QM Serie 3 Tipps

(Löse zuerst b))

3.1 Spin-Orbit

$SU(2) \times SU(2)$

$$\mathcal{H}_E(L,S) = \mathcal{D}_L \otimes \mathcal{D}_S \leftarrow \psi_L^{m_L} \otimes \psi_S^{m_S}$$

b)

$$= \bigoplus_{J=|L-S|}^{L+S} \mathcal{D}_J \leftarrow \psi_J^{m_J}(S,L) = \sum_{m_L m_S} (\;)$$

$$H_{S\text{-}O} = \tau_E(L,S)\, \vec{L}\cdot\vec{S}$$

$$\Delta E(L,S) = \tau_E(L,S) \langle \psi_J^{m_J}, \vec{L}\cdot\vec{S}, \psi_J^{m_J} \rangle$$

$$\hat{J}^2 = (L+S)^2 \qquad \vec{L}\cdot\vec{S} = \frac{1}{2}(\underset{j(j+1)\mathbb{1}}{J^2} - \underset{s(s+1)\mathbb{1}}{S^2} - \underset{l(l+1)\mathbb{1}}{L^2})$$

a) $H_Z \ll H_{SO}$

$$H_Z = -\mu_B(\underbrace{L_z + \overset{g_e}{2} S_z}) \cdot B$$

$= A$ in Formel (3)

$J_k \Rightarrow$ Drehimpulsoperator

Sei $A_k = T_{l=1}^{m=k}$ Wigner-Eckart:

$$\langle \psi_j^{m'}, A_k, \psi_j^m \rangle = (j m' \mathbb{1} k \,|\, j m)(-1)^{2j} \cdot \frac{\langle \tilde{\psi}_j \| A \| \psi_j \rangle}{\sqrt{2j+1}}$$

$\vec{J}$: $\quad J_{\pm 1} = \mp \frac{1}{\sqrt{2}} J_{\pm} \quad , \quad J_0 = J_3$

$$\langle \psi_j^{m'}, J_k \psi_j^m \rangle = (jm' \, 1 k \mid jm)(-1)^{2j} \frac{\langle \tilde{\psi} \| J \| \psi \rangle}{\sqrt{2j+1}}$$

(wieder Wigner-Eckart, aber für J)

P_J: Projektion auf $\mathcal{D}_J$

$$P_J A_k P_J = \tau P_J P_K P_J$$

$$\Rightarrow \quad P_J \vec{A} \cdot \vec{J} P_J = \tau P_J J^2 P_J = \tau j(j+1) P_J$$

$$\langle \tilde{\psi}_J^{m_J}, \vec{A} \cdot \vec{J}, \psi_J^{m_J} \rangle = \tau j(j+1)$$ ← Formel für τ

(→ auflösen
→ das was auf'm Blatt steht (Formel (3)))

Wie löst man damit

$H_Z = -\mu_B (\underbrace{L_z}_{\to J_z + S_z} + 2S_z) B$?

$\longrightarrow J_z + S_z \quad (J_z = S_z + L_z)$

$$\Delta E = \langle \psi_j^m | H_z | \psi_j^m \rangle$$

$$= -\mu_B B \langle \psi_j^m | J_z + S_z | \psi_j^m \rangle$$

$$\langle \psi_j^m | S_z | \psi_j^m \rangle = \underbrace{\frac{\langle \psi_j^m | \vec{S}\cdot\vec{J} | \psi_j^m \rangle}{j(j+1)}} \underbrace{\langle \psi_j^m | J_3 | \psi_j^m \rangle}_{= m}$$

$$\left\{ \vec{S}\cdot\vec{J} = \frac{1}{2}\Big(\underbrace{(J-S)^2}_{= L} - \underbrace{J^2 - S^2}_{\text{bekannt}} \Big) \right\}$$

$$= -\frac{1}{2} \cdot \frac{\ell(\ell+1) - j(j+1) - s(s+1)}{j(j+1)} \cdot m$$

$\Rightarrow$ Aufgabe 1 vollständig vorgerechnet :-)

Take-home message von dieser Aufgabe:

Proportionalität der Operatoren wegen Wigner-Eckart

② $$U_B \otimes U_S \big| \mathcal{H}_a^{(N)} (\text{geg. Kcht}) = \bigoplus_{LS} m_{LS} \mathcal{D}_L \otimes \mathcal{D}_S$$

$$\chi_{n_1,l_1 \ldots n_N l_N}(\varphi_B, \varphi_S)$$

$$\chi_{n_1 l_1, \ldots, n_N l_N}(\varphi_B, \varphi_S) = \sum_{LS} m_{LS}\, \chi_{\mathcal{D}_L}(\varphi_B)\, \chi_{\mathcal{D}_S}(\varphi_S)$$

$$\chi_{\mathcal{D}_L}(A), \quad A \in SU(2)$$

$$\parallel$$

$$\chi_{\mathcal{D}_L}(\underbrace{UAU^*}_{\text{Diagonal}})$$

Rotation um z-Achse

$$= \begin{pmatrix} e^{i\varphi\frac{B}{2}} & 0 \\ 0 & e^{-i\varphi\frac{B}{2}} \end{pmatrix} \xrightarrow{R(\cdots)} SO(3) \quad \varphi_B$$

$$\chi_{\mathcal{D}_L}(\varphi_B) = \sum_{m_L=-L}^{L} e^{-im_L\varphi_B} \quad (\text{QM } 1)$$

$$\chi_{\mathcal{D}_L} \otimes \chi_{\mathcal{D}_S}(\varphi_B, \varphi_S) = \chi_{\mathcal{D}_L}(\varphi_B)\, \chi_{\mathcal{D}_S}(\varphi_S)$$

$$= \sum_{m_L=-L}^{L} \sum_{m_S=-S}^{S} e^{-im_L\varphi_B - im_S\varphi_S}$$

$$\varphi_{\alpha_1 \ldots \alpha_N} \xmapsto{\varphi_B, \varphi_S} \left(e^{-iL_z\varphi_B} \otimes e^{-iS_z\varphi_S}\right) \varphi_{\alpha_1 \ldots \alpha_N}$$

$$L_z = \sum_{i=1}^{N} L_z^i \qquad \varphi_{\alpha_1} = \psi_{n_1 l_1 m_{l_1}} \otimes u_{m_{s_1}} \mapsto e^{-iL_z^1\varphi_B} \psi_{n_1 l_1 m_{l_1}}$$

$$\otimes\, e^{-iS_z^1\varphi_S} u_{m_{s_1}} \qquad =$$

$$e^{-im_{l_1}\varphi_B}\, e^{-im_{s_1}\varphi_S} \underbrace{\left(\psi_{n_1 l_1 m_{l_1}} \otimes u_{m_{s_1}}\right)}_{\varphi_{\alpha_1}}$$

$$\varphi_{\alpha_1} \cdots \varphi_N \longmapsto \prod_{j=1}^{N} e^{-im_{l_j}\varphi_B} \cdot \prod_{k=1}^{N} e^{-im_{s_k}\varphi_S}\, \varphi_{\alpha_1} \cdots \varphi_{\alpha_N}$$

$$\underbrace{\sum}_{\substack{\text{alle Det die} \\ \text{in der Konfiguration} \\ (n_1, l_1) \ldots (n_N, l_N) \\ \text{auftreten}}} \left\langle \varphi_{\alpha_1 \cdots \alpha_N},\, U_B(\varphi_B) \otimes U_S(\varphi_S)\, \varphi_{\alpha_1 \cdots \alpha_N} \right\rangle = \sum e^{-i\left(\sum_{i=1}^{N} m_{l_i}\right)\varphi_B} \cdot e^{-i\left(\sum_{i=1}^{N} m_{s_i}\right)\varphi_S}$$

Bsp $\quad 2p: \quad (1,1)(1,1)$

$$(\underbrace{n_1}_{=1}, \underbrace{l_1}_{=1}, m_{l_1}, m_{s_1})(\underbrace{n_2}_{=1}, \underbrace{l_2}_{=1}, m_{l_2}, m_{s_2}) = (m_{l_1}, m_{s_1})(m_{l_2}, m_{s_2})$$

Symbolreihe	$\sum_{i=1,2} m_{l_i}$ *	$\sum_{i=1,2} m_{s_i} = m_S$
$(1,\frac{1}{2})(1,-\frac{1}{2})$	2	0
$(1,\frac{1}{2})(0,\frac{1}{2})$	1	1
$(1,\frac{1}{2})(0,-\frac{1}{2})$	1	0
$(0,\frac{1}{2})(0,-\frac{1}{2})$	0	0
$(1,-\frac{1}{2})(-1,\frac{1}{2})$	0	0
$(1,-\frac{1}{2})(0,\frac{1}{2})$	1	0
$(1,\frac{1}{2})(-1,\frac{1}{2})$	0	1
$(1,\frac{1}{2})(-1,-\frac{1}{2})$ ...	0	0

$* = m_L$

$m_S \backslash m_L$	2	1	0
1	0	0 1	0 1
0	1	2	3
	0	1 0	2 1

rot

$$\mathcal{D}_L \otimes \mathcal{D}_S$$

$$m_L = -L, -L+1, \dots, L$$

$$m_S = -S, \dots, S$$

$1\times$: $\mathcal{D}_2 \otimes \mathcal{D}_0$

$m_S \backslash m_L$	2	1	0	-1	-2
0	1	1	1	1	1

- rot: nach Abzug von $\mathcal{D}_2 \otimes \mathcal{D}_0$
- blau: nach Abzug von $\mathcal{D}_1 \otimes \mathcal{D}_1$

$1\times$: $\mathcal{D}_1 \otimes \mathcal{D}_1$

$m_S \backslash m_L$	2	1	0	-1	1

$$\Rightarrow \quad U_B \otimes U_S \Big|_{\chi_a^{(2)}\,(1,1)(1,1)} = \mathcal{D}_2 \otimes \mathcal{D}_0 \oplus \mathcal{D}_1 \otimes \mathcal{D}_1 \oplus \mathcal{D}_0 \otimes \mathcal{D}_0$$

Endresultat

Alternativ: Merkt PC III Skript