$\Longrightarrow$ VORLESUNG 22 QM

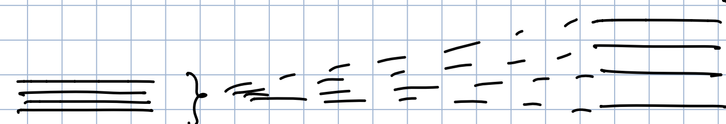
ZEIT UNABHÄNGIGE STÖRUNGSTHEORIE

$$H^0 |\psi^0\rangle = E^0 |\psi^0\rangle$$

$$H^1 |\psi^1\rangle = E^1 |\psi^1\rangle$$

$$H^0 \longrightarrow H^0 + H^1$$

E^0



$\psi_1^0, \dots, \psi_n^0$ $\qquad\qquad$ $\psi_1^1, \dots \psi_n^1$

$$E_1^1 \dots E_n^1$$

$$E^0 + E^1$$

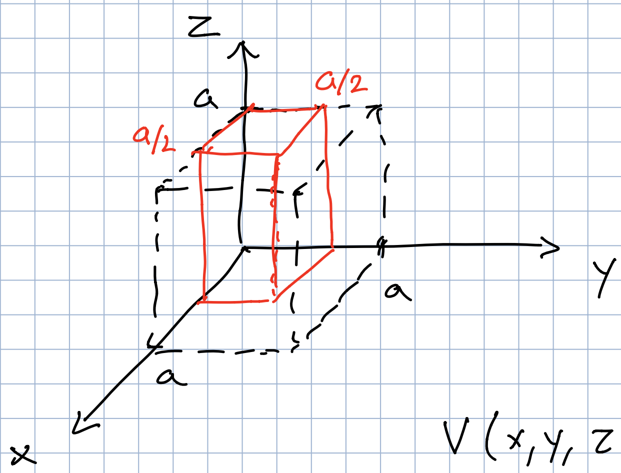
$\longrightarrow$ 1.) $\quad W_{ij} \equiv \langle \psi_i^0 | H^1 | \psi_j^0 \rangle$

$$i, j = 1 \dots n$$

2) $\quad |\psi^0\rangle = \alpha_1 |\psi_1^0\rangle + \dots + \alpha_n |\psi_n^0\rangle$

$$\begin{pmatrix} W_{11} & \cdots & W_{1n} \\ & & \\ W_{n1} & \cdots & W_{nn} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = E^1 \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}$$

⇒ BEISPIEL   3 DIM POT. TOPF



$$V(x,y,z) = \begin{cases} 0, & 0<x<a \\ & 0<y<a \\ & 0<z<a \\ \infty, & \text{AUSSERHALB} \end{cases}$$

$$H^0 = \frac{\hat{p}^2}{2m} + V(x,y,z)$$

$$\psi^0_{n_x n_y n_z}(x,y,z) = \left(\frac{2}{a}\right)^{3/2} \sin\Big(\underbrace{n_x \frac{\pi}{a}}_{k_x} x\Big) \sin\Big(\underbrace{n_y \frac{\pi}{a}}_{k_y} y\Big) \sin\Big(\underbrace{n_z \frac{\pi}{a}}_{k_z} z\Big)$$

$$n_x = 1, 2, \ldots$$

$$E^0_{n_x n_y n_z} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$= \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \left(n_x^2 + n_y^2 + n_z^2\right)$$

STÖRUNG $\quad H^1 = \begin{cases} V_0 & 0 < x < a/2 \\ & 0 < y < a/2 \\ & 0 < z < a \\ 0 & \text{AUSSERHALB} \end{cases}$

• GRUNDZUSTAND

$$n_x = n_y = n_z = 1$$

$$E^0_{111} = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 3$$

$$E^1 = \langle \psi^0_{111} | H^1 | \psi^0_{111} \rangle$$

• 1° ANREGUNG

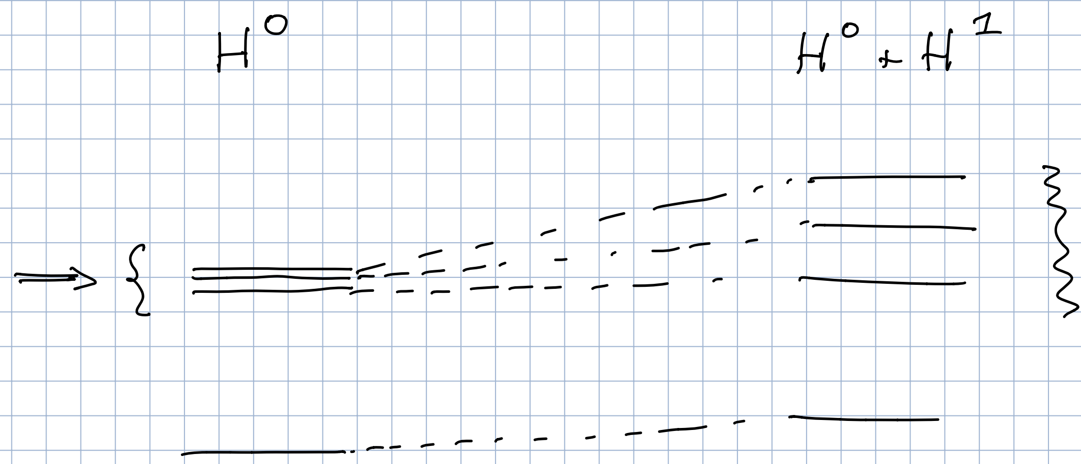
$\psi^0_{112} =: \psi^0_a : n_x = 1, \; n_y = 1, \; n_z = 2$

$\psi^0_{121} =: \psi^0_b : n_x = 1, \; n_y = 2, \; n_z = 1$

$\psi^0_{211} =: \psi^0_c : n_x = 2, \; n_y = 1, \; n_z = 1$

3 - FACH ENTARTUNG

$$E_a^0 = E_b^0 = E_c^0 = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 6$$



1) $W_{ij} = \langle \psi_i^0 | H^1 | \psi_j^0 \rangle$

2) $|\psi^0\rangle = \alpha |\psi_a^0\rangle + \beta |\psi_b^0\rangle + \gamma |\psi_c^0\rangle$

$$\begin{pmatrix} W_{aa} & W_{ab} & W_{ac} \\ W_{ab}^* & W_{bb} & W_{bc} \\ W_{ac}^* & W_{bc}^* & W_{cc} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$$\Rightarrow \quad W_{aa} = \langle \psi_a^0 | H^1 | \psi_a^0 \rangle$$

$$= \left(\frac{2}{a}\right)^3 V_0 \int^{a/2} dx \quad \sin^2\left(\frac{\pi}{a} x\right)$$

$$\cdot \int^{a/2} dy \quad \sin^2\left(\frac{\pi}{a} y\right)$$

$$\cdot \int_0^{a} dz \quad \sin^2\left(\frac{2\pi}{a} z\right)$$

$$\sin^2 x = \frac{1}{2}\left(1 - \cos 2x\right)$$

$$W_{aa} = \left(\frac{2}{a}\right)^3 V_0 \left(\frac{1}{2}\ \frac{a}{2}\right)\left(\frac{1}{2}\ \frac{a}{2}\right)\left(\frac{1}{2}\, a\right)$$

$$= \frac{V_0}{4}$$

$$W_{aa} = W_{bb} = W_{cc} = \frac{V_0}{4}$$

$$W_{ab} = \langle \psi_a^0 \,|\, H^1 \,|\, \psi_b^0 \rangle$$

$$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \ \sin^2\left(\frac{\pi}{a} x\right)$$

$$\cdot \int_0^{a/2} dy \ \sin\left(\frac{\pi}{a} y\right) \sin\left(\frac{2\pi}{a} y\right)$$

$$\cdot \int_0^{a} dz \ \underbrace{\sin\left(\frac{2\pi}{a} z\right) \sin\left(\frac{\pi}{a} z\right)}_{-\frac{1}{2}\left(\cancel{\cos\left(\frac{3\pi}{a} z\right)} - \cos\cancel{\left(\frac{\pi}{a} z\right)}\right)}$$

$$= 0$$

$$W_{ac} = 0$$

$$W_{bc} = \langle \psi_b^0 | H^1 | \psi_c^0 \rangle$$

$$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \; \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{2\pi}{a} x\right)$$

$$\cdot \int_0^{a/2} dy \; \sin\left(\frac{\pi}{a} y\right) \sin\left(\frac{2\pi}{a} y\right)$$

$$\cdot \int_0^{a} dz \; \underbrace{\sin^2\left(\frac{\pi}{a} z\right)}_{\downarrow \; \frac{1}{2}}$$

$$\int_0^{a/2} dx \; \underbrace{\sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{2\pi}{a} x\right)}_{-\frac{1}{2}\left(\cos \frac{3\pi}{a} x \; - \; \cos \frac{\pi}{a} x\right)}$$

$$= -\frac{1}{2} \frac{a}{\pi} \left(\frac{1}{3} \sin\left(\frac{3\pi}{a} x\right) - \sin\left(\frac{\pi}{a} x\right)\right)\Bigg|_0^{a/2}$$

$$\left(- \frac{1}{3} - 1 \right)$$

$$= \left(\frac{a}{\pi}\right) \frac{2}{3}$$

$$W_{bc} = \left(\frac{2}{a}\right)^3 V_0 \left(\frac{a}{\pi}\frac{2}{3}\right)\left(\frac{a}{\pi}\frac{2}{3}\right)\left(\frac{1}{2}a\right)$$

$$= \frac{16}{9}\,\frac{V_0}{\pi^2}$$

$$= \frac{V_0}{4}\,\underbrace{\left(\frac{8}{3\pi}\right)^2}_{K}$$

$$W = \frac{V_0}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix}$$

$$\Rightarrow \qquad E^1 = \frac{V_0}{4}\,\omega$$

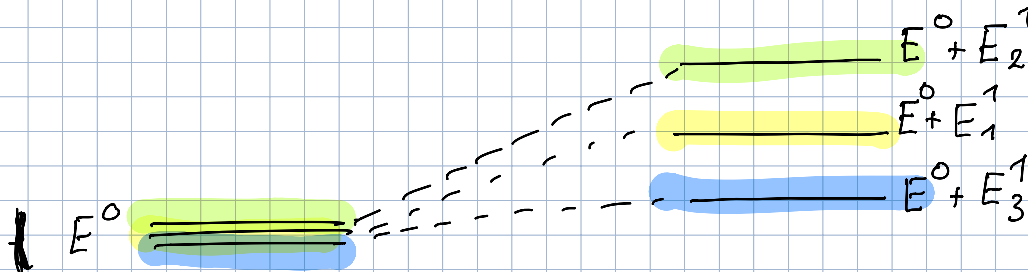
$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \omega \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$$
\begin{vmatrix} 1-w & 0 & 0 \\ 0 & 1-w & K \\ 0 & K & 1-w \end{vmatrix} = 0
$$

$$
(1-w)^3 - K^2(1-w) = 0
$$

$$
(1-w)\left((1-w)^2 - K^2\right) = 0
$$

$$
\begin{cases}
w_1 = 1 & \longrightarrow \quad E_1^1 = \dfrac{V_0}{4} \\
w_2 = 1 + K & \longrightarrow \quad E_2^1 = \dfrac{V_0}{4}(1+K) \\
w_3 = 1 - K & \longrightarrow \quad E_3^1 = \dfrac{V_0}{4}(1-K)
\end{cases}
$$



- $\omega_1 = 1$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$$\beta + K\gamma = \beta \Rightarrow \gamma = 0$$

$$K\beta + \gamma = \gamma \Rightarrow \beta = 0$$

$$\alpha = 1$$

$$\omega_1 = 0 \Rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|\Psi_a^0\rangle$$

- $\omega_{\substack{2\\3}} = 1 \pm K$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = (1 \pm K) \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$$\alpha = (1 \pm K)\,\alpha \implies \alpha = 0$$

$$\beta + K\gamma = (1 \pm K)\,\beta$$

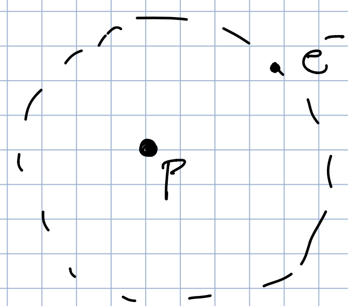
$$(1+K) \longrightarrow \beta = \gamma = \frac{1}{\sqrt{2}}$$

$$(1-K) \longrightarrow \beta = -\gamma = \frac{1}{\sqrt{2}}$$

$$\omega_2 = 1 + K \qquad \frac{1}{\sqrt{2}}\left(|\psi_b^0\rangle + |\psi_c^0\rangle\right)$$

$$\omega_3 = 1 - K \qquad \frac{1}{\sqrt{2}}\left(|\psi_b^0\rangle - |\psi_c^0\rangle\right)$$

$\Longrightarrow$ FEINSTRUKTUR DES H-ATOM



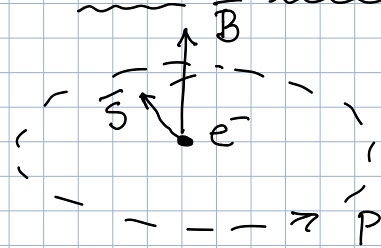
BOHR $E_n = \frac{E_1}{n^2}$ $n = 1, \dots, \infty$

$\rightsquigarrow$ $E_1 = -\left(\frac{1}{2} mc^2\right) \alpha^2 \simeq -13.6\ eV$

$T = \frac{p^2}{2m}$

FEINSTRUKTUR

DIRAC $\left\{ \begin{array}{l} \text{1) RELATIVISTISCHE KORREKTUR} \\ \text{2) SPIN-BAHN KOPPLUNG} \end{array} \right.$



1) REL. KORREKTUREN

N. REL. $\quad T = \frac{p^2}{2m}$

$$E = \frac{p^2}{2m} + mc^2$$

REL.

$$E = \sqrt{c^2 p^2 + m^2 c^4} = m_{rel}\, c^2 \qquad m_{rel} = \frac{m}{\sqrt{1 - v^2/c^2}}$$

$$= mc^2 \sqrt{1 + \frac{p^2}{m^2 c^2}}$$

$$\Big\downarrow \quad p \ll mc$$

$$\simeq mc^2 \left(1 + \frac{1}{2} \frac{p^2}{m^2c^2} - \frac{1}{8} \left(\frac{p^2}{m^2c^2} \right)^2 + \dots \right)$$

$$E = \underbrace{mc^2 + \frac{p^2}{2m}}_{\text{N. REL}} - \underbrace{\frac{1}{8} \frac{p^4}{m^3 c^2}}_{1^\circ\ \text{KORREKTUR}} + \dots$$

$$= mc^2 + \frac{p^2}{2m} \left(1 - \frac{1}{2} \frac{p^2/2m}{mc^2} \right)$$

$$\langle T \rangle = \langle \frac{p^2}{2m} \rangle \sim 10 \text{ eV}$$

$$mc^2 \simeq 511 \text{ keV}$$

$$\frac{\langle T \rangle}{mc^2} \sim 0.2 \quad 10^{-4}$$

NICHT REL

GUTE NÄHERUNG !

$$\Rightarrow \begin{cases} H^0 = \dfrac{\hat{p}^2}{2m} - \dfrac{\alpha \hbar c}{r} \\ H^1_{rel} = -\dfrac{1}{8} \dfrac{\hat{p}^4}{m^3 c^2} \end{cases}$$

THEOREM

$$\to [H^0, A] = 0 \qquad A^\dagger = A$$

$$\to [H^1, A] = 0$$

$$H^0 \quad \underbrace{|\psi_a^0\rangle , \ |\psi_b^0\rangle}_{\text{SELBE } E^0} \rightsquigarrow$$

AUCH EIGENF. VON A

$$\begin{cases} A\,|\psi_a^0\rangle = \underline{\underline{\mu}}\,|\psi_a^0\rangle \\ A\,|\psi_b^0\rangle = \underline{\underline{\nu}}\,|\psi_b^0\rangle \end{cases}$$

$$\underline{\underline{\mu \neq \nu}} \implies W_{ab} = \langle \psi_a^0 | H^1 | \psi_b^0 \rangle$$
$$= 0$$

$$\longrightarrow \begin{pmatrix} W_{aa} & 0 \\ 0 & W_{bb} \end{pmatrix}$$

$$W_{ab} = \langle \psi_a^0 | H^1 | \psi_b^0 \rangle$$

$$0 = \langle \psi_a^0 | [A, H^1] | \psi_b^0 \rangle$$

$$= \langle \psi_a^0 | A H^1 - H^1 A | \psi_b^0 \rangle$$

$$= (\mu - \nu) \underbrace{\langle \psi_a^0 | H^1 | \psi_b^0 \rangle}_{\underline{W_{ab}}}$$

$$\mu \neq \nu$$

$$[H^0, L^2] = 0 \qquad [H^0, L_z] = 0$$

$$\psi_{n\ell m}$$

$$[H^1, L^2] = [H^1, L_z] = 0$$

$$E_n^0$$

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

$$= -\frac{1}{8} \frac{1}{m^3 c^2} \langle \psi^0 | \hat{p}^4 | \psi^0 \rangle$$

$$\left(\frac{\hat{p}^2}{2m} + \hat{V} \right) |\psi^0\rangle = E^0 |\psi^0\rangle$$

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

$$E^1_{rel} = -\frac{1}{2} \frac{1}{mc^2} \langle \psi^0 | \underbrace{(E^0 - \hat{V})^2}_{(E^0)^2 - 2E^0\hat{V} + \hat{V}^2} | \psi^0 \rangle$$

$$\rightsquigarrow \quad \hat{V} = -\frac{\alpha \hbar c}{r}$$

$$E^1_{rel} = -\frac{1}{2mc^2}\left\{ (E^0)^2 - 2E^0 \langle \hat{V} \rangle + \langle \hat{V}^2 \rangle \right\}$$

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

$$\left\langle \frac{1}{r} \right\rangle = \left\langle \psi^0 \middle| \frac{1}{r} \middle| \psi^0 \right\rangle$$