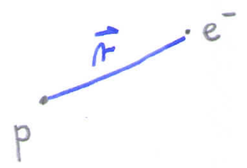
Kvantno mehanski model vodikovega atoma



$$\hat{H}\psi = E\psi$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(r)$$

$$V = \frac{-e_0^2}{4\pi\varepsilon_0 r}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-\frac{e_0^2}{4\pi\varepsilon_0 r}$$

$\vec{r} = (x, y, z)$

$r = \sqrt{x^2+y^2+z^2}$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)-\frac{e_0^2\psi}{4\pi\varepsilon_0\sqrt{x^2+y^2+z^2}} = E\psi \rightarrow$$

uvedemo sferične koordinate:

$x = r\sin\vartheta\cos\varphi$

$y = r\sin\vartheta\sin\varphi$

$z = r\cdot\cos\vartheta$

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)+\frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)-\frac{e_0^2}{4\pi\varepsilon_0 r}}$$

$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$ $\quad [\hat{H}, \hat{L}_z] = 0$, saj noben del $\hat{H}$ja nima spremenljivke φ!

$$\hat{H}\ \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2} \Rightarrow -\frac{\hbar^2}{2m}\frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2} = \frac{1}{2mr^2\sin^2\vartheta}\hat{L}_z^2$$

; ker $[\hat{L}_z^2, \hat{L}_z] = 0 \Rightarrow$

$$\left.\begin{aligned}&[\hat{H}, \hat{L}_z] = 0\\ &[\hat{H}, \hat{L}^2] = 0\end{aligned}\right\}$$ vedno velja, če $V \neq f(\vartheta, \varphi)$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\psi}{\partial\vartheta}\right)+\frac{1}{r^2\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right)-\frac{e_0^2}{4\pi\varepsilon_0 r}\psi = E\psi$$

$$\boxed{\psi(r,\vartheta,\varphi) = R(r)\,Y(\vartheta,\varphi)}$$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)\right) - \frac{\hbar^2}{2mr^2}\underbrace{\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\psi}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right)}_{\hat{L}^2} - \frac{e_0^2}{4\pi\varepsilon_0 r}\psi = E\psi$$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)\right)+\frac{\hat{L}^2\psi}{2mr^2}-\frac{e_0^2\psi}{4\pi\varepsilon_0 r} = E\psi$$

, kjer je $\psi = RY$

$$= -\frac{\hbar^2}{\cancel{YR}\,2m}\frac{\cancel{Y}}{\cancel{r^2}}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{\cancel{R}\hat{L}^2\cancel{r^2}Y}{\cancel{YR}\,2m\cancel{r^2}}-\frac{e_0^2\cancel{RY}r}{\cancel{YR}\,4\pi\varepsilon_0\cancel{r}} = \frac{E\cancel{RY}r^2}{\cancel{YR}} \quad \Big/ \cdot r^2,\ : YR$$

$$= \underbrace{-\frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-\frac{e_0^2 r}{4\pi\varepsilon_0}-Er^2}_{f(r)} = \underbrace{-\frac{\hat{L}^2Y}{2mY}}_{g(\vartheta,\varphi)}$$

$$\frac{-\hat{L}^2 Y}{2mY} = j \qquad -\frac{\hat{L}^2 Y}{2m} = jY \nearrow Y_{l,m}$$

$$[\hat{L}^2, \hat{H}] = 0 \qquad [\hat{L}_z, \hat{H}] = 0$$

$$\psi = R(r)\cdot Y_{l,m}(\theta,\varphi)$$

$$\hat{L}_z\psi = \hat{L}_z R(r) Y_{l,m}(\theta,\varphi) =$$

$$= R(r)\hat{L}_z Y_{l,m} =$$

$$= R(r)\, m\hbar\, Y_{l,m} =$$

$$\boxed{\hat{L}_z\psi = m\hbar R(r) Y_{l,m}}$$

$$R_{nl} = C x^l \cdot e^{-\frac{x}{2}} L^{2l+1}_{n+l}(x)$$

Laguerrovi polinomi

$$x = \frac{2me_0^2}{n\hbar^2 4\pi\varepsilon_0} r$$

$$L^{2l+1}_{n+l} = \frac{x^{-(2l+1)}e^{x}}{(n+1)!}\,\frac{d^{n+l}\left(e^{-x}x^{n+l+2\,+1}\right)}{dx^{n+l}}$$

$n \in \mathbb{N} = \{1,2,3\ldots\}$

$n \geq l+1$

$-l \leq m \leq l$

$$\boxed{E_n = \frac{-me_0^4}{2n^2(4\pi\varepsilon_0)^2\hbar^2} = -\frac{13{,}6\,eV}{n^2}}$$

ujemanje z Bohrovim modelom atoma

$\boxed{n=1}$, saj $n \geq l+1$

$l=0$ $\quad -l \leq m \leq l$

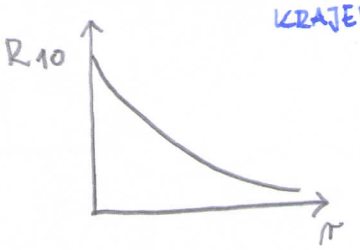
$m=0$

$\Downarrow$

$$Y_{00} = \frac{1}{\sqrt{2}\sqrt{2\pi}}$$

$$R_{10} = 2\cdot\left(\frac{1}{a_0}\right)^{\frac{3}{2}}\cdot e^{-\frac{r}{a_0}} \quad ; \quad a_0 = \frac{me_0^2}{4\pi\varepsilon_0\hbar^2}$$

KRAJEVNI DEL



$$\psi_{100} = R_{10}\cdot Y_{00} = 2\cdot\left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-\frac{r}{a_0}}\frac{1}{\sqrt{2}\sqrt{2\pi}}$$

$$E_{100} = E_{n=1} = \frac{-13{,}6\,eV}{n^2} = \underline{\underline{-13{,}6\,eV}}$$

$\boxed{n=2}$

$n \geq l+1$

$2 \geq l+1$

$1 \geq l$

$l=0$

$m=0$

$$R_{20} = 2\cdot\left(\frac{1}{a_0}\right)^{\frac{3}{2}}\left(1-\frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}$$

$$Y_{00} = \frac{1}{\sqrt{2}\sqrt{2\pi}}$$

$$\psi_{200} = R_{20}Y_{00}$$

$$E_{200} = E_{n=2} = \frac{-13{,}6\,eV}{4} = \underline{\underline{-3{,}4\,eV}}$$

1. vzbujeno stanje

$\boxed{n=2}$

$\ell = 1$

$m = -1, 0, 1$

$$\left.\begin{matrix} 2\,1\,1 \\ 2\,1\,0 \\ 2\,1\,-1 \end{matrix}\right\} \text{ isti } R(r)$$

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

$$\left.\begin{matrix} \psi_{211} = R_{21} Y_{11} \\ \psi_{210} = R_{21} Y_{10} \\ \psi_{21-1} = R_{21} Y_{1-1} \end{matrix}\right\} E_{211} = E_{210} = E_{21-1} = E_{200} = \underline{\underline{-3{,}4\,eV}}$$

Degeneracija $n=2$ je 4, saj imamo štiri valovne funkcije: $\psi_{200}, \psi_{211}, \psi_{210}, \psi_{21-1}$.

$\boxed{n=3}$ $\quad 3\ell \geq \ell+1$

$\ell = 0, 1, 2$

$$\left.\begin{matrix} n=3 \\ \ell=0 \\ m=0 \end{matrix}\right\} R_{30} = 2\left(\frac{1}{3a_0}\right)^{\frac{3}{2}}\left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right) e^{-\frac{r}{a_0}}$$

$$\psi_{300} = R_{30} Y_{00} \quad \Big\} \quad E_{300} = E_{n=3} = \frac{-13{,}6\,eV}{3^2} = \underline{\underline{-1{,}5\,eV}}$$

$$\left.\begin{matrix} n=3 \\ \ell=1 \\ m=-1,0,1 \end{matrix}\right\} R_{31} = \frac{4\sqrt{2}}{9}\left(\frac{1}{3a_0}\right)^{\frac{3}{2}} \frac{r}{a_0}\left(1 - \frac{r}{6a_0}\right) e^{-\frac{r}{3a_0}}$$

$$\left.\begin{matrix} \psi_{311} = R_{31} Y_{11} \\ \psi_{310} = R_{31} Y_{10} \\ \psi_{31-1} = R_{31} Y_{1-1} \end{matrix}\right\} E_{311} = E_{310} = E_{31-1} = E_{300} = \underline{\underline{-1{,}5\,eV}}$$

$n=3$

$\ell=2$

$m=-2,-1,0,1,2$

$$R_{32} = \left(\frac{2\sqrt{2}}{27\sqrt{5}}\right)\left(\frac{1}{3a_0}\right)^{\frac{3}{2}}\left(\frac{r}{a_0}\right)^2 e^{-\frac{r}{3a_0}}$$

$$\left.\begin{matrix} \psi_{32-2} = R_{32} Y_{2-2} \\ 3\psi_{32-1} = R_{32} Y_{2-1} \\ \psi_{320} = R_{32} Y_{20} \\ \psi_{321} = R_{32} Y_{21} \\ \psi_{322} = R_{32} Y_{22} \end{matrix}\right\} E_{32-2} = E_{32-1} = E_{320} = E_{321} = E_{322} = E_{300} = \underline{\underline{-1{,}5\,eV}}$$

Degeneracija $n=3$ je 9, saj imamo 9 valovnih funkcij.

n - gl. kv. število

$n =$ gl. kv. št. $\} \ 1, 2 \ldots$ DOLOČA ENERGIJO

$l =$ stransko oz. orbitalno kv. št. $\} \ n \geq l + 1$ DOLOČA OBLIKO STANJA V PROSTORU

$l = 0 \ \ldots \ s$ - sferično simetrična

$l = 1 \ \ldots \ p$ - usmerjeno v eno smer

$l = 2 \ \ldots \ d$ - v dve -||-

$l = 3 \ \ldots \ f$ - v tri -||-

$l = 4 \ \ldots \ g$ - v štiri -||-

$m =$ magnetno kv. št. $\} \ -l \leq m \leq l$

DOLOČA USMERITEV V PROSTORU

ψ_{100} 1s

ψ_{200} 2s

ψ_{210} $2p_z$

$\left.\begin{matrix}\psi_{211} \\ \psi_{21-1}\end{matrix}\right\}$ $\begin{matrix} 2p_x \\ 2p_y \end{matrix}$ lin. kombinacija

$$\langle \psi_{nlm} | \psi_{n'l'm'} \rangle = \delta_{nn'} \delta_{ll'} \cdot \delta_{mm'}$$

$$\langle \psi_{210} | \psi_{320} \rangle = 0$$

$$\langle \psi_{210} | \psi_{211} \rangle = 0$$

$$\langle \psi_{211} | \psi_{211} \rangle = 1$$

ψ_{nlm} so ORTOGONALNE

$\Downarrow$

če se razlikujejo v enem kv. št so PRAVOKOTNE ENA na DRUGO

$$\hat{H} \psi_{nlm} = E_{nlm} \psi_{nlm} = \boxed{E_n} \psi_{nlm}$$

$$\hat{L}^2 \psi_{nlm} = \hat{L}^2 R_{nl} Y_{lm} = R_{nl} \hat{L}^2 Y_{lm} = R_{nl} \cdot l(l+1) \hbar^2 Y_{l,m}$$

$$\hat{L}^2 \psi_{nlm} = l(l+1) \hbar^2 \psi_{nlm}$$

določa vrtilno količino

$$\hat{L}_z \psi_{nlm} = m \hbar \psi_{nlm}$$

$$\langle \psi_{nlm} | \psi_{n'l'm'} \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^*_{nlm} \psi_{n'l'm'} \cdot r^2 dr \sin\vartheta \, d\vartheta \, d\varphi$$

INTEGRIRAMO PO CELOTNEM PROSTORU

$$\psi^*_{nlm} = (R_{nl} Y_{lm})^* = R^*_{nl} Y^*_{lm} \Rightarrow \underline{R^*_{nl} = R_{nl}}$$ (R_{nl} so same $\mathbb{R}$ vrednosti)

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} R_{nl}^{(r)} \cdot Y^*_{l,m}(\vartheta,\varphi) \, R_{n'l'}^{(r)} Y_{l'm'}(\vartheta,\varphi) \, r^2 dr \sin\vartheta \, d\vartheta \, d\varphi$$

$$\int_0^\infty R_{nl} R_{n'l'} r^2 dr \int_0^\pi \int_0^{2\pi} Y^*_{l,m} Y_{l',m'} \sin\vartheta \, d\vartheta \, d\varphi$$

$$\left. \begin{aligned} \langle R_{nl} | R_{n'l'} \rangle &= \int_0^\infty R_{nl} R_{n'l'} r^2 dr \\ \langle Y_{lm} | Y_{l'm'} \rangle &= \int_0^\pi \int_0^{2\pi} Y^*_{lm} Y_{l'm'} \sin\vartheta \, d\vartheta \, d\varphi \end{aligned} \right\}$$ pogoji za normiranje

Vodikov atom

$\hat{H}\Psi = E\Psi$

$\Downarrow$

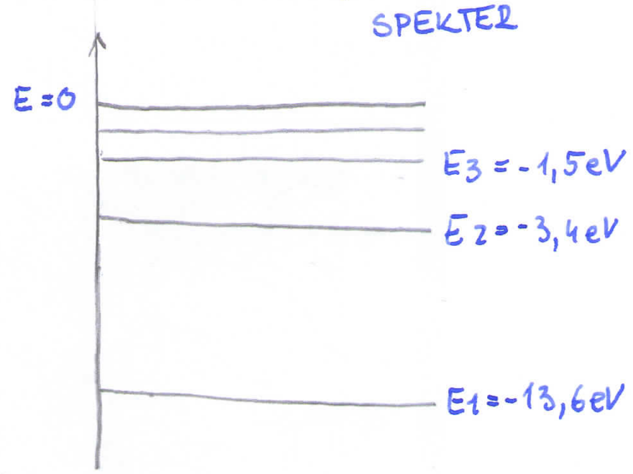
Ψ_{nlm}

$$E_n = -\frac{13{,}6\,\text{eV}}{n^2} \qquad n \in \mathbb{N}$$

$$n \geq l+1$$

$$-l \leq m \leq l$$

ENERGIJSKI SPEKTER



Ko je $E > 0 \Rightarrow$ delec NI VEZAN.

Valovne funkcije si ne moremo predstavljati, lahko pa si predstavljamo ELEKTRONSKO GOSTOTO.

$$\rho_{nlm} = |\Psi_{nlm}|^2 = \Psi^*_{nlm}\Psi_{nlm} = R^*_{nl} Y^*_{lm} R_{nl} Y_{lm} = R_{nl}^2 \, |Y_{lm}|^2 = f(r, \vartheta)$$

$$\boxed{Y_{lm} = g(\vartheta)\, e^{im\varphi}}$$

$$\boxed{Y^*_{lm} = g(\vartheta)\, e^{-im\varphi}}$$

$\Rightarrow$ ko zmnožimo, izgubimo odvisnost od spremenljivke φ

$$P(V) = \iiint \rho_{nlm}\, dV = \iiint \rho_{nlm}\, r^2 \sin\vartheta \, dr\, d\vartheta\, d\varphi =$$

$$= \iiint \underbrace{R_{nl}^2}_{\text{odvisna } (r)} \underbrace{|Y_{lm}|^2}_{\text{odvisna } (\vartheta)} r^2 dr \sin\vartheta\, d\vartheta\, d\varphi = \int r^2 R_{nl}^2\, dr \cdot \int |Y_{lm}|^2 \sin\vartheta\, d\vartheta \cdot \int d\varphi$$

Orbitala je definirana kot prostor, kjer lahko z 95% verjetnostjo trdimo, da se tu nahaja e^-.

$$\boxed{\frac{dw}{dr} \text{ - radialna verjetnostna gostota}}$$

$$\boxed{1 = \int_0^\infty \frac{dw}{dr}\, dr}$$

$$\underset{\text{ves prostor}}{P(V)} = 1 = \int_0^\infty r^2 R_{nl}^2\, dr \underbrace{\int_0^\pi |Y_{lm}|^2 \sin\vartheta\, d\vartheta \int_0^{2\pi} d\varphi}_{1} =$$

$$\langle Y_{lm} | Y_{l'm'} \rangle = \delta_{ll'}\, \delta_{mm'}$$

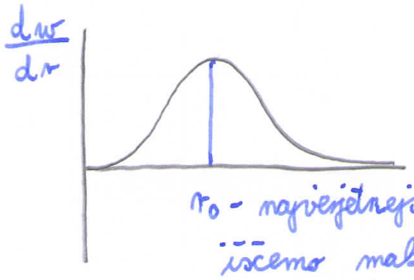
$$\int_0^\pi \int_0^{2\pi} Y^*_{lm} Y_{l'm'} \sin\vartheta\, d\vartheta\, d\varphi = 1$$

$$= \boxed{\int_0^\infty r^2 R_{nl}^2\, dr}$$

$$\boxed{r^2 R_{nl}^2 = \frac{dw}{dr}}$$

Zapišemo to za osnovno stanje $n=1$, $l=0$.

$$R_{10} = 2\left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-\frac{r}{a_0}}$$



$$\frac{dw}{dr} = r^2 4 \frac{1}{a_0^3} e^{-\frac{2r}{a_0}}$$

r_0 - najverjetnejši radij => iščemo maksimum => odvod = 0

$$\left(\frac{dw}{dr}\right)' = 4\cdot\frac{1}{a_0^3}\left(2re^{-\frac{2r}{a_0}} + r^2 e^{-\frac{2r}{a_0}}\left(-\frac{2}{a_0}\right)\right) = 0$$

$$4\cdot\frac{1}{a_0^3} e^{-\frac{2r}{a_0}} r \left(2 - \frac{2r}{a_0}\right) = 0$$

$r \to \infty$ //

$r = 0$ //

$\underline{r = a_0}$

Radij (najverjetnejši) je v osnovnem stanju ($n=1$, $l=0$) je enak BOHROVEM RADIJU.

Zanima nas pov. radij:

$$\langle\hat{r}\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \Psi_{nlm}^* \hat{r} \Psi_{nlm} r^2 dr \sin\vartheta d\vartheta d\varphi =$$

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

$$= \int_0^\infty r R_{nl}^2 r^2 dr \underbrace{\int_0^\pi \int_0^{2\pi} Y_{lm}^* Y_{lm} \sin\vartheta d\vartheta d\varphi}_{1} = \int_0^\infty r R_{nl}^2 r^2 dr$$

osnovno stanje:

$$\langle\hat{r}\rangle = \int_0^\infty r R_{10}^2 r^2 dr = \int_0^\infty r 4 \frac{1}{a_0^3} e^{-\frac{2r}{a_0}} r^2 dr = \frac{4}{a_0^3}\int_0^\infty r^3 e^{-\frac{2r}{a_0}} dr =$$

$$= \frac{4}{a_0^3} \frac{3!}{\left(\frac{2}{a_0}\right)^4} = \frac{\cancel{4}}{\cancel{a_0^3}} \frac{6 a_0^{\cancel{4}}}{2^{\cancel{4}2}} = \frac{6}{4} a_0 = \underline{\underline{\frac{3}{2} a_0}}$$ ~ ocena radija

gama integral:

$$\int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}}$$

$$\Gamma(n+1) = n!$$

$$\langle\hat{r}^2\rangle = \int_0^\infty r^2 R_{10}^2 r^2 dr = \int_0^\infty 4\cdot\frac{1}{a_0^3} r^4 e^{-\frac{2r}{a_0}} dr = \frac{4}{a_0^3}\cdot\frac{4!}{\left(\frac{2}{a_0}\right)^5} =$$

$$= \frac{\cancel{4}}{\cancel{a_0^3}}\cdot\frac{\cancel{4}\cdot 3\cdot\cancel{2}\cdot a_0^{\cancel{5}2}}{\cancel{2^5}} = \underline{\underline{3a_0^2}}$$

$$\sqrt{\langle\hat{r}^2\rangle} = \underline{\underline{\sqrt{3}\, a_0}}$$ - ocena radija

$$P(r<r_0) = \int_0^{r_0} R_{nl}^2 r^2 dr \underbrace{\int_0^{\pi}\int_0^{2\pi} |Y_{lm}|^2 \sin\vartheta \, d\vartheta \, d\varphi}_{1} = \int_0^{r_0} r^2 R_{nl}^2 dr$$

100 :

$$\int_0^{r_0} r^2 R_{10}^2 dr = \int_0^{r_0} r^2 \frac{4}{a_0^3} e^{-\frac{2r}{a_0}} dr = \frac{4}{a_0^3}\int_0^{r_0} r^2 e^{-\frac{2r}{a_0}} dr =$$ Bronštejn

$$= \frac{4}{a_0^3}\left(e^{-\frac{2r}{a_0}} \left(\frac{r^2}{\left(-\frac{2}{a_0}\right)} - \frac{2r}{\left(-\frac{2}{a_0}\right)^2} + \frac{2}{\left(-\frac{2}{a_0}\right)^3} \right) \right)\Big|_0^{r_0} =$$

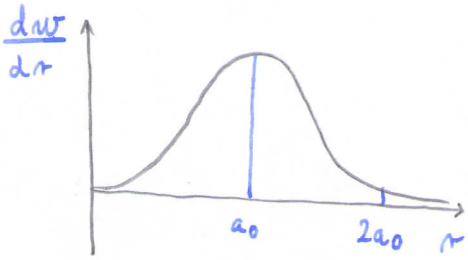
$$= e^{-\frac{2r}{a_0}}\left(-\frac{2r^2}{a_0^2} - \frac{2r}{a_0} - 1\right)\Big|_0^{r_0} = e^{-\frac{2r}{a_0}}\left(1 + \frac{2r}{a_0} + \frac{2r^2}{a_0^2}\right)\Big|_{r_0}^{0} =$$

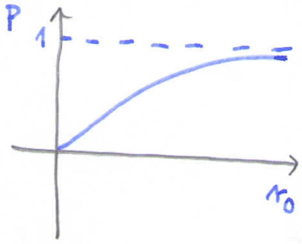
številke:

$r_0 = 2a_0$

$\underline{P = 0{,}76}$

$$= \underline{1 - e^{-\frac{2r_0}{a_0}}\left(1 + \frac{2r_0}{a_0} + \frac{2r_0^2}{a_0^2}\right)}$$



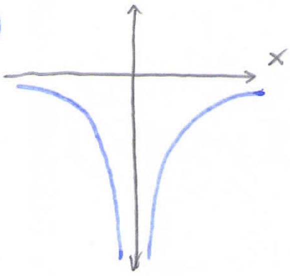


$$\boxed{0{,}95 = 1 - e^{-\frac{2r_0}{a_0}}\left(1 + \frac{2r_0}{a_0} + \frac{2r_0^2}{a_0^2}\right)}$$

ORBITALA

potrebno numerično izračunati

$\langle \hat{p}_x \rangle = 0$



$$\hat{p}^2 = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)$$

$$\psi_{100} = R_{10}\cdot Y_{00} = f(r)$$

$$\hat{p}^2\psi_{100} = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R_{10}Y_{00}}{\partial r}\right) + \cancel{\frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial R_{10}Y_{00}}{\partial\vartheta}\right)} + \cancel{\frac{1}{r^2\sin^2\vartheta}\frac{\partial^2 R_{10}Y_{00}}{\partial\varphi^2}}\right)$$

$$\hat{p}^2\psi_{100} = \frac{-\hbar^2 Y_{00}}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R_{10}\right)\right)$$

$$\langle\hat{p}^2\rangle = \int R_{10}Y_{00}^* \, \hat{p}^2 R_{10}Y_{00} \, dV$$

$$\langle\hat{p}^2\rangle = \int_0^{\infty} R_{10}\left(-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R_{10}\right)\right)\right) r^2 dr =$$

$$= -\frac{\hbar^2}{2m}\int \frac{2}{a_0^{\frac{3}{2}}} e^{-\frac{r}{a_0}}$$

$$= -\frac{\hbar^2}{2m}\int_0^\infty \frac{2}{a^{\frac{3}{2}}} e^{-\frac{r}{a_0}} \left(-\frac{2e^{-\frac{r}{a_0}}}{a_0^{\frac{5}{2}}}\left(\frac{2}{r}-\frac{1}{a_0}\right) r^2 dr\right) =$$

$$= \frac{\hbar^2}{2m}\frac{4}{a_0^4}\int_0^\infty e^{-\frac{2r}{a_0}}\left(2r^{-1}-\frac{1}{a_0}\right) r^2 dr =$$

$$= \frac{2\hbar^2}{m a_0^4}\int_0^\infty \left(2r^1 e^{-\frac{2r}{a_0}} - \frac{1}{a_0} r^2 e^{-\frac{2r}{a_0}}\right) dr =$$

gama integral $$= \frac{2\hbar^2}{m a_0^4}\left(2\frac{1!}{\left(\frac{2}{a_0}\right)^2} - \frac{1}{a_0}\frac{2!}{\left(\frac{2}{a_0}\right)^3}\right) =$$

$$= \frac{2\hbar^2}{m a_0^4}\left(\frac{a_0^2}{2} - \frac{a_0^2}{4}\right) =$$

$$= \frac{2\hbar^2}{m a_0^4}\frac{a_0^2}{4} = \boxed{\frac{\hbar^2}{2 m a_0^2} = \langle \hat{W}_k \rangle}$$

napaka pri računanju

13,6 eV

$\Downarrow$

$E_1 = -13{,}6\,\text{eV}$

$$\boxed{\langle \hat{p}^2 \rangle = \frac{\hbar^2}{a_0^2}}$$

$R_{10} = \frac{2}{a_0^{\frac{3}{2}}} e^{-\frac{r}{a_0}}$

$\frac{\partial R_{10}}{r} = \frac{-2}{a_0 a_0^{\frac{3}{2}}} e^{-\frac{r}{a_0}}$

$r^2 \frac{\partial R_{10}}{\partial r} = \frac{-2r^2}{a_0^{\frac{5}{2}}} e^{-\frac{r}{a_0}}$

$\frac{\partial}{\partial r}\left(r^2 \frac{\partial R_{10}}{\partial r}\right) = \frac{-2}{a_0^{\frac{5}{2}}}\left(2r e^{\frac{-r}{a_0}} - \frac{r^2}{a_0} e^{-\frac{r}{a_0}}\right)$

$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial R_{10}}{\partial r}\right) = \frac{-2e^{\frac{-r}{a_0}}}{a_0^{\frac{5}{2}}}\left(2r^{-1} - \frac{1}{a_0}\right)$

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{\hbar^2}{a_0^2}} = \frac{\hbar}{a_0}$$

$$\Delta r = \sqrt{\langle \hat{r}^2 \rangle - \langle r \rangle^2} = \sqrt{3a_0^2 - \frac{9}{4}a_0^2} = \sqrt{\frac{3}{4}a_0^2} = \sqrt{3}\,\frac{a_0}{2}$$

$$\boxed{\Delta p \Delta r = \frac{\sqrt{3}}{2}\hbar \geq \frac{\hbar}{2}}$$

USTREZA HEISENBERGOVI NEENAKOSTI

$\langle \hat{W}_p \rangle = \langle \hat{V} \rangle = -27{,}2\,\text{eV}$; saj je

DOKAZ $E_1 = \langle \hat{W}_k \rangle + \langle \hat{W}_p \rangle$

$\langle \hat{H} \rangle = E_1$

$\hat{H} = \hat{W}_k + \hat{W}_p$

$$\boxed{\hat{W}_p = \hat{V}}$$

$$\boxed{\langle \hat{H} \rangle = \langle \hat{W}_k \rangle + \langle \hat{W}_p \rangle = E_1}$$

$$\langle \hat{V} \rangle = \int_0^\infty \frac{-e_0^2}{4\pi\varepsilon_0 r} R_{10}^2 r^2 dr = \frac{-e_0^2}{4\pi\varepsilon_0 a_0}$$

$\left(\frac{dw}{dr}\right) \to n a_0 \Rightarrow$

gl. kv. št. pove tudi vrednost max. $\frac{dw}{dr} \Rightarrow$

$n = 1$, max pri a_0

$n = 2$ pri $2a_0$

$\vdots$

ATOM SE Z VZBUJANJEM NAPIHUJE