Plenum 4 – Musterlösung

$$\underbrace{\left[c\,\vec{\alpha}\,\vec{p} + \beta mc^2 + V(r)\right]}_{H_D}\psi(\vec{r}) = E\,\psi(\vec{r})$$

a) $[H_D, \vec{S}_D^2] = ?$

$$\vec{S}_D^2 = \frac{\hbar^2}{4}\begin{pmatrix} \vec{\sigma}^2 & 0 \\ 0 & \vec{\sigma}^2 \end{pmatrix} = \frac{3\hbar^2}{4}\mathbb{1}_{4\times 4} \Rightarrow [H_D, \vec{S}_D^2] = 0$$

Erhaltungsgröße!

$[H_D, S_i] = ?$

$$S_i = \frac{\hbar}{2}\begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix} ; \quad [S_i, \beta mc^2] = 0$$

$$[S_i, V(r)] = 0$$

$$[\alpha_j p_j, S_i] = \frac{\hbar}{2}\left[\begin{pmatrix} 0 & \sigma_j p_j \\ \sigma_j p_j & 0 \end{pmatrix}, \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}\right] = \frac{\hbar}{2}\begin{pmatrix} 0 & [\sigma_j, \sigma_i] p_j \\ [\sigma_j, \sigma_i] p_j & 0 \end{pmatrix} =$$

$$= \frac{\hbar}{2}\begin{pmatrix} 0 & 2i\,\varepsilon_{jik}\sigma_k p_j \\ 2i\,\varepsilon_{jik}\sigma_k p_j & 0 \end{pmatrix} = \frac{-2i\hbar}{2}(\vec{\alpha}\times\vec{p})_i \neq 0$$

$$[H_D, \vec{S}] = -ic\hbar(\vec{\alpha}\times\vec{p})$$

$$[H_D, L_i] = ? \qquad [V(r), L_i] = 0, \quad [\beta mc^2, L_i] = 0$$

$$[\alpha_j p_j, L_i] = [\alpha_j p_j, \varepsilon_{ikl} r_k p_l] = \alpha_j \varepsilon_{ikl}\underbrace{[p_j, r_k]}_{i\hbar\delta_{jk}} p_l =$$

$$= i\hbar\,\varepsilon_{ijl}\,\alpha_j p_l$$

$$\Rightarrow \quad [H_D, L_i] = ic\hbar(\vec{\alpha} \times \vec{p})_i \neq 0$$

$$[H_D, \vec{L}_D^2] = [H_D, L_i L_i] = [H_D, L_i]L_i + L_i[H_D, L_i] =$$

$$= ic\hbar\left((\vec{\alpha} \times \vec{p}) \cdot \vec{L} + \vec{L} \cdot (\vec{\alpha} \times \vec{p})\right) \neq 0$$

b) $$[H_D, \vec{J}_D] = [H_D, \vec{S}_D] + [H_D, \vec{L}_D] = 0 \;!$$

$\vec{J}_D$ ist Erhaltungsgröße

c) Pauli Darstellung : $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$

$$(E - V)\varphi = mc^2\varphi + c\vec{\sigma}\vec{p}\chi$$
$$(E - V)\chi = -mc^2\chi + c\vec{\sigma}\vec{p}\varphi$$

$$\varepsilon := E - mc^2$$

$$(\varepsilon - V)\varphi = c\vec{\sigma}\vec{p}\chi$$
$$(\varepsilon - V + 2mc^2)\chi = c\vec{\sigma}\vec{p}\varphi$$

$$\chi = \frac{1}{\varepsilon - V + 2mc^2} c\vec{\sigma}\vec{p}\varphi$$

Wir entwickeln um $\left(\frac{\varepsilon - V}{2mc^2}\right) << 1$

$$\frac{1}{\varepsilon - V + 2mc^2} = \frac{1}{2mc^2}\left(\frac{1}{1 + \frac{\varepsilon - V}{2mc^2}}\right) = \frac{1}{2mc^2}\left(1 - \frac{\varepsilon - V}{2mc^2}\right) + O\left(\frac{1}{m^3c^6}\right)$$

$$(\varepsilon - V)\varphi = \frac{c^2}{2mc^2}(\vec{\sigma}\vec{p})\left(1 - \frac{\varepsilon - V}{2mc^2}\right)(\vec{\sigma}\vec{p})\varphi = \overbrace{\frac{1}{2m}\underbrace{(\vec{\sigma}\vec{p})(\vec{\sigma}\vec{p})}_{\vec{p}^2}\varphi}^{1} +$$
$$\underbrace{-\frac{1}{4m^2c^2}(\vec{\sigma}\vec{p})(\varepsilon - V)(\vec{\sigma}\vec{p})\varphi}_{2}$$

$$-\frac{1}{4m^2c^2}(\vec\sigma\vec p)(\varepsilon - V)(\vec\sigma\vec p) = \overbrace{-\frac{1}{4m^2c^2}(\vec\sigma\vec p)(\vec\sigma\vec p)(\varepsilon - V)}^{2a} +$$

$$\left\{ V\vec\sigma\vec p = \vec\sigma\vec p\, V + \vec\sigma\,[V,\vec p] \right\}$$

$$\underbrace{-\frac{1}{4m^2c^2}(\vec\sigma\vec p)\cdot(\vec\sigma\cdot[V,\vec p])}_{2b}$$

$$2a = -\frac{1}{4m^2c^2}\,\vec p^{\,2}(\varepsilon - V)$$

$\Rightarrow$ Korrektur zu kinetische Energie

$$\varepsilon - V = E - V - mc^2 = \sqrt{p^2c^2 + m^2c^4} - mc^2 = mc^2\sqrt{1+\frac{p^2}{m^2c^2}} - mc^2 =$$

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

$$2a \cong -\frac{1}{4m^2c^2}\frac{(\vec p^{\,2})^2}{2m} = -\frac{1}{8m^3c^2}(\vec p^{\,2})^2$$

2b : von $(\vec\sigma\vec a)(\vec\sigma\vec b) = \vec a\cdot\vec b\,\mathbb{1} + i\vec\sigma\cdot(\vec a\times\vec b)$

wir bekommen :

$$(\vec\sigma\vec p)\cdot(\vec\sigma\cdot[V,\vec p]) = \underbrace{\vec p\,[V,\vec p]\,\mathbb{1}}_{\text{Darwin Term} \sim \Delta V} + i\vec\sigma\left(\vec p\times[V,\vec p]\right)$$

$$[V,p_i]\varphi = -i\hbar\left[V(r),\frac{\partial}{\partial r_i}\right]\varphi = -i\hbar\left(V\frac{\partial}{\partial r_i}\varphi - \frac{\partial}{\partial r_i}(V\varphi)\right) =$$

$$= i\hbar\left(\frac{\partial}{\partial r_i}V\right)\varphi = i\hbar\frac{\partial V}{\partial r}\frac{\partial r}{\partial r_i}\varphi = i\hbar\frac{\partial V}{\partial r}\frac{\partial\sqrt{r_i r_i}}{\partial r_i}\varphi = i\hbar\frac{1}{r}\frac{\partial V}{\partial r}r_i\varphi$$

$$[V, p_i] = i\hbar \frac{1}{r}\frac{\partial V}{\partial r} r_i$$

$$[V, \vec{p}] = i\hbar \frac{1}{r}\frac{\partial V}{\partial r}\vec{r}$$

$$i\vec{\sigma}\left(\vec{p}\times[V,\vec{p}]\right) = -i\vec{\sigma}\left([V,\vec{p}]\times\vec{p}\right) = \hbar\underbrace{\vec{\sigma}}_{2\vec{S}}\frac{1}{r}\frac{\partial V}{\partial r}\underbrace{(\vec{r}\times\vec{p})}_{\vec{L}}$$

$$(2b) = -\frac{1}{4m^2c^2}\Delta V \mathbb{1} - \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{S}\cdot\vec{L}$$

Zusammen:

$$\varepsilon\varphi = \left\{\Big[\underbrace{V + \frac{\vec{p}^2}{2m}}_{\text{nicht-relativistischer Teil}} \underbrace{- \frac{1}{8m^3c^2}(\vec{p}^2)^2}_{\text{Korrektur zu Kinetische Energie}} \underbrace{- \frac{1}{4m^2c^2}\Delta V}_{\text{Darwin Term}}\Big]\mathbb{1} \underbrace{- \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{S}\cdot\vec{L}}_{\text{Spin-Bahn Kopplung}}\right\}\varphi$$

d) $[\vec{p}^2, \vec{L}] = 0$, $[(\vec{p}^2)^2, \vec{L}] = 0$, $\underbrace{[V, \vec{L}] = 0 \;, [\Delta V, \vec{L}] = 0}_{\text{weil } V(r) \text{ Zentralpotential ist}}$

$$[\vec{L}\cdot\vec{S}, L_i] = [L_j S_j, L_i] = [L_j, L_i] S_j = i\varepsilon_{jik} L_k S_j = -i\vec{S}\times\vec{L}$$

$$[\vec{L}\cdot\vec{S}, S_i] = [L_j S_j, S_i] = L_j[S_j, S_i] = i\,\varepsilon_{jik} S_k L_j = -i\vec{L}\times\vec{S} = i\vec{S}\times\vec{L}$$

$$[\vec{L}\cdot\vec{S}, \vec{J}] = [\vec{L}\cdot\vec{S}, \vec{L}+\vec{S}] = 0\,!$$

$\vec{J}$ ist Erhaltungsgrösse

Auch:

$[\vec{L}^2, \vec{L}\cdot\vec{S}] = 0$ und $[\vec{S}^2, \vec{L}\cdot\vec{S}] = 0$

also auch $\vec{L}^2$ und $\vec{S}^2$ sind Erhalten

c) Was sind die gute Quantenzahlen?

Ohne Spin-Bahn Kopplung	Mit Spin-Bahn-Koppl
$\vert l, m_l; s, m_s\rangle$	$\vert l, s; j, m_j\rangle$

$$\mathcal{Y}_{\substack{l,s\\ j,m_j}}(\theta,\phi) = \underbrace{C_{\substack{j=l\pm\frac{1}{2}\\ m_l,\, m_s=+\frac{1}{2}}}} \cdot Y_{l m_l} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \underbrace{C_{\substack{j=l\pm\frac{1}{2}\\ m_l+1,\, m_s=-\frac{1}{2}}}} \cdot Y_{l\, m_l+1} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Clebsch-Gordan Koeffiziente