Wdh.: Dirac - Gleichung

$$i\hbar \frac{\partial}{\partial t}\psi = -i\hbar c \underline{\alpha}\,\underline{\nabla}\psi + m_0 c^2 \beta \psi$$

wobei $\alpha^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \sigma^\mu & 0 \end{pmatrix}$

$\beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$

Pauli - Spinmatrizen

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ; \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Bahn - Drehimpuls : $\underline{L} = \underbrace{\underline{r} \times \underline{p}}_{\text{Bahnraum}} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\text{Spinor Raum}}$

Spin - Operator: $\underline{\tilde{\sigma}} = \begin{pmatrix} \underline{\sigma} & 0 \\ 0 & \underline{\sigma} \end{pmatrix}$ $\qquad \tilde{\sigma}^1 = \begin{pmatrix} \sigma^1 & 0 \\ 0 & \sigma^1 \end{pmatrix}$

Gesamt Drehimpuls $\underline{J} = \underline{L} + \frac{\hbar}{2}\underline{\tilde{\sigma}}$ ist Erhaltungsgröße

d.h. $[J, H] = 0$

Einschub: Beweis der Beziehung

$$\boxed{i\underbrace{(\underline{\alpha}\,\underline{r})}\,\underline{r}\,\underline{p} - i r^2 \underbrace{(\underline{\alpha}\,\underline{p})} = i(\underline{\alpha}\,\underline{r})(\underline{\underline{\tilde{\sigma}}\,\underline{L}})}$$

$$\boxed{\underline{\alpha}\,\underline{r}} = \underbrace{\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix} x_1 + \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix} x_2 + \begin{pmatrix} 0 & \sigma^3 \\ \sigma^3 & 0 \end{pmatrix} x_3}_{\underline{\sigma}\,\underline{r}}$$

$$= \begin{pmatrix} \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} \\ (\;" \;) & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \end{pmatrix} = \begin{pmatrix} 0 & \underline{\sigma}\underline{r} \\ \underline{\sigma}\underline{r} & 0 \end{pmatrix}$$

$$\underline{\alpha}\underline{p} = \begin{pmatrix} \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & \overbrace{\begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}}^{\underline{\sigma}\underline{p}} \\ (\underline{\sigma}\underline{p}) & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \end{pmatrix} = \begin{pmatrix} 0 & \underline{\sigma}\underline{p} \\ \underline{\sigma}\underline{p} & 0 \end{pmatrix}$$

$$\tilde{\underline{\sigma}}\underline{L} = \begin{pmatrix} \sigma^1 & 0 \\ 0 & \sigma^1 \end{pmatrix} L_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix} L_2 + \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} L_3$$

$$= \begin{pmatrix} \begin{matrix} L_3 & L_1 - iL_2 \\ L_1 + iL_2 & -L_3 \end{matrix} & 0 \\ 0 & " \end{pmatrix} = \begin{pmatrix} \underline{\sigma}\underline{L} & 0 \\ 0 & \underline{\sigma}\underline{L} \end{pmatrix}$$

$$(\underline{\alpha}\underline{r})(\tilde{\underline{\sigma}}\underline{L}) = \begin{pmatrix} 0 & \overbrace{(\underline{\sigma}\underline{r})(\underline{\sigma}\underline{L})}^{M} \\ (\underline{\sigma}\underline{r})(\underline{\sigma}\underline{L}) & 0 \end{pmatrix} \qquad M = \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} \begin{pmatrix} L_3 & L_1 - iL_2 \\ L_1 + iL_2 & -L_3 \end{pmatrix}$$

$$M_{11} = x_3 (x_1 p_2 - x_2 p_1) + (x_1 - ix_2)(x_2 \underline{p_3} - \underline{x_3 p_3} + i \underline{x_3 p_1} - i x_1 \underline{p_3})$$

$$= x_3 (x_1 p_2 - x_2 p_1 + (x_1 - ix_2)(ip_1 - p_2)) + \underline{p_3} (x_2 - ix_1)(x_1 - ix_2)$$

$$= x_3 (i x_1 p_1 + i x_2 p_2) + x_3 i x_3 p_3 - x_3 i x_3 p_3 - p_3 (i x_2^2 + i x_1^2)$$

$$= \underline{\underline{i x_3 (\underline{r}\underline{p}) - i p_3 (\underline{r})^2}}$$

Rest analog

- nützliche Beziehung

$$\sigma^i \sigma^j = \delta_{ij} + i\varepsilon^{ijk}\sigma^k$$

$$\Rightarrow (\underline{\sigma}\,\underline{a})(\underline{\sigma}\,\underline{b}) = \underline{a}\,\underline{b} + i\underline{\sigma}(\underline{a}\times\underline{b})$$

7.5. Wasserstoffatom

Rotationssymm. Potenzial: $H = c\,\underline{\alpha}\,\underline{p} + m_0c^2\beta + V(r)$

$\boxed{\text{Def.:}}$

$$\left.\begin{aligned} p_r &:= \frac{1}{r}(\underline{r}\,\underline{p} - i\hbar) \\ \alpha_r &:= \frac{1}{r}\,\underline{\alpha}\,\underline{r} \\ \hbar Q &:= \beta(\underline{\tilde{\sigma}}\,\underline{L} + \hbar) \end{aligned}\right\}$$ hermitesche Operatoren

$$\Rightarrow \boxed{H = \underbrace{c\,\alpha_r p_r + \frac{ic}{r}\alpha_r\beta\hbar Q}_{c\cdot\underline{\alpha}\,\underline{p}} + m_0c^2\beta + V(r)}$$

Beweis:

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

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

$$= \frac{1}{r^2}\Big((\underline{\alpha}\,\underline{r})(\underline{r}\,\underline{p}) + i\underbrace{(\underline{\alpha}\,\underline{r})(\underline{\tilde{\sigma}}\,\underline{L})}_{i(\underline{\alpha}\,\underline{r})(\underline{r}\,\underline{p}) - ir^2(\underline{\alpha}\,\underline{p})}\Big)$$

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

$\blacksquare$

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

$\Rightarrow$ es existieren gemeinsame Eigenzustände zu $H, \hbar Q$

Eigenwerte von $\hbar Q$:

$$(\hbar Q)^2 = \beta(\tilde{\underline{\sigma}}\underline{L} + \hbar)\beta(\tilde{\underline{\sigma}}\underline{L} + \hbar) = \beta^2(\tilde{\underline{\sigma}}\underline{L} + \hbar)^2 \qquad \text{denn } [\beta, \tilde{\underline{\sigma}}] = 0$$

$$= \underbrace{(\tilde{\underline{\sigma}}\underline{L})(\tilde{\underline{\sigma}}\underline{L})}_{L^2 + i\sigma \underbrace{(\underline{L}\times\underline{L})}_{i\hbar\underline{L}}} + 2\hbar(\tilde{\underline{\sigma}}\underline{L}) + \hbar^2 \qquad \underline{L} = (\underline{r}\times\underline{p})\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$= L^2 + \hbar(\tilde{\underline{\sigma}}\underline{L}) + \hbar^2 = \underbrace{\left(\underline{L} + \frac{\hbar}{2}\tilde{\underline{\sigma}}\right)^2}_{\underline{J}} + \frac{\hbar^2}{4}$$

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

J^2 hat die Eigenwerte $\hbar j(j+1)$ mit $j = \ell \pm s$
$= \frac{1}{2}, \frac{3}{2}, \ldots$

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

$$\boxed{\hbar Q|j\rangle = \hbar q|j\rangle} \qquad \text{mit } q = \pm 1, \pm 2, \ldots$$

Es bleibt das radiale Eigenwertproblem für

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

Geeignete Darstellung für α_r: $\qquad \alpha_r := \frac{1}{r}\underline{\alpha}\,\underline{r}$

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

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

$$2\delta^{\mu\nu}$$

$$= \frac{1}{r^2} x^\mu x^\mu = \underline{\mathbb{1}} \qquad \left(\underline{\alpha}\,\underline{r} = \begin{pmatrix} 0 & \underline{\sigma}\,\underline{r} \\ \underline{\sigma}\,\underline{r} & 0 \end{pmatrix} \right)$$

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

Für $\beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$ lässt sich durch die Darstellung $\alpha_r = \begin{pmatrix} 0 & -i\mathbb{1} \\ i\mathbb{1} & 0 \end{pmatrix}$,

$\alpha_r = \alpha_r^+$ erfüllen.

$$\alpha_r\beta = \begin{pmatrix} 0 & i\mathbb{1} \\ i\mathbb{1} & 0 \end{pmatrix}, \qquad \beta\alpha_r = \begin{pmatrix} 0 & -i\mathbb{1} \\ -i\mathbb{1} & 0 \end{pmatrix}$$

- Es gilt: $p_r = \frac{1}{r}(\underbrace{\underline{r}\,\underline{p}}_{\frac{\hbar}{i} r \frac{\partial}{\partial r}} - i\hbar) = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$

$$\Rightarrow \boxed{\begin{array}{l} \text{Dirac gleichung für Radialanteil} \\ H = \hbar c \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \left(\frac{\partial}{\partial r} + \frac{1}{r}\right) - c\frac{\hbar q}{r}\begin{pmatrix} 0 & \mathbb{1} \\ 1 & 0 \end{pmatrix} + m_0 c^2 \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \\ \qquad + V\begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix} \end{array}}$$

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

eingesetzt in Eigenwertgleichung für H:

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

$$\Rightarrow \left[\begin{aligned} -\frac{\hbar c}{r}\frac{dG}{dr} - \frac{c\hbar q}{r^2}G + \frac{m_0c^2}{r}F + \frac{V}{r}F &= E\frac{F}{r} \\ \frac{\hbar c}{r}\frac{dF}{dr} - \frac{c\hbar q}{r^2}F - \frac{m_0c^2}{r}G + \frac{V}{r}G &= E\frac{G}{r} \end{aligned}\right.$$

bzw.:

$$(E - m_0c^2 - V)F + \hbar c\frac{dG}{dr} + \frac{c\hbar q}{r}G = 0$$

$$(E + m_0c^2 - V)G - \hbar c\frac{dF}{dr} + \frac{c\hbar q}{r}F = 0$$

Skalentransformation: $a_1 = \dfrac{m_0c^2 + E}{\hbar c}$

$a_2 = \dfrac{m_0c^2 - E}{\hbar c}$

$\rho := ar$ $\qquad a = \sqrt{a_1a_2} = \dfrac{\sqrt{m_0^2c^4 - E^2}}{\hbar c}$

$V = -\dfrac{e^2}{4\pi\varepsilon_0}\dfrac{1}{r}$ $\quad , \gamma := \dfrac{e^2}{4\pi\varepsilon_0\hbar c} \approx \dfrac{1}{137}$

$\dfrac{V}{\hbar c a} = -\dfrac{\gamma}{\rho}$ $\qquad \gamma$: „Feinstrukturkonstante"

$$\boxed{\begin{aligned} \left(\frac{d}{d\rho} + \frac{q}{\rho}\right)G - \left(\frac{a_2}{a} - \frac{\gamma}{\rho}\right)F &= 0 \\ \left(\frac{d}{d\rho} - \frac{q}{\rho}\right)F - \left(\frac{a_1}{a} + \frac{\gamma}{\rho}\right)G &= 0 \end{aligned}}$$

<u>Randbed.</u>: $F(\rho), G(\rho)$ regulär bei $\rho \to 0$

$\rightarrow 0$ für $\varrho \rightarrow \infty$

Betrachte $|E| < m_0 c^2 \Rightarrow \alpha_1, \alpha_2 > 0 \quad , \quad \alpha \in \mathbb{R}$

<u>gebundene Zustände</u>

Asymptotisches Verhalten:

- $\varrho \rightarrow \infty \Rightarrow \left.\boxed{\begin{aligned} G' &= \frac{\alpha_2}{\alpha} F \\ F' &= \frac{\alpha_1}{\alpha} G \end{aligned}}\right\} \quad \begin{aligned} G'' &= G \quad \rightarrow G \sim e^{-\varrho} \\ F'' &= F \quad \rightarrow F \sim e^{-\varrho} \end{aligned}$

  (e^{ϱ} divergiert → keine Lösung)

- $\varrho \rightarrow 0 \Rightarrow \boxed{\begin{aligned} G' + \frac{\kappa}{\varrho} G + \frac{\gamma}{\varrho} F &= 0 \\ F' - \frac{\kappa}{\varrho} F - \frac{\gamma}{\varrho} G &= 0 \end{aligned}}$