

Blatt 5

16) a) Nur Winkelabhängigkeit: $Y_{l,m}(\theta, \varphi)$, $l=2$, $\varphi=0$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$$

$$\theta = 0: 3 \cos^2 \theta - 1 = 2$$

$$\theta = 90^\circ: 3 \cos^2 \theta - 1 = -1$$

$$3 \cos^2 \theta - 1 = 0: \theta = 54,74^\circ$$

$$Y_{2,\pm 1} = \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta e^{\pm i\varphi}$$

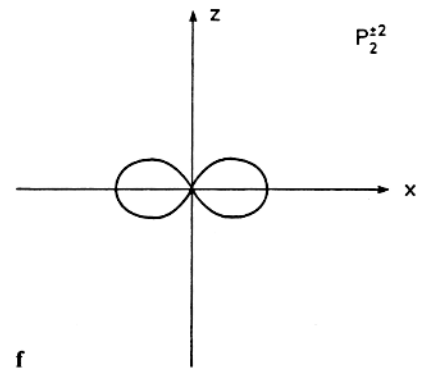
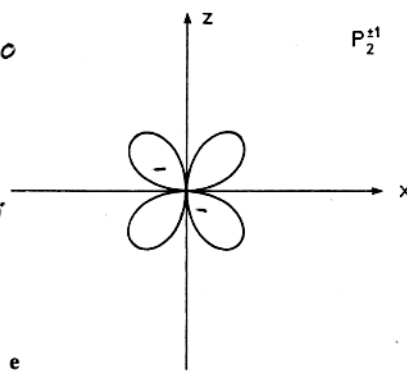
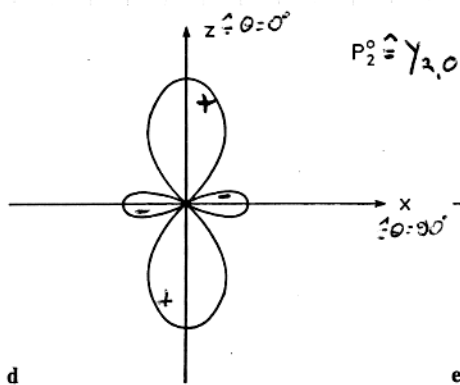
$$= 0 \text{ für } \theta = 0$$

$$= 0 \text{ für } \theta = 90^\circ$$

$$= \frac{1}{2} \text{ für } \theta = 45^\circ$$

$$= \frac{\sqrt{3}}{4} = 0,43 \text{ für } \theta = 30^\circ$$

$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm i2\varphi}$$



aus Haken Woff: "Atom -
und Quantenphysik"

b)

Kugelsymmetrisch, ungleich von Null für $r \rightarrow 0$: s-Orbital ($l=0$)

Aus Vorlesung: Anzahl nicht-triviale Nullstellen:

$$n - (l+1) \stackrel{!}{=} 4 \Rightarrow n=5$$

 $\Rightarrow$ 5s-Orbital

17)

$$L_z \stackrel{!}{=} \frac{\hbar}{i} \partial_\varphi$$

$$L_z \psi = \frac{\hbar}{i} \partial_\varphi \left[A r^2 e^{-\frac{r}{3a_0}} \sin \theta \cos \theta e^{i\varphi} \right]$$

$$= \frac{\hbar}{i} i \psi = \hbar \psi \Rightarrow \underline{m=1}, \text{ denn } \psi \propto e^{i\varphi}$$

$$\text{denn } \langle L_z \rangle = \iiint \psi^* L_z \psi dV = m \hbar$$

$$\stackrel{\text{S.O.}}{=} \iiint \psi^* \hbar \psi dV = \hbar \iiint \psi^* \psi dV = \hbar$$

$$\langle \vec{L}^2 \rangle = l(l+1) \hbar^2$$

(nicht $\vec{L} \psi$, da nur Betrag und eine Komponente bestimmbar)

wie oben:

$$\vec{L}^2 \psi = -\hbar^2 \left(\underbrace{\frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta)}_{1. \text{ Teil}} + \underbrace{\frac{1}{\sin^2 \theta} \partial_\varphi^2}_{2. \text{ Teil}} \right) \psi$$

 $\vec{L}^2$ im Kugelkoordinaten
z.B. aus Nolting „QM 2“

$$1. \text{ Teil: } \frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta) \sin \theta \cos \theta$$

$$= \frac{1}{\sin \theta} \partial_\theta \sin \theta (\cos^2 \theta - \sin^2 \theta)$$

$$= \frac{\cos \theta}{\sin \theta} (\cos^2 \theta - \sin^2 \theta) - 4 \cos \theta \sin \theta$$

$$2. \text{ Teil: } \frac{1}{\sin^2 \theta} \partial_\varphi^2 \sin \theta \cos \theta e^{i\varphi} = -\frac{\cos \theta}{\sin \theta} e^{i\varphi}$$

$$\Rightarrow \vec{L}^2 \psi = A r^2 e^{-\frac{r}{3a_0}} \left[\frac{\cos \theta}{\sin \theta} (1 - 2 \sin^2 \theta) - 4 \cos \theta \sin \theta - \frac{\cos \theta}{\sin \theta} \right] e^{i\varphi} (-\hbar^2)$$

$$= 6 \hbar^2 \psi \stackrel{!}{=} l(l+1) \hbar^2 \psi \rightarrow \underline{\underline{l=2}}$$

$$"e^{-\frac{r}{3a_0}}" \Rightarrow n=3$$

18) a) orthogonal: mit $\iint Y_{l,m}^*(u, \varphi) Y_{l',m'}(u, \varphi) du d\varphi = \delta_{l,l'} \delta_{m,m'}$

d_{z^2} und d_{xy}

$$\begin{aligned} \iint Y_{2,0}^* \frac{1}{\sqrt{2}} (Y_{2,-2} + Y_{2,2}) du d\varphi &= \frac{1}{\sqrt{2}} \iint [Y_{2,0}^* Y_{2,-2} + Y_{2,0}^* Y_{2,2}] du d\varphi \\ &= \frac{1}{\sqrt{2}} [\delta_{2,2} \delta_{0,-2} + \delta_{2,2} \delta_{0,2}] = 0 \quad \checkmark \end{aligned}$$

$d_{x^2-y^2}$ und d_{xy}

$$\begin{aligned} \iint \frac{1}{\sqrt{2}} (Y_{2,-2}^* + Y_{2,2}^*) \left(\frac{i}{\sqrt{2}}\right) (Y_{2,-2} - Y_{2,2}) du d\varphi \\ = \iint \frac{i}{2} (Y_{2,-2}^* Y_{2,-2} - Y_{2,2}^* Y_{2,2}) du d\varphi = 0 \quad \checkmark \end{aligned}$$

u.s.w. ...

normiert:

$$\iint Y_{2,0}^* Y_{2,0} du d\varphi = 1 \quad \checkmark \text{ (klar)}$$

$$\begin{aligned} \iint \frac{1}{\sqrt{2}} (Y_{2,-2}^* + Y_{2,2}^*) \frac{1}{\sqrt{2}} (Y_{2,-2} + Y_{2,2}) du d\varphi \\ = \frac{1}{2} \iint [Y_{2,-2}^* Y_{2,2} + Y_{2,-2}^* Y_{2,2} + Y_{2,2}^* Y_{2,2}] du d\varphi \\ = \frac{1}{2} \cdot [1 + 0 + 0 + 1] = 1 \quad \checkmark \end{aligned}$$

$$\begin{aligned} \iint -\frac{i}{\sqrt{2}} (Y_{2,-1}^* - Y_{2,1}^*) \frac{i}{\sqrt{2}} (Y_{2,-1} - Y_{2,1}) du d\varphi \\ = \frac{1}{2} \iint (Y_{2,-1}^* Y_{2,-1} + Y_{2,1}^* Y_{2,1}) du d\varphi = 1 \quad \checkmark \end{aligned}$$

u.s.w.

$$b) \vec{L}^2 Y_{l,m} = l(l+1) \hbar^2 Y_{l,m}$$

$$d_z: \langle \vec{L}^2 \rangle = \iint Y_{2,0}^* \vec{L}^2 Y_{2,0} d\mu d\varphi = 2 \cdot 3 \cdot \hbar^2 \cdot \underbrace{\iint Y_{2,0}^* Y_{2,0} d\mu d\varphi}_1 \\ = 2 \cdot 3 \cdot \hbar^2 \quad \checkmark$$

$$d_{x^2-y^2}: \langle \vec{L}^2 \rangle = \iint \frac{1}{\sqrt{2}} (Y_{2,-2}^* + Y_{2,2}^*) \vec{L}^2 \frac{1}{\sqrt{2}} (Y_{2,-2} + Y_{2,2}) d\mu d\varphi \\ = \frac{1}{2} \cdot 2 \cdot 3 \cdot \hbar^2 [1 + 0 + 0 + 1] = 2 \cdot 3 \cdot \hbar^2 \quad \checkmark$$

$$d_{xy}: \langle \vec{L}^2 \rangle = \iint -\frac{i}{\sqrt{2}} (Y_{2,-1}^* - Y_{2,1}^*) \frac{i}{\sqrt{2}} (2 \cdot 3 \cdot \hbar^2) (Y_{2,-1} - Y_{2,1}) d\mu d\varphi \\ = \frac{1}{2} \cdot 2 \cdot 3 \cdot \hbar^2 \cdot (1+1) = 2 \cdot 3 \cdot \hbar^2 \quad \checkmark$$

usw.

$$d_z: \langle L_z \rangle = \iint Y_{2,0}^* \underbrace{L_z Y_{2,0}}_0 d\mu d\varphi = 0 \quad \checkmark$$

$$d_{x^2-y^2}: \langle L_z \rangle = \iint \frac{1}{\sqrt{2}} (Y_{2,-2}^* + Y_{2,2}^*) L_z \frac{1}{\sqrt{2}} (Y_{2,-2} + Y_{2,2}) d\mu d\varphi \\ = \frac{1}{2} \iint (Y_{2,-2}^* + Y_{2,2}^*) (-2\hbar Y_{2,-2} + 2\hbar Y_{2,2}) d\mu d\varphi \\ = \frac{1}{2} (-2\hbar + 2\hbar) = 0 \quad \checkmark$$

$$d_{xy}: \langle L_z \rangle = \iint \frac{i}{\sqrt{2}} (Y_{2,1}^* - Y_{2,-1}^*) \frac{i}{\sqrt{2}} (-\hbar Y_{2,-1} - \hbar Y_{2,1}) d\mu d\varphi \\ = -\frac{1}{2} \hbar (1-1) = 0 \quad \checkmark$$

usw.

$$c) \text{ mit } Y_{l,m}(\theta, \varphi) = A_{l,m} P_l^{|m|}(\cos \theta) e^{im\varphi}$$

$$\Rightarrow Y_{l,m}(\theta, \varphi + \alpha) = A_{l,m} P_l^{|m|}(\cos \theta) e^{im(\varphi + \alpha)} = Y_{l,m}(\theta, \varphi) e^{im\alpha}$$

$$d_{xy}: \frac{1}{\sqrt{2}} (Y_{2,-2}(\theta, \varphi) + Y_{2,2}(\theta, \varphi)) \rightarrow \frac{1}{\sqrt{2}} (Y_{2,-2}(\theta, \varphi - \frac{\pi}{4}) + Y_{2,2}(\theta, \varphi - \frac{\pi}{4}))$$

$$= \frac{1}{\sqrt{2}} (Y_{2,-2}(\theta, \varphi) \underbrace{e^{i\frac{\pi}{2}}}_{i} + Y_{2,2}(\theta, \varphi) \underbrace{e^{-i\frac{\pi}{2}}}_{-i})$$

$$= \frac{i}{\sqrt{2}} (Y_{2,-2} - Y_{2,2}) \hat{=} d_{xy} \quad \checkmark$$

d) Betrachtung nach Winkelabhängigkeit:

$$\frac{x}{r} = \sin \theta \cos \varphi$$

$$\frac{y}{r} = \sin \theta \sin \varphi$$

$$\frac{z}{r} = \cos \theta$$

$$\Rightarrow p_z \sim \cos \theta \quad p_y \sim \sin \theta \sin \varphi \quad p_x \sim \sin \theta \cos \varphi$$

$$\text{mit } Y_{1,0} \sim \cos \theta$$

$$Y_{1,1} \sim \sin \theta e^{i\varphi}$$

$$Y_{1,-1} \sim \sin \theta e^{-i\varphi}$$

und

$$\frac{1}{2i} (e^{i\varphi} - e^{-i\varphi}) = \sin \varphi$$

$$\frac{1}{2} (e^{i\varphi} + e^{-i\varphi}) = \cos \varphi$$

folgt:

$$p_z = Y_{1,0}$$

$$p_y = \frac{i}{\sqrt{2}} (Y_{1,1} - Y_{1,-1}) \sim \frac{i}{\sqrt{2}} \sin \theta (e^{i\varphi} - e^{-i\varphi}) \sim \sin \theta \sin \varphi$$

$$p_x = \frac{1}{\sqrt{2}} (Y_{1,1} + Y_{1,-1}) \sim \frac{1}{\sqrt{2}} \sin \theta (e^{i\varphi} + e^{-i\varphi}) \sim \sin \theta \cos \varphi$$

19) Resonanz: $g \mu_B B_0 = h \nu$

$$g = \frac{h \nu}{\mu_B B_0} = \frac{h}{\mu_B} \frac{9,2 \text{ GHz}}{327,74 \text{ mT}} = 2,0056$$

Resonanzbedingung für $\nu = 9,80 \text{ GHz}$ für diesen g -Faktor:

$$B_0 (9,80 \text{ GHz}) = 349,11 \text{ mT}$$