

English Summary:

$$\text{Dirac eq. } i\hbar \frac{\partial}{\partial t} \psi = (c \underline{\alpha} \cdot \underline{p} + m_0 c^2 \beta) \psi$$

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\text{probab. continuity eq. } \partial_k j^k = 0$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \text{ spinor}$$

7.4 Nonrelativistic limit

$$i\hbar \frac{\partial}{\partial t} \psi = (c \underline{\alpha} \cdot \underline{\Pi} + m_0 c^2 \beta + e\phi) \psi$$

$$\underline{\Pi} := \underline{p} - e \underline{A}, \quad \psi = \begin{pmatrix} \varphi_a \\ \varphi_b \end{pmatrix} \begin{array}{l} E > 0 \text{ particle} \\ E < 0 \text{ antipart.} \end{array}$$

$$\text{nonrelativist.: } \begin{array}{l} E - m_0 c^2 \ll m_0 c^2 \\ e\phi \ll m_0 c^2 \end{array}$$

$$\Rightarrow i\hbar \dot{\varphi}_a = \left[\frac{1}{2m_0} (\underline{p} - e \underline{A})^2 - \frac{e\hbar}{2m_0} \underline{\sigma} \cdot \underline{B} + e\phi \right] \varphi_a$$

$$\text{Pauli eq. } \varphi_a = \begin{pmatrix} \varphi_{a+} \\ \varphi_{a-} \end{pmatrix}$$

7.5 H-Atom

$$\text{Rotationssymm. Pot.: } H = c \underline{\alpha} \cdot \underline{p} + m_0 c^2 \beta + V(r)$$

$$p_r := \frac{1}{r} (\underline{r} \cdot \underline{p} - i\hbar)$$

$$\alpha_r := \frac{1}{r} \underline{\alpha} \cdot \underline{r}$$

$$\hbar Q := \beta (\underline{\sigma} \cdot \underline{L} + \hbar)$$

} hermitesche Op.

$$\Rightarrow H = c \alpha_r p_r + \frac{i\hbar}{r} \alpha_r \beta \hbar Q + m_0 c^2 \beta + V(r)$$

$$\text{Beweis: } \alpha_r p_r + \frac{i}{r} \alpha_r \beta \hbar Q = \alpha_r \left[\frac{1}{r} (\underline{r} \cdot \underline{p} - i\hbar) + \frac{i}{r} \beta^2 (\underline{\sigma} \cdot \underline{L} + \hbar) \right]$$

$$= \frac{\alpha_r}{r} (\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L})$$

$$= \frac{1}{2} \left[(\underline{\alpha} \cdot \underline{r})(\underline{\alpha} \cdot \underline{p}) + \underbrace{i(\underline{\alpha} \cdot \underline{r})(\underline{\sigma} \cdot \underline{L})}_{i(\underline{\alpha} \cdot \underline{r})(\underline{\sigma} \cdot \underline{p}) - i r^2 (\underline{\alpha} \cdot \underline{p})} \right]$$

$$= \underline{\alpha} \cdot \underline{p}$$

Es gilt $[\hbar Q, H] = 0$

\Rightarrow es ex. gemeinsame Eigenzustände zu $H, \hbar Q$.

Eigenwerte von $\hbar Q$:

$$\begin{aligned}(\hbar Q)^2 &= \beta(\underline{\sigma} \cdot \underline{L} + \hbar) \beta(\underline{\sigma} \cdot \underline{L} + \hbar) = \underbrace{\beta^2}_{1} (\underline{\sigma} \cdot \underline{L} + \hbar)^2 \quad \text{denn } [\beta, \underline{\sigma}] = 0 \\ &= \underbrace{(\underline{\sigma} \cdot \underline{L})(\underline{\sigma} \cdot \underline{L})}_{L^2 + i\underline{\sigma}(\underline{L} \times \underline{L})} + 2\hbar \underline{\sigma} \cdot \underline{L} + \hbar^2 \\ &= L^2 + \hbar(\underline{\sigma} \cdot \underline{L}) + \hbar^2 = \underbrace{J^2}_{\substack{= \\ =}} \left(\underline{L} + \frac{\hbar}{2} \underline{\sigma} \right)^2 + \frac{\hbar^2}{4}\end{aligned}$$

$$= \begin{pmatrix} [1, \underline{\sigma}] & 0 \\ 0 & -[1, \underline{\sigma}] \end{pmatrix}$$

$$\text{denn } \left(\underline{L} + \frac{\hbar}{2} \underline{\sigma} \right)^2 = L^2 + \hbar(\underline{\sigma} \cdot \underline{L}) + \frac{\hbar^2}{4} \underbrace{\underline{\sigma}^2}_3$$

$$\boxed{(\hbar Q)^2 = J^2 + \frac{\hbar^2}{4}}$$

J^2 hat die Eigenwerte $\hbar^2 j(j+1)$ mit $j = l \pm s$

$$\Rightarrow (\hbar Q)^2 |j\rangle = \left(\hbar^2 j(j+1) + \frac{\hbar^2}{4} \right) |j\rangle = \hbar^2 \underbrace{\left(j + \frac{1}{2} \right)^2}_{= \frac{1}{2}, \frac{3}{2}, \dots}} |j\rangle$$

$$\Rightarrow \boxed{\hbar Q |j\rangle = \hbar q |j\rangle} \quad \text{mit } q = \pm \frac{1}{2}, \pm \frac{3}{2}, \dots$$

Es bleibt das radiale Eigenwertproblem für

$$H = c \alpha_r p_r + \frac{i\hbar c}{r} \alpha_q \alpha_r \beta + m_0 c^2 \beta + V(r)$$

Geignete Darstellung für α_r :

$$(\alpha_r)^2 = \frac{1}{2} (\underline{\alpha} \cdot \underline{r})(\underline{\alpha} \cdot \underline{r}) = \frac{1}{2} \sum_{\mu, \nu=1}^3 \alpha^\mu \alpha^\nu x^\mu x^\nu$$

$$= \frac{1}{2r^2} \sum_{\mu\nu} (\alpha^\mu \alpha^\nu + \alpha^\nu \alpha^\mu) x^\mu x^\nu$$

$$= \frac{1}{r^2} \sum_{\mu\nu} x^\mu x^\nu = 1$$

$$\alpha_r \beta + \beta \alpha_r = \frac{1}{r} (\alpha \beta + \beta \alpha) r = 0$$

Für $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ lässt sich dies durch die Darstellung

$$\alpha_r = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \alpha_r = \alpha_r^\dagger \text{ erfüllen:}$$

$$\alpha_r \beta = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad \beta \alpha_r = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$$

$$\text{Es gilt } p_r = \frac{1}{r} (\underbrace{c p_r}_{\frac{\hbar r}{i}} - i \hbar) = -i \hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right)$$

$$\Rightarrow H = \hbar c \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) - \frac{e \hbar g}{r} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + m_0 c^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + V \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Ansatz für den Radialanteil: $\begin{pmatrix} \varphi_a \\ \varphi_b \end{pmatrix} \sim \frac{1}{r} \begin{pmatrix} F(r) \\ G(r) \end{pmatrix}$

eingesetzt in Eigenwertgl. für H:

$$H \begin{pmatrix} F/r \\ G/r \end{pmatrix} = E \begin{pmatrix} F/r \\ G/r \end{pmatrix}$$

$$- \frac{\hbar c}{r} \frac{dG}{dr} - \frac{e \hbar g}{r^2} G + \frac{m_0 c^2}{r} F + \frac{V}{r} F = E \frac{F}{r}$$

$$\frac{\hbar c}{r} \frac{dF}{dr} - \frac{e \hbar g}{r^2} F - \frac{m_0 c^2}{r} G + \frac{V}{r} G = E \frac{G}{r} \quad \left(V = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r} \right)$$

also:

$$(E - m_0 c^2 - V) F + \hbar c \frac{dG}{dr} + \frac{e \hbar g}{r} G = 0$$

$$(E + m_0 c^2 - V) G - \hbar c \frac{dF}{dr} + \frac{e \hbar g}{r} F = 0$$

$$\text{Skalentransf.} : a_1 = \frac{m_0 c^2 + E}{\hbar c}, \quad a_2 = \frac{m_0 c^2 - E}{\hbar c}$$

$$a = \sqrt{a_1 a_2} = \frac{\sqrt{m_0^2 c^4 - E^2}}{\hbar c}$$

$$\rho := a r, \quad \gamma := \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137} \quad \text{„Feinstrukturkonstante“},$$

$$\frac{V}{\hbar c a} = -\frac{\lambda}{\rho}$$

$$\left(\frac{d}{d\rho} + \frac{\rho}{\rho}\right) G - \left(\frac{a_2}{a} - \frac{\lambda}{\rho}\right) F = 0$$

$$\left(\frac{d}{d\rho} - \frac{\rho}{\rho}\right) F - \left(\frac{a_1}{a} + \frac{\lambda}{\rho}\right) G = 0$$

Randbed. : $F(\rho), G(\rho)$ regulär bei $\rho \rightarrow 0$
 $\rightarrow 0$ für $\rho \rightarrow \infty$

Betrachte $|E| < m_0 c^2 \rightarrow a_1, a_2 > 0, a \in \mathbb{R}$
gebundene Zustände

Asymptot. Verhalten :

$$\rho \rightarrow \infty \Rightarrow \left. \begin{aligned} G' &= \frac{a_2}{a} F \\ F' &= \frac{a_1}{a} G \end{aligned} \right\} \Rightarrow \begin{aligned} G'' &= G \Rightarrow G \sim e^{-\rho} \\ F'' &= F \Rightarrow F \sim e^{-\rho} \end{aligned} \quad (e^{+\rho} \text{ divergiert!})$$

$$\rho \rightarrow 0 \Rightarrow G' + \frac{\rho}{\rho} G + \frac{\lambda}{\rho} F = 0$$

$$F' - \frac{\rho}{\rho} F - \frac{\lambda}{\rho} G = 0$$

$$\text{Ansatz: } F(\rho) = f_0 \rho^\lambda, \quad G(\rho) = g_0 \rho^\lambda$$

$$\Rightarrow (\lambda + \rho) f_0 + \gamma f_0 = 0$$

$$(\lambda - \rho) f_0 - \gamma g_0 = 0$$

Nichttriviale Lösungen f_0, g_0, λ

$$(\lambda+q)(\lambda-q) + \gamma^2 = \lambda^2 - q^2 + \gamma^2 \stackrel{!}{=} 0$$

$$\lambda = \pm \sqrt{q^2 - \gamma^2} \quad \begin{matrix} ! \\ > 0 \\ \text{regulär bei } \gamma \rightarrow 0 \end{matrix}$$

$$\underline{\text{Ansatz}}: \begin{cases} F(\varrho) = \varrho^2 e^{-\varrho} f(\varrho) \\ G(\varrho) = \varrho^2 e^{-\varrho} g(\varrho) \end{cases} \left\{ \begin{array}{l} g' - g + \frac{\lambda+q}{\varrho} g - \left(\frac{a_2}{\lambda} - \frac{a_1}{\varrho}\right) f = 0 \\ f' - f + \frac{\lambda-q}{\varrho} f - \left(\frac{a_1}{\lambda} + \frac{a_2}{\varrho}\right) g = 0 \end{array} \right.$$

Lösung mit Potenzreihenansatz:

$$f(\varrho) = \sum_{k=0}^{\infty} f_k \varrho^k, \quad g(\varrho) = \sum_{k=0}^{\infty} g_k \varrho^k$$

$$f'(\varrho) = \sum_{k=1}^{\infty} k f_k \varrho^{k-1} = \sum_{k=0}^{\infty} (k+1) f_{k+1} \varrho^k$$

$$\frac{f(\varrho)}{\varrho} = \sum_{k=0}^{\infty} f_k \varrho^{k-1} = \frac{f_0}{\varrho} + \sum_{k=0}^{\infty} f_{k+1} \varrho^k$$

usw. für $g'(\varrho)$, $g(\varrho)/\varrho$

Koeffizientenvergleich:

$$\underline{O\left(\frac{1}{\varrho}\right)}: \begin{cases} (\lambda+q)g_0 + \gamma f_0 = 0 \\ (\lambda-q)f_0 - \gamma g_0 = 0 \end{cases}$$

$\Rightarrow f_0, g_0$ (bis auf Norm.)
falsch

$O(\varrho^k)$, $k=0,1,\dots$:

$$\boxed{\begin{cases} (\lambda+q+k+1)g_{k+1} - g_k + \gamma f_{k+1} - \frac{a_2}{\lambda} f_k = 0 & (1) \\ (\lambda-q+k+1)f_{k+1} - f_k - \gamma g_{k+1} - \frac{a_1}{\lambda} g_k = 0 & (2) \end{cases}}$$

Rekursion!

$$(1) \cdot a - (2) \cdot a_2: [a(\lambda+q+k+1) + a_2 \gamma] g_{k+1} = [a_2(\lambda-q+k+1) - a \gamma] f_{k+1} \quad (3)$$

Verhalten für große k : $a k g_{k+1} \approx a_2 k f_{k+1} \Rightarrow f_k \approx \frac{a}{a_2} g_k$

eingesetzt in (1): $(k+1)g_{k+1} \approx 2g_k$
 $\rightarrow \frac{g_{k+1}}{g_k} \approx \frac{2}{k+1} \Rightarrow g_{k+1} \approx \frac{2^{k+1}}{(k+1)!} g_0$

$\Rightarrow g(\rho) \sim \exp(2\rho)$
 $f(\rho) \sim \exp(2\rho)$

Falls die Pot.reihe $g(\rho) = \sum_k g_k \rho^k$, $f(\rho) = \sum_k f_k \rho^k$ nicht
abbrechen, divergiert $G(\rho) = \rho^2 \underset{F}{=} \underset{f}{=} g(\rho) \sim e^{+2\rho}$ für $\rho \rightarrow \infty$
 \nrightarrow Randbed.!

Daher Abbruch bei $k=n' \in \mathbb{N}_0$:

$f_{n'+1} = 0$, $g_{n'+1} = 0$

(1) $\Rightarrow -g_{n'} - \frac{a_2}{a} f_{n'} = 0 \Rightarrow a_2 f_{n'} = -a g_{n'}$ (1')

(2) $\Rightarrow -f_{n'} - \frac{a_1}{a} g_{n'} = 0 \Rightarrow a f_{n'} = -a_1 g_{n'}$, stimmt
mit (1') überein wegen $\frac{a_2}{a} = \frac{a_1}{a}$

(1') in (3) für $k+1=n'$:

$$\frac{a(\lambda + \gamma + n') + a_2 \gamma}{a} = - \frac{a_2(\lambda - \gamma + n') - a \gamma}{a_2}$$

$$2a(\lambda + n') = \left(\frac{a^2}{a_2} - a_2 \right) \gamma = \frac{2E}{\hbar c} \gamma$$

quadriert:

$$\frac{a^2(\lambda + n')^2}{\left(\frac{\hbar^2 c^4}{4E^2} - E^2 \right)^2} = \frac{E^2}{(\hbar c)^2} \gamma^2$$

$$E = \frac{m_0 c^2}{\sqrt{1 + \left(\frac{\gamma}{\lambda + n'} \right)^2}}$$

Feinstrukturformel

$\gamma \approx \frac{1}{137}$ Feinstrukturkonst.

$\lambda = \sqrt{q^2 - \gamma^2} = \sqrt{\left(\gamma + \frac{1}{2}\right)^2 - \gamma^2}$

erlaubte Energie-Eigenwerte $n' \in \mathbb{N}_0$ $\left(\begin{array}{l} j = \frac{1}{2}, \frac{3}{2}, \dots \\ j = l \pm s \end{array} \right)$

Entwicklung nach der Feinstrukturkonst. bis $O(\alpha^4)$:

$$E = m_0 c^2 \left[1 - \frac{1}{2} \left(\frac{\alpha}{n'+2} \right)^2 + \frac{3}{8} \left(\frac{\alpha}{n'+2} \right)^4 + O(\alpha^6) \right]$$

$$\lambda(\alpha) = |\gamma| \sqrt{1 - \left(\frac{\alpha}{n'} \right)^2} = |\gamma| \left[1 - \frac{1}{2} \left(\frac{\alpha}{n'} \right)^2 \right] + O(\alpha^4)$$

$$\frac{1}{(n'+2)^2} = \frac{1}{(n'+|\gamma| - \frac{\alpha^2}{2|\gamma|})^2} + O(\alpha^4)$$

$$= \frac{1}{n^2} \left(1 - \frac{\alpha^2}{2|\gamma|n} \right)^{-2} + O(\alpha^4)$$

$$= \frac{1}{n^2} \left(1 + \frac{\alpha^2}{|\gamma|n} \right) + O(\alpha^4)$$

Eingesetzt in E:

$$n = n' + |\gamma|$$

$$\begin{aligned} n' &= 0, 1, 2, \dots \\ |\gamma| &= j + \frac{1}{2} = 1, 2, \dots \\ &= l \pm s + \frac{1}{2} \end{aligned}$$

$$E = m_0 c^2 \left[1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^3} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) \right] + O(\alpha^6)$$

$$n = 1, 2, 3, \dots ; j = \frac{1}{2}, \frac{3}{2}, \dots, n - \frac{1}{2} \text{ (wegen } n = n' + j + \frac{1}{2} \text{)}$$

$$= l \pm s$$

Diskussion:

$$O(\alpha^0): E = m_0 c^2$$

$$O(\alpha^2): \Delta E^{(2)} = - m_0 c^2 \frac{\alpha^2}{2n^2} = - \frac{R_H}{n^2}$$

$$O(\alpha^4): \Delta E^{(4)} = - m_0 c^2 \frac{\alpha^4}{2n^3} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right)$$

Ruheenergie

nichtrelativist.
Energiespektrum
(entartet)

Feinstruktur-
Aufspaltung

(Aufhebung der j -Entartung)

$2(2j+1)$ -fache m_j -Entartung bleibt

Spektroskop. Bezeichnung der Feinstrukturterme $[n, l, j]$

$$n=1 \quad j = \frac{1}{2} : 1s_{1/2} \quad (n'=0)$$

$$n=2 \quad j = \frac{1}{2} : 2s_{1/2} \quad 2p_{1/2} \quad (n'=0)$$

$$j = \frac{3}{2} : \quad \quad \quad 2p_{3/2} \quad (n'=0)$$

...

