$\Longrightarrow$ VORLESUNG 23 QM

FEIN STRUKTUR DES H – ATOM

1) REL. KORREKTUREN

2) SPIN – BAHN KOPPLUNG

1) REL. KORREKTUREN

$$H^0 = \frac{\hat{P}^2}{2m} - \frac{\alpha}{r}\hbar c$$

$$H^1_{rel} = -\frac{1}{8}\frac{\hat{P}^4}{m^3c^2}$$

$$E = \sqrt{c^2p^2 + m^2c^4}$$

$$T = \frac{p^2}{2m} - \frac{1}{8}\frac{p^4}{m^3c^2} + \dots$$

$$= \frac{p^2}{2m}\left(1 - \underbrace{\frac{(cp)^2}{(2mc^2)^2}}_{\sim 10^{-4}} + \dots\right)$$

$$2mc^2 \simeq 10^6\ \mathrm{eV}$$

$$(cp) \sim m\alpha$$

$$E^1_{rel} = \langle \psi^0 | H^1_{rel} | \psi^0 \rangle$$

$$0 = [H^1, L^2] = [H^1, L_z] \quad \psi_{n\ell m}$$

$$\frac{p^2}{2m} \psi^0 = (E - \hat{V}) \psi^0$$

$$\frac{p^4}{4m^2} \psi^0 = (E - \hat{V})^2 \psi^0$$

$$E^1_{rel} = -\frac{1}{2mc^2} \left\{ (E^0)^2 + 2E^0 \alpha \hbar c \left\langle \frac{1}{r} \right\rangle + \alpha^2 \hbar^2 c^2 \left\langle \frac{1}{r^2} \right\rangle \right\}$$

$$\left\langle \frac{1}{r} \right\rangle$$

$$\left\langle \frac{1}{r^2} \right\rangle$$

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

$$a = \frac{1}{m\alpha} \frac{\hbar c}{c^2}$$

$$C^2 \int dr \; r^2 \; e^{-2r/a} = 1$$

$$\Rightarrow \quad x = 2r/a.$$

$$C^2 \left(\frac{a}{2}\right)^3 \underbrace{\int dx \; x^2 \, e^{-x}}_{2} = 1$$

$$C^2 = \frac{4}{a^3} \longrightarrow C = \frac{2}{a^{3/2}}$$

$$\rightsquigarrow \psi_{100}(\vec{r}) = \frac{1}{(\pi a^3)^{1/2}} \, e^{-r/a}$$

$\Rightarrow$ FEYNMAN - HELLMANN THEOREM

H HÄNGT AB VOM PARAMETER λ

$$H^0 = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{\alpha \hbar c}{r} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$$

$$\alpha \; , \; \ell$$

$$E_n(\lambda) \; , \; \psi_n(\lambda) \qquad E_1 = -\frac{1}{2} m c^2 \alpha^2$$

$$\Downarrow$$

$$\boxed{\frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial H^0}{\partial \lambda} | \psi_n \rangle}$$

$$\lambda = \underbrace{\lambda_0} + d\lambda$$

$$H(\lambda) = H(\lambda_0) + \underbrace{d\lambda \left.\frac{\partial H}{\partial \lambda}\right|_{\lambda_0}}_{H^1} + O(d\lambda)^2$$

$$\underbrace{dE_n}_{d\lambda \left.\frac{\partial E_n}{\partial \lambda}\right|_{\lambda=\lambda_0}} = \langle \psi_n | \underbrace{H^1}_{d\lambda \left.\frac{\partial H}{\partial \lambda}\right|_{\lambda_0}} | \psi_n \rangle$$

$$\Rightarrow \quad \left\langle \frac{1}{r} \right\rangle$$

$$\frac{\partial H^0}{\partial \alpha} = -\frac{\hbar c}{r}$$

$$\frac{\partial E_n}{\partial \alpha} = -\hbar c \left\langle \frac{1}{r} \right\rangle$$

$$E_n = -\frac{1}{2} m c^2 \alpha^2 \frac{1}{n^2}$$

$$\frac{\partial E_n}{\partial \alpha} = -\alpha m c^2 \frac{1}{n^2}$$

$$-\alpha \frac{mc^2}{n^2} = -\hbar c \left\langle \frac{1}{r} \right\rangle$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{\alpha mc}{\hbar} \frac{1}{n^2} = \frac{1}{an^2}$$

$$\Longrightarrow \left\langle \frac{1}{r^2} \right\rangle$$

$$\frac{\partial H^0}{\partial l} = \frac{\hbar^2}{\cancel{2}m} \cancel{2} \left(l + \frac{1}{2}\right) \frac{1}{r^2}$$

$$\frac{\partial E_n}{\partial l} = \frac{\hbar^2}{m} \left(l + \frac{1}{2}\right) \left\langle \frac{1}{r^2} \right\rangle$$

$$E_n = \frac{E_1}{(\underbrace{j_{max} + l + 1}_{n})^2}$$

$$l = 0, \dots, \underline{\underline{n-1}}$$

$$\frac{\partial E_n}{\partial l} = -2\,\frac{E_1}{(j_{max}+l+1)^3} = -2\,\frac{E_1}{n^3}$$

$$-2\,\frac{E_1}{n^3} = \frac{\hbar^2}{m}\left(l+\frac{1}{2}\right)\left\langle \frac{1}{r^2}\right\rangle$$

$$\Big\downarrow \qquad -2E_1 = (mc^2)\,\alpha^2$$

$$\frac{m^2c^2\,\alpha^2}{\hbar^2}\,\frac{1}{n^3}\,\frac{1}{\left(l+\frac{1}{2}\right)} = \left\langle \frac{1}{r^2}\right\rangle$$

$$\left\langle \frac{1}{r^2}\right\rangle = \frac{1}{a^2}\,\frac{1}{n^3\left(l+\frac{1}{2}\right)}$$

$$\left\langle \frac{1}{r}\right\rangle = \frac{1}{a}\,\frac{1}{n^2}$$

$$E^1_{rel} = -\frac{1}{2mc^2}\left\{ (E^0)^2 + 2E^0\alpha\hbar c\left\langle \frac{1}{r}\right\rangle + \alpha^2\hbar^2c^2\left\langle \frac{1}{r^2}\right\rangle \right\}$$

$$E^0 = E_n = \frac{E_1}{n^2}$$

$$\rightsquigarrow \quad \frac{1}{a n^2} = \alpha m \frac{c}{\hbar} \frac{1}{n^2} = -\frac{2E_n}{\hbar c} \frac{1}{\alpha}$$

$$E_n = \frac{E_1}{n^2} = -\frac{1}{2} m c^2 \alpha^2 \frac{1}{n^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{(a n^2)^2} \frac{n}{l + \frac{1}{2}}$$

$$= \frac{4 E_n^2}{(\hbar c)^2} \frac{1}{\alpha^2} \frac{n}{l + 1/2}$$

$$\therefore \quad E^1_{rel} = -\frac{E_n^2}{2mc^2} \left\{ 1 + 2\alpha\hbar c \left(-\frac{2}{\hbar c} \frac{1}{\alpha} \right) + \alpha^2 (\hbar c)^2 \frac{4}{(\hbar c)^2 \alpha^2} \frac{n}{l + \frac{1}{2}} \right\}$$

$$= -\frac{E_n^2}{2mc^2} \left\{ 1 - 4 + 4 \frac{n}{l + 1/2} \right\}$$

$$\boxed{E^1_{rel} = -\frac{E_n^2}{2mc^2} \left\{ -3 + \frac{4n}{l + 1/2} \right\}}$$

• $n = 1$, $\ell = 0$

$$\{\ \} = -3 + 8 = 5$$

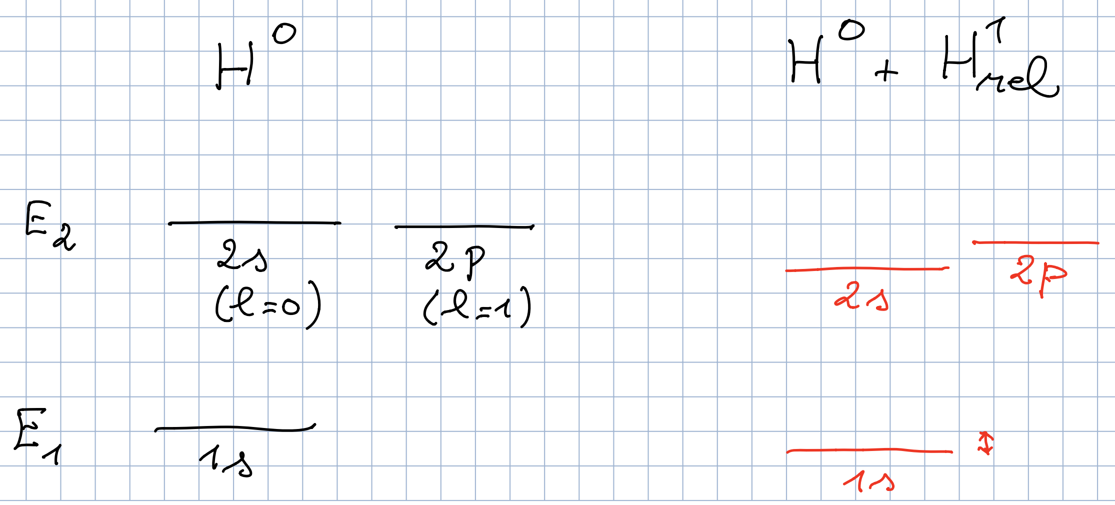
$$\frac{E_1^2}{2mc^2} \cdot 5 \simeq \frac{(13.6\ eV)^2}{(10^6\ eV)} \sim \underline{\underline{10^{-4}\ eV}}$$

$$E_1 \sim \alpha^2$$

• $n = 2$

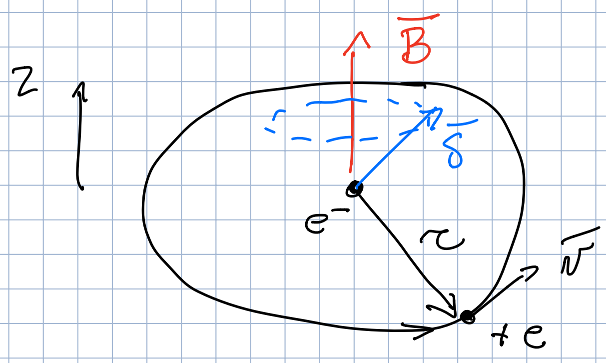
$\ell = 0$ $\qquad \{\ \} = -3 + 16 = \underline{\underline{13}}$

$\ell = 1$ $\qquad \{\ \} = -3 + 8 \cdot \frac{2}{3} = \underline{\underline{\frac{7}{3}}}$



2) SPIN - BAHN KOPPLUNG

RUHESYSTEM DES e^-



$$I = \frac{e}{T} \qquad v\,T = 2\pi r$$

- $\vec{B}$ - FELD (BIOT - SAVART) AM e^-

$$\vec{B} = \mu_0 \frac{I}{2r} \; \vec{e}_z \quad , \quad \varepsilon_0 \mu_0 = \frac{1}{c^2}$$

- $\vec{L}$ DES e^- IM RUHESYSTEM DES p

$$\vec{L} = m v r \; \vec{e}_z$$
$$= 2\pi m \frac{r^2}{T} \; \vec{e}_z$$

- $$\underbrace{\bar{B}}_{} = \mu_0 \, \frac{e}{\underbrace{2r}_{}} \, \frac{1}{\underbrace{2\pi m r^2}_{}} \underbrace{\left(\frac{2\pi m r^2}{T} \, \bar{e}_z \right)}_{\bar{L}}$$

$$\bar{B} = \frac{e}{4\pi \varepsilon_0 c^2} \, \frac{1}{m r^3} \, \bar{L}$$

- $$\bar{\mu} = \gamma \, \bar{S}$$

$\Uparrow$

→ KLASSISCHE ELECTRO $\quad \gamma = \frac{q}{2m}$

$$= -\frac{e}{2m}$$

$q = -e$

$(e > 0)$

→ QM $\quad \underline{\underline{\gamma}} = \underset{\substack{\| \\ 2}}{g} \left(-\frac{e}{2m} \right)$

$$(\overset{\text{DIRAC}}{2}.\underbrace{0023}_{\text{QFT}}\ldots)$$

$$\bar{\mu}_e = -\frac{e}{m} \, \bar{S}$$

- $H^1_{SO} = - \underbrace{\bar{\mu}_e} \cdot \bar{B}$

$$= \underbrace{\frac{e}{m}} \frac{e}{4\pi \varepsilon_0 c^2} \frac{1}{\underbrace{m} r^3} \bar{L} \cdot \bar{S}$$

$$\alpha = \frac{e^2}{4\pi \varepsilon_0 \hbar c}$$

$$H^1_{SO} = \frac{1}{2} \alpha \frac{\hbar}{c} \frac{1}{m^2 r^3} \bar{L} \cdot \bar{S}$$

↑

(THOMAS PRÄZESSION)

! RECHNUNG OBEN NUR QUALITATIV !

$$\bar{J} = \bar{L} + \bar{S}$$

↓

$$J^2 = L^2 + S^2 + 2 \underbrace{\bar{L} \cdot \bar{S}}$$

$$\bar{L} \cdot \bar{S} = \frac{1}{2} \left(J^2 - L^2 - S^2 \right)$$

↓ EIGENWERTE

$$= \frac{\hbar^2}{2} \left(j(j+1) - \ell(\ell+1) - 3/4 \right)$$

$$J^2,\ J_z,\ L^2,\ S^2$$

KOMMUTIEREN

$$|\psi^0\rangle = |\psi_{n j m_j \ell s}\rangle$$

$$\left[H^1_{SO} ,\ \begin{matrix} J^2 \\ J_z \\ L^2 \\ S^2 \end{matrix} \right] = 0$$

$$E^1_{SO} = \langle \psi_{n j m_j \ell s} | H^1_{SO} | \psi_{n j m_j \ell s} \rangle$$

$$= \frac{1}{2} \alpha \frac{\hbar}{c} \frac{1}{m^2} \frac{\hbar^2}{2} \left[j(j+1) - \ell(\ell+1) - \frac{3}{4} \right]$$

$$\cdot \left\langle \frac{1}{r^3} \right\rangle$$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\ell(\ell+1)(\ell+\frac{1}{2})} \frac{1}{a^3 n^3}$$

$$E_n^2 \qquad E_n = -\frac{1}{2} m c^2 \alpha^2 \frac{1}{n^2}$$

$$\frac{1}{a n^2} = \alpha m \frac{c}{\hbar} \frac{1}{n^2} = -2 \frac{E_n}{\hbar c} \frac{1}{\alpha}$$

$$\frac{1}{(a n)^3} = \frac{n}{a} \left(\frac{1}{a n^2} \right)^2 = \frac{n}{a} \frac{4 E_n^2}{(\hbar c)^2 \alpha^2}$$

$$E^1_{SO} = E_n^2 \frac{n}{\alpha a} \frac{1}{m^2} \frac{\hbar^3}{c} \frac{1}{(\hbar c)^2}$$

$$\cdot \frac{1}{l(l+1)(l+\frac{1}{2})} \left[j(j+1) - l(l+1) - \frac{3}{4} \right]$$

$$a = \frac{1}{m \alpha} \frac{\hbar}{c}$$

$$\alpha a m^2 = m \frac{\hbar}{c}$$

$$E^1_{SO} = \frac{E_n^2}{m c^2} n \frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+1)(l+\frac{1}{2})}$$