Imamo e^- v H atomu; je v stanju s kv. št. 211. Kakšna je valovna funkcija tega stanja v atm., kje je ρ najmanjša, kakšna je povprečna radialna verjetnostna gostota na jedru in kje je največja? Kakšna je $\rho\, e^-$ 1,5 atm. stran od jedra pri $\varphi=60°$ in $\vartheta=75°$? Kolikšna je povprečna vrednost radija?

$n=2$
$l=1$
$m=1$

$$E_2 = \frac{-13{,}6\,eV}{4} = \underline{-3{,}4\,eV} \quad \} \text{ vsota kin. in pot. energije}$$

$$\sqrt{\langle \hat{L}^2 \rangle} = \sqrt{(l+1)l\,\hbar^2} = \underline{\sqrt{2}\,\hbar} \quad \} \text{ velikost vrt. količine}$$

$$\langle \hat{L}_z \rangle = m\hbar = \underline{\hbar} \quad \} \text{ projekcija vrt. količine}$$

$$\Psi_{nlm} = R_{nl} Y_{lm} = R_{12} Y_{11}$$

Merimo v atm:

$\boxed{r = x\, a_0}$ pretvorba v atm

$\underline{\frac{r}{a_0} = x}$

$$R_{21}\ (\text{v učbeniku}) = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{\frac{3}{2}} \frac{r}{a_0}\, e^{-\frac{r}{2a_0}}$$

$$Y_{11} = \sqrt{\frac{3}{4}}\, \sin\vartheta \frac{1}{\sqrt{2\pi}} e^{i\varphi}$$

$$R_{21} = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{\frac{3}{2}} x\, e^{-\frac{x}{2}}$$

val. f. v atm

$$\Psi_{211} = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{\frac{3}{2}} x\, e^{-\frac{x}{2}} \cdot \sqrt{\frac{3}{4}} \sin\vartheta \frac{1}{\sqrt{2\pi}} e^{i\varphi}$$

$$\rho_{211} = \underline{\Psi^*_{211}}\, \Psi_{211} = \frac{1}{\cancel{3}}\left(\frac{1}{2a_0}\right)^{3} x^2 e^{-x} \cdot \frac{\cancel{3}}{4} \sin^2\vartheta \frac{1}{2\pi} =$$

konjugirana vrednost

(vse kar nima i-ja je na kvadrat; drugo se pokrajša)

$$= \frac{1\, x^2 e^{-x} \sin^2\vartheta}{64\,\pi} \rightarrow \rho \text{ je najmanjša} \Rightarrow \underline{\rho = 0}$$

Kje je ρ 0?

1) $x = 0$
2) $x \to \infty$
3) $\vartheta = 0$
4) $\vartheta = 180°$

211 = p_x orbitala

$$\frac{dw}{dr} = r^2 R_{nl}^2 = x^2 \cdot a_0^2\, \frac{1}{3}\left(\frac{1}{2a_0}\right)^3 x^2 e^{-x} =$$

$$= \frac{1}{24} \cdot \frac{1}{a_0} \cdot x^4 e^{-x} = \boxed{0}$$

pov. rad. verjetnost

povprečna rad. verjetnostna gostota je 0, saj je na jedru $r=0$

največja $\frac{dw}{dr}$: $\left(\frac{1}{24}\frac{1}{a_0}x^4 e^{-x}\right)' = 0$ odvod je $0 \Rightarrow$ iščemo max

$$4x^3e^{-x} - e^{-x}x^4 = 0$$

$$e^{-x}(4x^3 - x^4) = 0$$

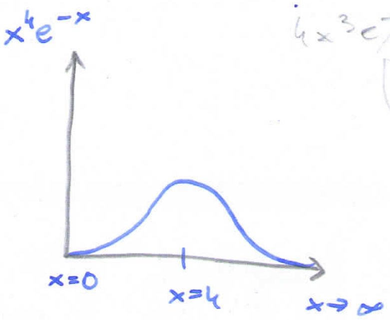
$4x^3 e^{-x} = e^{-x}x^4$

$\boxed{4 = x}$

$x = \infty$

$x = 0$

$\boxed{x = 4}$ max



$x = 1{,}5$

$\varphi = 60^\circ$

$\vartheta = 75^\circ$

$\rho(x, \vartheta, \varphi) = ?$

$$\rho_{211} = \frac{1}{64\pi (0{,}529 \cdot 10^{-10}\,m)^3} \cdot 1{,}5^2 \cdot e^{-1{,}5} \cdot \sin^2 75^\circ = 1{,}57 \cdot 10^{28}\,m^{-3}$$

v atm: $\rho_{211} = \frac{1}{64\pi} 1{,}5^2 \cdot e^{-1{,}5} \sin^2 75^\circ \cdot \frac{1}{a_0^3} = 2{,}3 \cdot 10^{-3} a^{-3}$

št. e^- na volumen

radij:

$$\langle r \rangle = \langle \hat{r} \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^*_{nlm} \hat{r} \psi_{nlm} dV =$$

$$= \int_0^\infty \int_0^\pi \int_0^{2\pi} R_{nl} Y^*_{lm} r R_{nl} Y_{lm} r^2 dr \sin\vartheta d\vartheta d\varphi =$$

$$= \int_0^\infty \int_0^\pi \int_0^{2\pi} R^2_{nl} r^3 \boxed{Y^*_{lm} Y_{lm} \sin\vartheta d\vartheta d\varphi} dr =$$

$= 1$ - ortogonalnost (SPLOŠNA FORMULA)

$$= \int_0^\infty R^2_{nl} r^3 dr =$$

$$= \int_0^\infty \frac{1}{3}\left(\frac{1}{2a_0}\right)^3 \frac{r^2}{a_0^2} e^{-\frac{r}{a_0}} r^3 dr \overset{\text{Bronštejn}}{=}$$

$\int_0^\infty x^n e^{-ax} = \frac{n!}{a^{n+1}}$

$$= \frac{1}{3}\frac{1}{8}\frac{1}{a_0^3}\frac{1}{a_0^2}\int_0^\infty r^2 r^3 e^{-\frac{r}{a_0}} dr = \frac{1}{24a_0^5}\int_0^\infty r^5 e^{-\frac{r}{a_0}} dr =$$

$$\langle \hat{r} \rangle = \frac{1}{24a_0^5} \cdot \frac{5!}{a_0^{-6}} = \frac{5!}{24} a_0 = 5a_0$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{24a_0^5}\int_0^\infty r^3 e^{-\frac{r}{a_0}} dr = \frac{3!}{24a_0^5 a^{-4}} = \frac{1}{4a_0}$$

$\boxed{\langle \hat{p}_x \rangle = \langle \hat{p}_y \rangle = \langle \hat{p}_z \rangle = 0}$; !

gib. kol.

$\boxed{V = \frac{-e_0^2}{4\pi\varepsilon_0 r} \quad \langle \hat{V} \rangle = \frac{-e_0^2}{4\pi\varepsilon_0}\left\langle \frac{1}{r} \right\rangle}$!

pot. E

$\boxed{\langle W_{kin} \rangle = E_n - \langle V \rangle}$ pov. kin. E