

# ⇒ VORLESUNG 18 QM

H-ATOM

$$R(r) = \frac{U(r)}{r}$$

$$U(r) = r^{l+1} \underline{e^{-\rho}} v(r)$$

$$\rho = Kr$$

$$E = -\frac{\hbar^2}{2m} K^2$$

$$\underline{v(r)} = \sum_{j=0}^{j_{\max}} c_j r^j$$

$$c_{j+1} = \frac{[2(j+l+1) - \rho_0]}{(j+1)(j+2l+2)} c_j$$

•  $j_{\max} \Rightarrow c_{j_{\max}+1} = 0$

$$2(j_{\max} + l + 1) = \rho_0$$

$$n = 1, 2, \dots$$

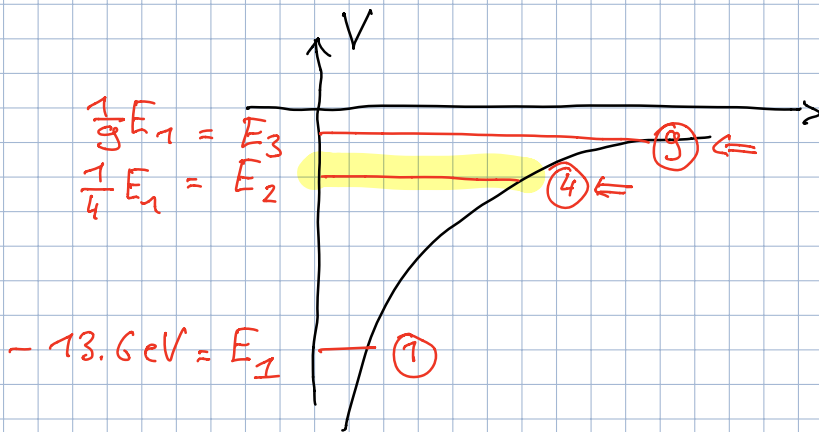
$$K = \frac{1}{an}$$

BOHR RADIUS

$$a = \frac{1}{m\alpha} \frac{\hbar c}{c^2} \approx 0.5 \cdot 10^{-10} \text{ m}$$

$$E_n = - \frac{E_1}{n^2} \quad n = 1, 2, \dots$$

$$E_1 = \left( \frac{1}{2} m c^2 \right) \alpha^2 = 13.6 \text{ eV} \quad \alpha = \frac{1}{137}$$



• GRUNDZUSTAND  $n=1$

$$n = j_{\max} + l + 1$$

$$j_{\max} = 0, \quad l = 0$$

$$v(r) = c_0$$

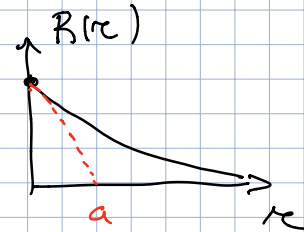
$$v(r) = c_0 e^{-r} e^{-l}$$

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$$p = k r = \frac{1}{a m} r = \frac{r}{a}$$

$$R(r) = \frac{1}{r} c_0 \left(\frac{r}{a}\right) e^{-r/a}$$

$$R(r) = \frac{c_0}{a} e^{-r/a}$$



NORMIERUNG

$$\int_0^{\infty} dr r^2 |R(r)|^2 = 1$$

$$1 = \frac{c_0^2}{a^2} \int_0^{\infty} dr r^2 e^{-2r/a}$$

$$= \frac{c_0^2}{a^2} \frac{a^3}{8} \int_0^{\infty} dx x^2 e^{-x}$$

$x = 2r/a$

$$= c_0^2 \frac{a}{4}$$

$$c_0 = \frac{2}{\sqrt{a}} \rightarrow R(r) = \frac{2}{a\sqrt{a}} e^{-r/a}$$

$$\Psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\theta, \phi)$$

$$n=1, l=0, m=0$$

$$= R_{10}(r) \underbrace{Y_{00}(\theta, \phi)}_{\frac{1}{\sqrt{4\pi}}}$$

$$\Psi_{100}(\vec{r}) = \frac{1}{\sqrt{4\pi}} \frac{2}{a\sqrt{a}} e^{-r/a}$$

• 1° ANREGUNG  $n=2$

$$n = j_{\max} + l + 1 = 2$$

$$\rightarrow l=0 \quad j_{\max}=1$$

$$\rightarrow l=1 \quad j_{\max}=0$$

$$\leadsto l=0$$

$$v(r) = c_0 + c_1 r$$

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$$c_{j+1} = \frac{[2(j+l+1) - 4]}{(j+1)(j+2l+2)} c_j$$

$$\rho_0 = 2m$$

$$c_1 = \frac{2(1) - 4}{1 \cdot (2)} c_0 = -c_0$$

$$v(r) = c_0 (1 - e^{-r})$$

$$\downarrow \quad \rho = \frac{K\mu}{am} = \frac{1}{a} \mu$$

$$\Rightarrow v(r) = c_0 \left(1 - \frac{\mu}{2a}\right), \quad \rho = \left(\frac{\mu}{2a}\right)$$

$$U(r) = \rho e^{-\rho r} v(r)$$

$$= \left(\frac{\mu}{2a}\right) e^{-\mu/2a} c_0 \left(1 - \frac{\mu}{2a}\right)$$

$$R_{20}(\mu) = \frac{c_0}{2a} \left(1 - \frac{\mu}{2a}\right) e^{-\frac{\mu}{2a}}$$

$\uparrow$   $\uparrow$   
 $\mu$   $r$

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$$C_0 = \frac{2}{\sqrt{2/a}}$$

$$R_{20}(0) = \frac{C_0}{2a}$$

↑  
l=0

→  $l=1$   $f_{\max} = 0$

$$v(r) = C_0$$

$$v(r) = r^2 e^{-\rho} C_0$$

$$\rho = \kappa r = \left(\frac{\mu}{a m}\right) r = \frac{\mu}{2a}$$

$$R_{21}(r) = \frac{1}{r} \left(\frac{\mu}{2a}\right)^2 e^{-r/2a} C_0$$

↑ ↑  
r r

$$R_{21}(r) = \frac{C_0}{4a^2} r e^{-r/2a}$$

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$$R_{nl}(r) \xrightarrow{r \ll} r^l$$

• BELIEBIGES  $n$

$$n = j_{\max} + l + 1$$

$$\leadsto l = n - 1 - j_{\max}$$

$$l = 0, \dots, n-1$$

$$n=1 \quad l=0$$

$$n=2 \quad l=0, 1$$

$$n=3 \quad l=0, 1, 2$$

$$\forall l \quad m = -l, \dots, +l$$

$$\underline{2l+1}$$

$$\Psi_{nlm} \leadsto E_n$$

ENTARTUNG

$$\text{FÜR } n \quad \sum_{l=0}^{n-1} (2l+1) = n^2$$

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$$n=1 \quad l=0 \quad m=0 \quad \textcircled{1}$$

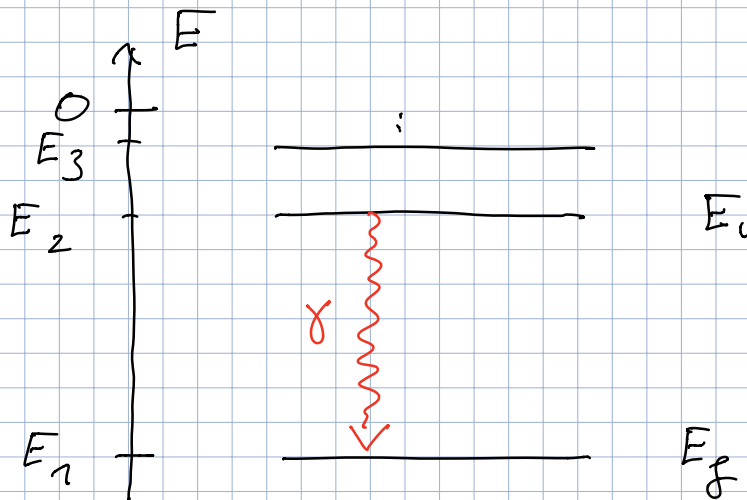
$$n=2 \quad \left. \begin{array}{l} l=0 \quad m=0 \quad 1 \\ l=1 \quad m=-1,0,1 \quad 3 \end{array} \right\} \textcircled{4}$$

$$n=3 \quad \left. \begin{array}{l} l=0 \quad 1 \\ l=1 \quad 3 \\ l=2 \quad 5 \end{array} \right\} \textcircled{9}$$

⋮

$v(l)$   $\Rightarrow$  ASSOZIIERTE  
LAGUERRE POLY.

$\Rightarrow$  SPEKTRUM DES H-ATOM



$$E_\gamma = E_i - E_f$$
$$= (-13.6) \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

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$$E_\gamma = \underbrace{h\nu} = \hbar\omega$$

$$\frac{1}{\lambda} = \frac{\nu}{c} = \frac{h\nu}{hc} = \frac{E_\gamma}{2\pi\hbar c}$$

$$\frac{1}{\lambda} = \underbrace{\frac{(-E_i)}{2\pi\hbar c}} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$R$  (RYDBERG)

$$-E_1 = \left( \frac{1}{2} mc^2 \right) \alpha^2$$

$$R \approx 1.1 \cdot 10^7 \text{ m}^{-1}$$

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⇒ SPIN

• ORBITAL  $\bar{L}$

EIGENZUSTÄNDE  $L^2, L_z$   
↓ ↓  
 $l$   $m$

$$\langle \bar{r} | l m \rangle = Y_{lm}(\hat{r})$$

$$\begin{cases} L^2 | l m \rangle = \hbar^2 l(l+1) | l m \rangle \\ L_z | l m \rangle = \hbar m | l m \rangle \end{cases}$$

$$l = 0, 1, 2, \dots$$

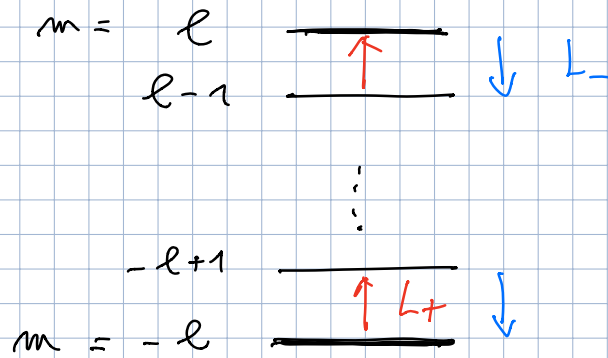
$$m = -l, \dots, +l$$

$$L_{\pm} = L_x \pm i L_y$$

$$L_{\pm} | l m \rangle = C_{\pm} | l m \pm 1 \rangle$$

$$C_{\pm} = \hbar \sqrt{l(l+1) - m(m \pm 1)}$$

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$2l+1$  ZUSTÄNDE

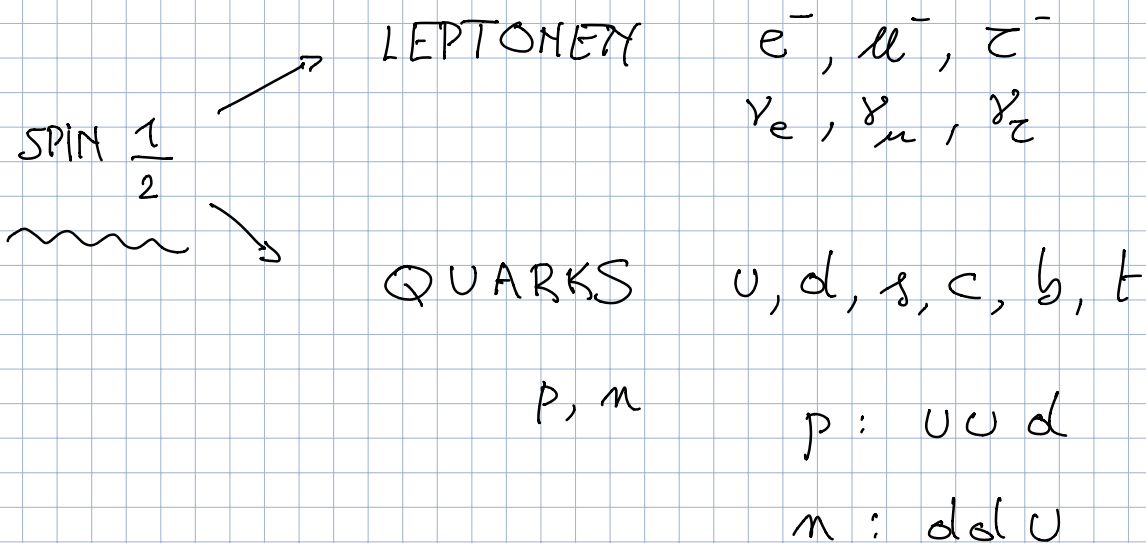
$2l$  SCHRITTE

$$2l \in \mathbb{N}$$

$$l = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$$

INTRINSISCHER SPIN

SICHTBARE MATERIE



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• SPIN  $\frac{1}{2}$

$$S = \frac{1}{2} \quad S_z = \pm \frac{\hbar}{2}$$

$$\text{—————} \quad S_z = +\frac{\hbar}{2}$$

$$\text{—————} \quad S_z = -\frac{\hbar}{2}$$

$$|SS_z\rangle \rightarrow \left| \frac{1}{2}, +\frac{1}{2} \right\rangle, \left| \frac{1}{2}, -\frac{1}{2} \right\rangle$$

$$\left\{ \begin{array}{l} S^2 \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle = \hbar^2 \frac{3}{4} \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle \\ S_z \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle = \pm \frac{\hbar}{2} \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle \end{array} \right.$$

$$\left| \frac{1}{2}, +\frac{1}{2} \right\rangle \longleftrightarrow \chi_{\uparrow} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{SPIN UP}$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle \longleftrightarrow \chi_{\downarrow} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{SPIN DOWN}$$

$$\chi^\dagger \chi = \underline{1}$$

$S^2, S_z$  IN MATRIX DARSTELLUNG

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$$\hookrightarrow \underbrace{S^2}_{2 \times 2} \underbrace{\chi_{\uparrow}}_{2 \times 1} = \hbar^2 \frac{3}{4} \chi_{\uparrow}$$

$$S^2 = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$S^2 \chi_{\uparrow} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ c \end{pmatrix}$$

$$= \hbar^2 \frac{3}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$c = 0, \quad a = \hbar^2 \frac{3}{4}$$

$$S^2 \chi_{\downarrow} = \hbar^2 \frac{3}{4} \chi_{\downarrow}$$

$$b = 0, \quad d = \hbar^2 \frac{3}{4}$$

$$S^2 = \hbar^2 \frac{3}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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$$\hookrightarrow S_z \chi_{\uparrow} = + \frac{\hbar}{2} \chi_{\uparrow}$$

$$S_z = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$S_z \chi_{\uparrow} = \begin{pmatrix} a \\ c \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$c = 0, \quad a = \frac{\hbar}{2}$$

$$S_z \chi_{\downarrow} = \begin{pmatrix} b \\ d \end{pmatrix} = - \frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$b = 0, \quad d = - \frac{\hbar}{2}$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hookrightarrow S_{\pm} = S_x \pm i S_y$$

$$L_{\pm} |l m\rangle = C_{\pm} |l m \pm 1\rangle$$

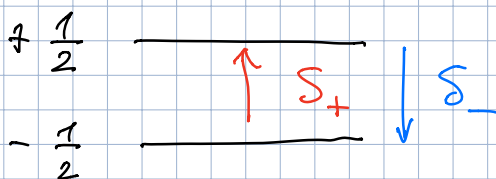
$$C_{\pm} = \hbar \sqrt{l(l+1) - m(m \pm 1)}$$

$$S = \frac{1}{2}$$

$$S_{\pm} |S S_z\rangle = \hbar \sqrt{\frac{3}{4} - S_z(S_z \pm 1)} |S S_z \pm 1\rangle$$

$$S_+ \left| \frac{1}{2} + \frac{1}{2} \right\rangle = 0$$

$$S_+ \left| \frac{1}{2} - \frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2} + \frac{1}{2} \right\rangle$$



$$S_- \left| \frac{1}{2} + \frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2} - \frac{1}{2} \right\rangle$$

$$S_- \left| \frac{1}{2} - \frac{1}{2} \right\rangle = 0$$

•  $S_+ \chi_{\uparrow} = 0$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ c \end{pmatrix} \Rightarrow \underline{\underline{a=c=0}}$$

$$S_+ \chi_{\downarrow} = \hbar \chi_{\uparrow}$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} b \\ d \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$d = 0$$
$$\underline{\underline{b = \hbar}}$$

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

•  $S_-$

$$S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\Rightarrow S_{\pm} = S_x \pm i S_y$$

$$S_x = \frac{1}{2} (S_+ + S_-)$$

$$S_y = \frac{1}{2i} (S_+ - S_-)$$



$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\vec{S} (S_x, S_y, S_z)$$

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma}$$



PAULI MATRIZEN

$$\left\{ \begin{array}{l} \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{array} \right.$$

