

2. Bsp. p-Orbital

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

↳ 1 Knoten

3. Bsp. d-Orbital

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

↳ 2 Knoten

Vorlesung 05.12.2013

Wellenfunktionen

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

$R(n, l)$: Radialer Teil der WF

assoziierte Laguerre-Polynome (normiert)

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

$$a_0 = 0,529 \text{ \AA}$$

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

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

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

zugeordnete Legendre-Polynome (normiert)

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

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

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

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

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

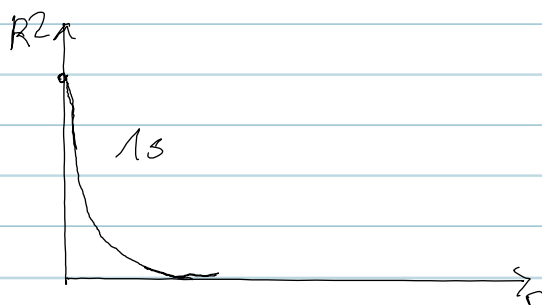
Bsp. 1s-Orbital (H-Atom)

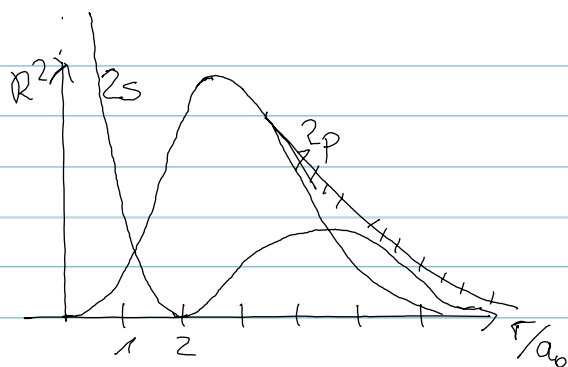
$$\psi(1,0,0) = \underbrace{2 \left(\frac{2}{a_0}\right)^{3/2} e^{-2r/a_0}}_{R(1,0)} \cdot \underbrace{\frac{1}{2} \sqrt{2}}_{\Theta(0,0)} \cdot \underbrace{\frac{1}{\sqrt{2\pi}}}_{\phi(0)}$$

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

Darstellung

radiale Wahrscheinlichkeitsdichte R^2

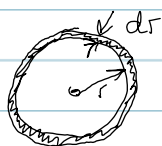




Radiale Verteilungsfunktion: P

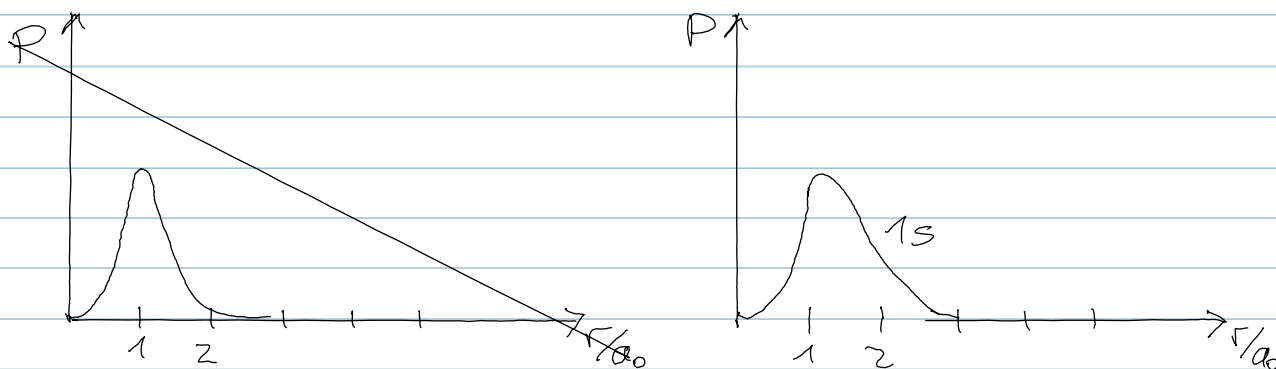
$$F = \int_0^{\pi} \int_0^{2\pi} R^2 r^2 \sin\vartheta \, d\vartheta \, d\varphi \, dr = \underbrace{4\pi r^2 R^2}_{P} dr$$

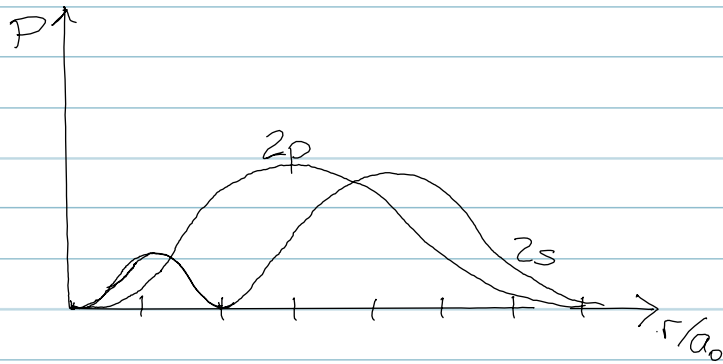
$$\int_0^{\pi} \sin\vartheta \, d\vartheta \int_0^{2\pi} d\varphi = [-\cos\vartheta]_0^{\pi} [\varphi]_0^{2\pi} \\ (1+1) \cdot 2\pi$$



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

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



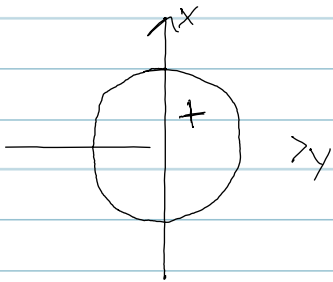


Winkelabhängigkeit

$$Y_{l,m}(\vartheta, \varphi) = \Theta \phi(l, m)$$

s-Orbital: $l=0, m=0$

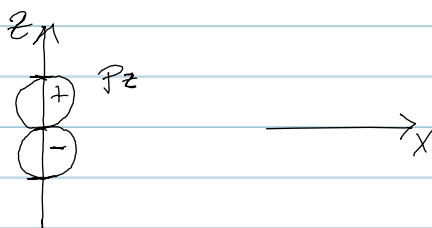
$$\Theta \phi = \text{const.}$$



p-Orbitale: $l=1, m=0, \pm 1$

p_z -Orbital: $l=1, m=0$

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



p_x u. p_y -Orbitale: $l=0, l=1, m=\pm 1$

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

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

↳ Darstellung s. Folie

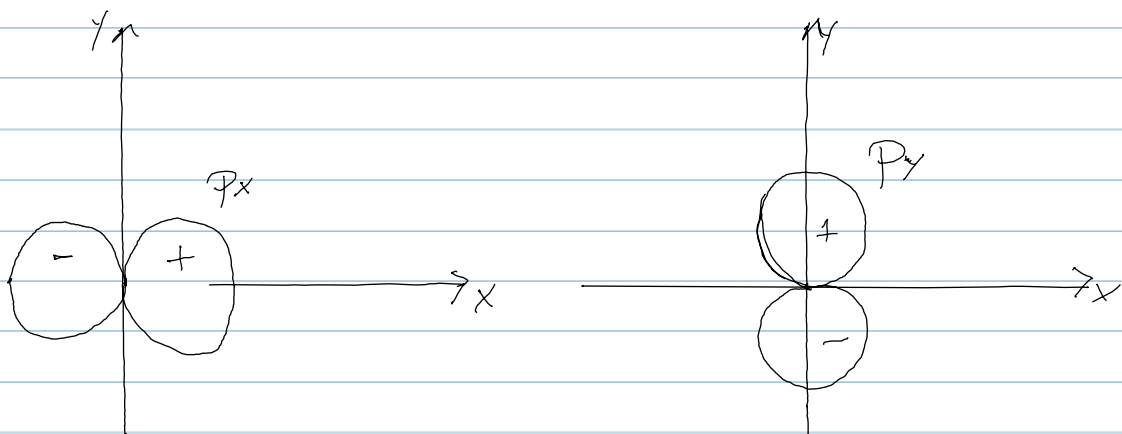
$\Theta\phi(1,\pm 1)$ sind entartet!

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

Linearkomb.

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

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



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

u.a. Linearkomb.

$$d_{z^2} = \Theta \phi(2,0)$$

$$= \left(\frac{15}{16\pi}\right)^{1/2} (3\cos^2\vartheta - 1)$$

$$d_{xz} = \frac{1}{\sqrt{2}} [\Theta \phi(2,1) + \Theta \phi(2,-1)]$$

$$= \left(\frac{15}{4\pi}\right)^{1/2} \sin\vartheta \cos\vartheta \cos\varphi$$

$$d_{yz} = \frac{1}{\sqrt{2}i} [\Theta \phi(2,1) - \Theta \phi(2,-1)]$$

$$= \left(\frac{15}{4\pi}\right)^{1/2} \sin\vartheta \cos\vartheta \sin\varphi$$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}} [\Theta \phi(2,2) + \Theta \phi(2,-2)]$$

$$= \left(\frac{15}{16\pi}\right)^{1/2} \sin^2\vartheta \cos 2\varphi$$

$$d_{xy} = \frac{1}{\sqrt{2}i} [\Theta \phi(2,2) - \Theta \phi(2,-2)]$$

$$= \left(\frac{15}{16\pi}\right)^{1/2} \sin^2\vartheta \sin 2\varphi$$

