2. Bsp. p-Orbital

$n=2, l=1, m=0: \psi_{210}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \cdot \cos\vartheta$

↳ 1 Knoten

3. Bsp: d-Orbital

$n=3, l=2, m=0: \psi_{320}(r) = \frac{1}{81\sqrt{6\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(\frac{r}{a_0}\right)^2 \cdot e^{-r/3a_0} (3\cos^2\vartheta - 1)$

↳ 2 Knoten

Vorlesung 05.12.2013

Wellenfunktionen

$\psi(n,l,m) = R(n,l)\, \Theta(l,m)\, \phi(m)$

R(n,l): Radiales Teil der WF

assoziierte Laguerre-Polynome (normiert)

$n=1, l=0: R(1,0) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$

$a_0 = 0{,}529\ \text{Å}$

$n=2, l=0: R(2,0) = \left(\frac{Z}{2a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$

$n=2, l=1: R(2,1) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0} \cdot e^{-Zr/2a_0}$

$\Theta(l,m)$: 1. winkelabh. Teil der WF

zugeordnete Legendre-Polynome (normiert)

$l=0, m=0: \quad \Theta(0,0) = \frac{1}{2}\sqrt{2}$

$l=1, m=0: \quad \Theta(1,0) = \sqrt{\frac{3}{2}} \cos\vartheta$

$l=1, m=\pm 1: \quad \Theta(1,\pm 1) = \sqrt{\frac{3}{4}} \sin\vartheta$

$\phi(m)$: 2. winkelabh. Teil der WF

$$A \cdot e^{im\varphi} = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

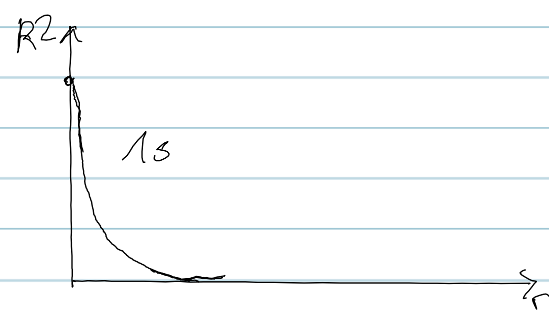
Bsp. 1s-Orbital (H-Atom)

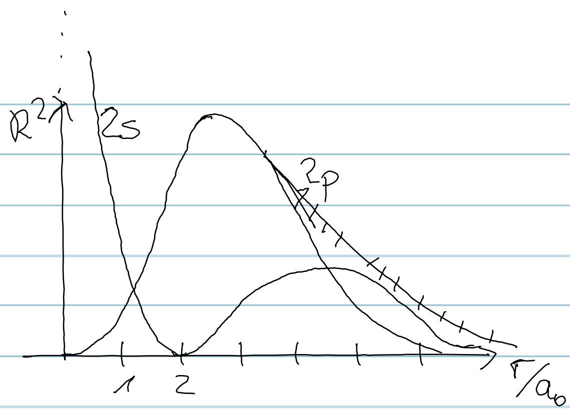
$$\psi(1,0,0) = \underbrace{2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}}_{R(1,0)} \cdot \underbrace{\frac{1}{2}\sqrt{2}}_{\Theta(0,0)} \cdot \underbrace{\frac{1}{\sqrt{2\pi}}}_{\phi(0)}$$

$$\psi(1,0,0) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$ (vgl. Abschnitt 2.3)

Darstellung

radiale Wahrscheinlichkeitsdichte $R^2$



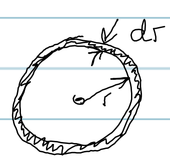



Radiale Verteilungsfunktion: P

$$F = \int_0^{\pi}\int_0^{2\pi} R^2 r^2 \sin\vartheta \, d\vartheta \, d\varphi \, dr = \underbrace{4\pi r^2 R^2}_{P} dr$$

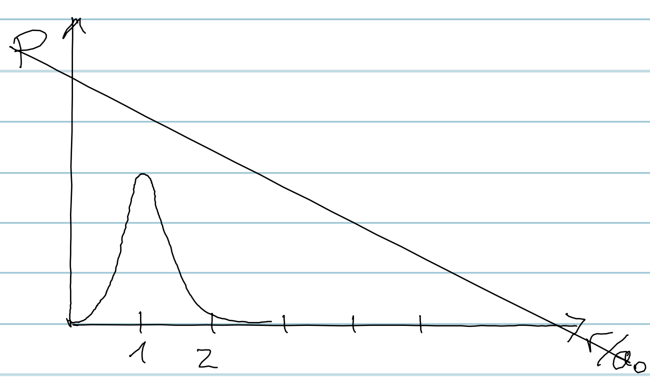
$$\int_0^{\pi} \sin\vartheta \, d\vartheta \int_0^{2\pi} d\varphi = [-\cos\vartheta]_0^{\pi} \, [\varphi]_0^{2\pi}$$

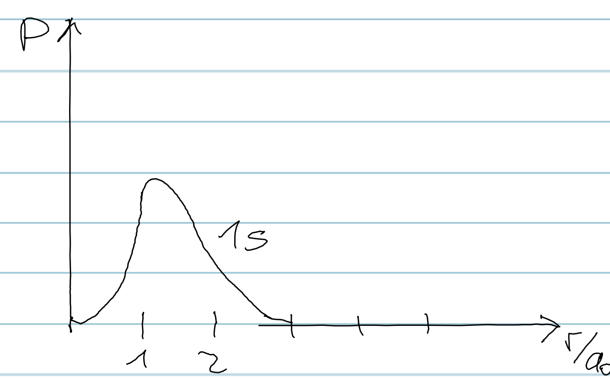
$$(1+1) \cdot 2\pi$$

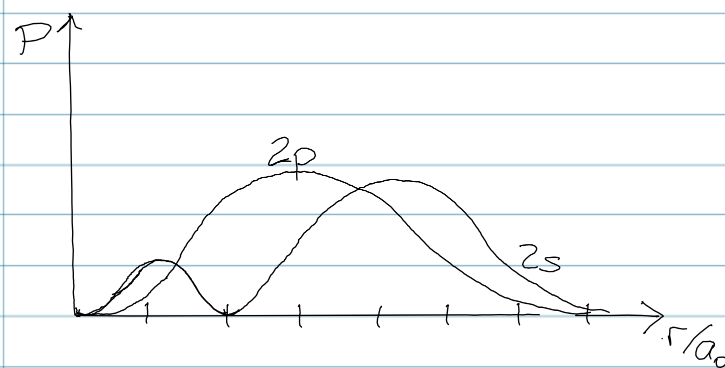



$P = 4\pi r^2 R^2$ rad. Dichteverteilung

= Wahrscheinlichkeit, das $e^-$ in einer „Hülle" der Dicke „dr" im Abstand „r" vom Kern zu finden



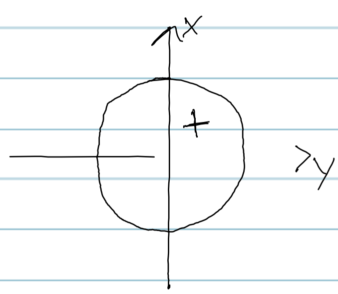



## Winkelabhängigkeit

$Y_{\ell,m}(\vartheta,\varphi)=\Theta\Phi(\ell,m)$

s-Orbital: $\ell=0, m=0$

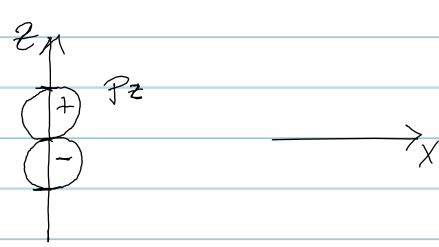
$\Theta\,\phi = \text{const.}$




p-Orbitale: $\ell=1, m=0,\pm1$

$p_z$-Orbital: $\ell=1,\ m=0$

$\Theta\,\phi(1,0)=\sqrt{\frac{3}{4\pi}}\cos\vartheta$



$p_x$ u. $p_y$ – Orbitale: $\cancel{l=0}$ $l = 1,\ m = \pm 1$

$$\Theta\phi\,(1,\pm 1) = -\sqrt{\tfrac{3}{8\pi}}\,\sin\vartheta\, e^{\pm i\varphi}$$

$$|\Theta\phi(1,1)|^2 = |\Theta\phi(1,-1)|^2 = \tfrac{3}{8\pi}\sin^2\vartheta$$

↪ Darstellung s. Folie

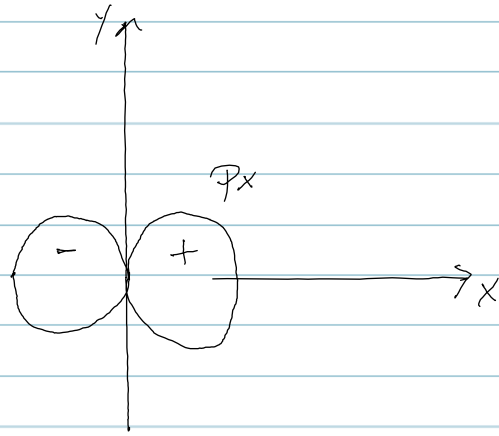
$\Theta\phi(1,\pm 1)$ sind entartet!

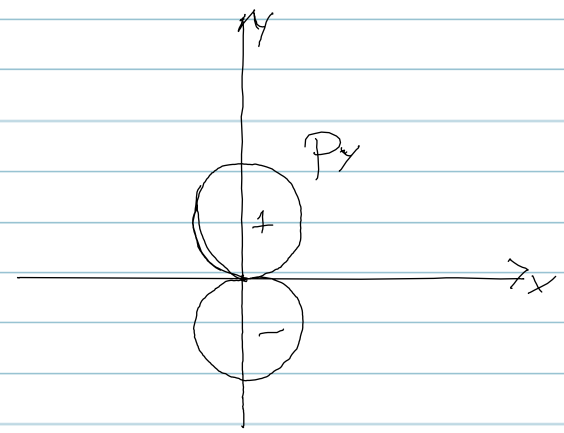
$$\hat{L}_z\Theta\phi = \underbrace{m\hbar}_{\text{Eigenwert}}\Theta\phi = \pm 1\hbar\,\Theta\phi$$

Linearkomb.

$$\psi_1 = \tfrac{1}{2}\left[\Theta\phi(1,1) + \Theta\phi(1,-1)\right] = A\sin\vartheta\cos\varphi \equiv p_x$$

$$\psi_2 = \tfrac{1}{2i}\left[\Theta\phi(1,1) - \Theta\phi(1,-1)\right] = A\sin\vartheta\sin\varphi \equiv p_y$$



d-Orbitale: $\ell = 2,\ m = 0, \pm 1, \pm 2$

u.a. Linearkomb.

$$d_{z^2} = \Theta\phi(2,0) = \left(\frac{15}{16\pi}\right)^{1/2}(3\cos^2\vartheta - 1)$$

$$d_{xz} = \frac{1}{\sqrt{2}}\left[\Theta\phi(2,1) + \Theta\phi(2,-1)\right] = \left(\frac{15}{4\pi}\right)^{1/2}\sin\vartheta\cos\vartheta\cos\varphi$$

$$d_{yz} = \frac{1}{\sqrt{2}\,i}\left[\Theta\phi(2,1) - \Theta\phi(2,-1)\right] = \left(\frac{15}{4\pi}\right)^{1/2}\sin\vartheta\cos\vartheta\sin\varphi$$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}\left[\Theta\phi(2,2) + \Theta\phi(2,-2)\right] = \left(\frac{15}{16\pi}\right)^{1/2}\sin^2\vartheta\cos 2\varphi$$

$$d_{xy} = \frac{1}{\sqrt{2}\,i}\left[\Theta\phi(2,2) - \Theta\phi(2,-2)\right] = \left(\frac{15}{16\pi}\right)^{1/2}\sin^2\vartheta\sin 2\varphi$$