \frac{1\ r_B^{\cancel{3}}}{\underset{16}{\cancel{32\pi}}\ \cancel{r_B^3}\, r_B}\underbrace{\int_0^{2\pi} d\varphi}_{\cancel{2\pi}}\ \underbrace{\int_{-1}^{1} d(\cos\theta)\cos^2\theta}_{\frac{2}{3}}\ \underbrace{\int_0^{\infty}\frac{dr}{r_B}\frac{r^2}{r_B^2}\left(\frac{r}{r_B}\right)^2 e^{-r/r_B}\frac{1}{r}}_{3!}$$

$$= \frac{\cancel{1}}{4\cancel{16}\cdot\cancel{3}}\cdot\cancel{3!}\ \frac{1}{r_B} = \frac{1}{4r_B} \Rightarrow \langle V\rangle = -\frac{\alpha\hbar c}{4r_B}$$

- in če uporabimo $r_B = \frac{\hbar c}{\alpha mc^2} \Rightarrow \langle V\rangle = -\left(\frac{\alpha}{2}\right)^2 mc^2.$

* Bohrov model:  $2\pi r = n\lambda,\quad \lambda = \frac{h}{p}$

De Broglie: $p = \frac{h}{\lambda} = \frac{\cancel{2\pi}\hbar n}{\cancel{2\pi} r} = \frac{n\hbar}{r},$

$$F_c = F_c \Rightarrow \frac{mv^2}{r} = \frac{p^2}{mr} = \frac{\alpha\hbar c}{r^2}\quad \text{ali: } \frac{(n\hbar)^2}{m\cancel{r^2}r} = \frac{\alpha\hbar c}{\cancel{r^2}}$$

$$\Rightarrow r_{\substack{\text{Bohrov}\\\text{model}}} = \frac{n^2\hbar^{\cancel{2}}c}{\alpha\cancel{\hbar}c^2 m} = n^2 r_B \Rightarrow \langle V\rangle_{\substack{\text{Bohr}\\\text{model}}} = -\frac{\alpha\hbar c}{r_{\substack{\text{Bohr}\\\text{model}}}} = -\frac{\alpha\hbar c}{n^2 r_B}$$

za $n=2 \Rightarrow \langle V\rangle_{\substack{\text{Bohr}\\\text{model}}} = -\frac{\alpha\hbar c}{4r_B}.$

∘ Poglejmo si še <u>virialni</u> <u>teorem</u> za atom H

$$V = a\, r^{p} \Rightarrow 2\langle T\rangle = p\,\langle V\rangle$$

dve konstanti

atom H : $\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} - \frac{\alpha\hbar c}{r}$

$$\hat{p}^2 = -\hbar^2\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \cancel{\frac{\hat{l}^2}{2mr^2}}^{\,\to 0},$$ osn. stanje $n=1,\ l=0,\ m=0$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\int dV\, \psi_{100}\left(\frac{d^2\psi_{100}}{dr^2} + \frac{2}{r}\frac{d\psi_{100}}{dr}\right)$$

$$\psi_{100} = \frac{1}{\sqrt{4\pi}}\, e^{-\frac{r}{r_B}}\, \frac{2}{r_B^{3/2}},\quad \psi_{100}' = \frac{2}{\sqrt{4\pi}\, r_B^{3/2}}\left(-\frac{1}{r_B}\right)e^{-\frac{r}{r_B}}$$

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

$r = \frac{r_B}{2}t,\ dr = \frac{r_B}{2}dt$

⇓

$$\langle T\rangle = -\frac{\hbar^2}{\cancel{2}m}\,\frac{\cancel{2}\cancel{4}\cdot \cancel{4\pi}}{\cancel{4\pi}\, r_B^3}\int_0^\infty dr\, r^2\, e^{-\overset{=t}{2r/r_B}}\left(\frac{1}{r_B^2} + \frac{2}{r}\left(-\frac{1}{r_B}\right)\right)$$

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

$$= -\frac{2\hbar^2\cancel{r_B^3}}{48\, m\, \cancel{r_B^3}\, r_B^2}\int_0^\infty dt\,(t^2 - 4t) = \frac{\hbar^2}{4m r_B^2}\underbrace{\int_0^\infty dt\,(4t - t^2)}_{4\cdot 1! - 2! = 2}$$

$$= \frac{\hbar^2\cancel{2}}{2\cancel{4}m r_B^2} = \frac{\cancel{\hbar^2}\,\alpha^2 m^2 c^{4\,2}}{2m\cancel{(\hbar c)^2}} = \frac{\alpha^2 m c^2}{2}.$$

Sedaj napravimo še podoben račun za $\langle V\rangle$ ↗