

Beispiel 1: Lösung

[1] Hamiltonoperator:

$$\mathbf{H} = -\frac{1}{\hbar} \mathbf{S}_z + \frac{1}{\hbar^3} \mathbf{S}_z^3 + \frac{4}{\hbar^4} \{ \underline{\mathbf{S}}^2 - (\underline{\mathbf{S}}^{(1)})^2 - (\underline{\mathbf{S}}^{(2)})^2 \}^2$$

[2a] CG-Koeffizienten:

$$\begin{aligned} \langle \tfrac{3}{2}, 2-s; \tfrac{1}{2}s | 22 \rangle &= \delta_{s,+1/2} & \dots & s=\pm \tfrac{1}{2} \\ \langle \tfrac{3}{2}, 1-s; \tfrac{1}{2}s | 21 \rangle &= \frac{\sqrt{3}}{2} & \dots & s=+\tfrac{1}{2} \\ \langle \tfrac{3}{2}, 1-s; \tfrac{1}{2}s | 21 \rangle &= \frac{1}{2} & \dots & s=-\tfrac{1}{2} \\ \langle \tfrac{3}{2}, -s; \tfrac{1}{2}s | 20 \rangle &= \frac{1}{\sqrt{2}} & \dots & s=\pm \tfrac{1}{2} \\ \langle \tfrac{3}{2}, -1-s; \tfrac{1}{2}s | 2-1 \rangle &= \frac{1}{2} & \dots & s=+\tfrac{1}{2} \\ \langle \tfrac{3}{2}, -1-s; \tfrac{1}{2}s | 2-1 \rangle &= \frac{\sqrt{3}}{2} & \dots & s=-\tfrac{1}{2} \\ \langle \tfrac{3}{2}, -2-s; \tfrac{1}{2}s | 2-2 \rangle &= \delta_{s,-1/2} & \dots & s=\pm \tfrac{1}{2} \end{aligned}$$

$$\begin{aligned} \langle \tfrac{3}{2}, 1-s; \tfrac{1}{2}s | 11 \rangle &= -\frac{1}{2} & \dots & s=+\tfrac{1}{2} \\ \langle \tfrac{3}{2}, 1-s; \tfrac{1}{2}s | 11 \rangle &= \frac{\sqrt{3}}{2} & \dots & s=-\tfrac{1}{2} \\ \langle \tfrac{3}{2}, -s; \tfrac{1}{2}s | 10 \rangle &= (-1)^{s+1/2} \frac{1}{\sqrt{2}} & \dots & s=\pm \tfrac{1}{2} \\ \langle \tfrac{3}{2}, -1-s; \tfrac{1}{2}s | 1-1 \rangle &= -\frac{\sqrt{3}}{2} & \dots & s=+\tfrac{1}{2} \\ \langle \tfrac{3}{2}, -1-s; \tfrac{1}{2}s | 1-1 \rangle &= \frac{1}{2} & \dots & s=-\tfrac{1}{2} \end{aligned}$$

[2b] Gesamtdrehimpuls-Basis:

$$|(\tfrac{3}{2}\tfrac{1}{2})SM\rangle = \sum_{s=-1}^{+1} \langle \tfrac{3}{2}, M-s; \tfrac{1}{2}s | SM \rangle | \tfrac{3}{2}, M-s; \tfrac{1}{2}s \rangle$$

$$\begin{aligned} |(\tfrac{3}{2}\tfrac{1}{2})22\rangle &= | \tfrac{3}{2}\tfrac{3}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle \\ |(\tfrac{3}{2}\tfrac{1}{2})21\rangle &= \frac{1}{2}(\sqrt{3}| \tfrac{3}{2}\tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + | \tfrac{3}{2}\tfrac{3}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle) \\ |(\tfrac{3}{2}\tfrac{1}{2})20\rangle &= \frac{1}{\sqrt{2}}(| \tfrac{3}{2}-\tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + | \tfrac{3}{2}\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle) \\ |(\tfrac{3}{2}\tfrac{1}{2})2-1\rangle &= \frac{1}{2}(| \tfrac{3}{2}-\tfrac{3}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + \sqrt{3}| \tfrac{3}{2}-\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle) \\ |(\tfrac{3}{2}\tfrac{1}{2})2-2\rangle &= | \tfrac{3}{2}-\tfrac{3}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle \end{aligned}$$

$$\begin{aligned} |(\tfrac{3}{2}\tfrac{1}{2})11\rangle &= \frac{1}{2}(-| \tfrac{3}{2}\tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + \sqrt{3}| \tfrac{3}{2}\tfrac{3}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle) \\ |(\tfrac{3}{2}\tfrac{1}{2})10\rangle &= \frac{1}{\sqrt{2}}(-| \tfrac{3}{2}-\tfrac{1}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + | \tfrac{3}{2}\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle) \\ |(\tfrac{3}{2}\tfrac{1}{2})1-1\rangle &= \frac{1}{2}(-\sqrt{3}| \tfrac{3}{2}-\tfrac{3}{2}; \tfrac{1}{2}\tfrac{1}{2} \rangle + | \tfrac{3}{2}-\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2} \rangle) \end{aligned}$$

[3a] EW-Gleichung:

$$\mathbf{H} |(\tfrac{3}{2}\tfrac{1}{2})SM\rangle = E_{SM} |(\tfrac{3}{2}\tfrac{1}{2})SM\rangle$$

$$E_{SM} = M(M^2 - 1) + [2S(S+1) - 9]^2$$

[3b] EWe, EVen, Entartung:

EWe	EVen	Entartung
$E_{2-2} = 3$	$ (\tfrac{3}{2}\tfrac{1}{2})2-2\rangle$	1
$E_{21}=E_{20}=E_{2-1} = 9$	$ (\tfrac{3}{2}\tfrac{1}{2})21\rangle, (\tfrac{3}{2}\tfrac{1}{2})20\rangle, (\tfrac{3}{2}\tfrac{1}{2})2-1\rangle$	3
$E_{22} = 15$	$ (\tfrac{3}{2}\tfrac{1}{2})22\rangle$	1
$E_{11}=E_{10}=E_{1-1} = 25$	$ (\tfrac{3}{2}\tfrac{1}{2})11\rangle, (\tfrac{3}{2}\tfrac{1}{2})10\rangle, (\tfrac{3}{2}\tfrac{1}{2})1-1\rangle$	3

[4] Wahrscheinlichkeit $(+\frac{\hbar}{2}, -\frac{\hbar}{2})$:

$$\mathbf{Q}_{+\frac{\hbar}{2}, -\frac{\hbar}{2}} = | \tfrac{3}{2}, +\tfrac{1}{2} \rangle^{(1)} \langle \tfrac{3}{2}, +\tfrac{1}{2} | \otimes | \tfrac{1}{2}, -\tfrac{1}{2} \rangle^{(2)} \langle \tfrac{1}{2}, -\tfrac{1}{2} |$$

$$W = \langle (\tfrac{3}{2}\tfrac{1}{2})2-2 | \mathbf{Q}_{+\frac{\hbar}{2}, -\frac{\hbar}{2}} | (\tfrac{3}{2}\tfrac{1}{2})2-2 \rangle = 0$$

Beispiel 2: Lösung

[1] Hamiltonoperator H_0 :
$$H_0 = -\frac{4}{\hbar} S_z + \frac{1}{\hbar^3} S_z^3 + \frac{4}{\hbar^4} \{ \underline{S}^2 - (\underline{S}^{(1)})^2 - (\underline{S}^{(2)})^2 \}^2$$

[2a] CG-Koeffizienten: (siehe Beispiel 1)

[2b] Gesamtdrehimpuls-Basis: (siehe Beispiel 1)

[3a] EW-Gleichung für H_0 :
$$H_0 \left| \left(\frac{3}{2} \frac{1}{2} \right) SM \right\rangle = E_{SM}^{(0)} \left| \left(\frac{3}{2} \frac{1}{2} \right) SM \right\rangle$$

$$E_{SM}^{(0)} = M(M^2 - 4) + [2S(S + 1) - 9]^2$$

[3b] EWe, EVen, Entartung:

EWe	EVen	Entartung
$E_{21}^{(0)} = 6$	$\left \left(\frac{3}{2} \frac{1}{2} \right) 21 \right\rangle$	1
$E_{22}^{(0)} = E_{20}^{(0)} = E_{2-2}^{(0)} = 9$	$\left \left(\frac{3}{2} \frac{1}{2} \right) 22 \right\rangle, \left \left(\frac{3}{2} \frac{1}{2} \right) 20 \right\rangle, \left \left(\frac{3}{2} \frac{1}{2} \right) 2-2 \right\rangle$	3
$E_{2-1}^{(0)} = 12$	$\left \left(\frac{3}{2} \frac{1}{2} \right) 2-1 \right\rangle$	1
$E_{11}^{(0)} = 22$	$\left \left(\frac{3}{2} \frac{1}{2} \right) 11 \right\rangle$	1
$E_{10}^{(0)} = 25$	$\left \left(\frac{3}{2} \frac{1}{2} \right) 10 \right\rangle$	1
$E_{1-1}^{(0)} = 28$	$\left \left(\frac{3}{2} \frac{1}{2} \right) 1-1 \right\rangle$	1

[4] Energiekorrektur $\varepsilon_{\min}^{(1)}(\xi)$:
$$\mathbf{W} \left| \frac{3}{2}, m; \frac{1}{2}, s \right\rangle = m \left| \frac{3}{2}, m; \frac{1}{2}, s \right\rangle$$

$$\mathbf{u}_{\min} = \left| \left(\frac{3}{2} \frac{1}{2} \right) 21 \right\rangle = \frac{1}{2} (\sqrt{3} \left| \frac{3}{2} \frac{1}{2}; \frac{1}{2} \frac{1}{2} \right\rangle + \left| \frac{3}{2} \frac{3}{2}; \frac{1}{2} - \frac{1}{2} \right\rangle)$$

$$\mathbf{W} \left| \left(\frac{3}{2} \frac{1}{2} \right) 21 \right\rangle = \frac{\sqrt{3}}{4} \left(\left| \frac{3}{2} \frac{1}{2}; \frac{1}{2} \frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2} \frac{3}{2}; \frac{1}{2} - \frac{1}{2} \right\rangle \right)$$

$$\varepsilon_{\min}^{(1)}(\xi) = \frac{3\xi}{4}$$

[5] Energiekorrekturen $\varepsilon_{\min+1,\ell}^{(1)}(\xi)$:
$$\mathbf{W} \left| \left(\frac{3}{2} \frac{1}{2} \right) 22 \right\rangle = \frac{3}{2} \left| \frac{3}{2} \frac{3}{2}; \frac{1}{2} \frac{1}{2} \right\rangle = \frac{3}{2} \left| \left(\frac{3}{2} \frac{1}{2} \right) 22 \right\rangle$$

$$\mathbf{W} \left| \left(\frac{3}{2} \frac{1}{2} \right) 20 \right\rangle = \frac{1}{2\sqrt{2}} \left(- \left| \frac{3}{2} - \frac{1}{2}; \frac{1}{2} \frac{1}{2} \right\rangle + \left| \frac{3}{2} \frac{1}{2}; \frac{1}{2} - \frac{1}{2} \right\rangle \right) =$$

$$= \frac{1}{2} \left| \left(\frac{3}{2} \frac{1}{2} \right) 10 \right\rangle$$

$$\mathbf{W} \left| \left(\frac{3}{2} \frac{1}{2} \right) 2-2 \right\rangle = -\frac{3}{2} \left| \frac{3}{2} - \frac{3}{2}; \frac{1}{2} - \frac{1}{2} \right\rangle = -\frac{3}{2} \left| \left(\frac{3}{2} \frac{1}{2} \right) 2-2 \right\rangle$$

Matrix $\mathbf{W}$ bezüglich ONB $\{ |2, 2\rangle, |2, 0\rangle, |2, -2\rangle \}$:

$$\mathbf{W} = \begin{bmatrix} +\frac{3}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{3}{2} \end{bmatrix}$$

$$\varepsilon_{\min+1,1}^{(1)}(\xi) = +\frac{3}{2}\xi$$

$$\varepsilon_{\min+1,2}^{(1)}(\xi) = 0$$

$$\varepsilon_{\min+1,3}^{(1)}(\xi) = -\frac{3}{2}\xi$$

Beachte: Vollständige Aufhebung der Entartung des EW's $E_{\min+1}^{(0)} = 9$

Beispiel 3: Lösung

[1] Schrödingergleichung: $\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x) - E\right)u(x) = 0$

Bereich 1: $(\partial_x^2 + k^2)u_1(x) = 0 \implies k = \sqrt{\frac{2mE}{\hbar^2}}$

Bereich 2: $(\partial_x^2 + K^2)u_2(x) = 0 \implies K = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$

Bereich 3: $(\partial_x^2 + Q^2)u_3(x) = 0 \implies Q = \sqrt{\frac{2m(E-V_0/4)}{\hbar^2}}$

Bereich 4: $(\partial_x^2 + k^2)u_4(x) = 0 \implies k = \sqrt{\frac{2mE}{\hbar^2}}$

[2] Energie EW: $K = 2k \implies E + V_0 = 4E \implies E = \frac{V_0}{3} \implies Q = \frac{k}{2}$

[3,1] Matrix $\mathbf{Q}(-a)$: $\mathbf{Q}(-a) = \frac{1}{2} \begin{bmatrix} 3e^{-ika} & -e^{+i3ka} \\ -e^{-i3ka} & 3e^{+ika} \end{bmatrix}$

[3,2] Matrix $\mathbf{Q}(0)$: $\mathbf{Q}(0) = \frac{1}{8} \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix}$

[3,3] Matrix $\mathbf{Q}(+a)$: $\mathbf{Q}(+a) = \frac{1}{2} \begin{bmatrix} 3e^{+ika/2} & -e^{-i3ka/2} \\ -e^{+i3ka/2} & 3e^{-ika/2} \end{bmatrix}$

[4,1] Matrix $\mathbf{Q}(-a)$: $\mathbf{Q}(-a) = \frac{1}{2} \begin{bmatrix} -3 & +1 \\ +1 & -3 \end{bmatrix}$

[4,2] Matrix $\mathbf{Q}(0)$: $\mathbf{Q}(0) = \frac{1}{8} \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix}$

[4,3] Matrix $\mathbf{Q}(+a)$: $\mathbf{Q}(+a) = \frac{1}{2} \begin{bmatrix} +3i & -i \\ +i & -3i \end{bmatrix}$

[4,4] Transfermatrix $\mathbf{M}$: $\mathbf{M} = \mathbf{Q}(-a) \mathbf{Q}(0) \mathbf{Q}(a)$
 $\mathbf{Q}(-a) \mathbf{Q}(0) = \frac{1}{4} \begin{bmatrix} -3 & -1 \\ -1 & -3 \end{bmatrix}$
 $\mathbf{Q}(-a) \mathbf{Q}(0) \mathbf{Q}(+a) = \frac{1}{4} \begin{bmatrix} -5i & +3i \\ -3i & +5i \end{bmatrix}$
 $\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} -5i & +3i \\ -3i & +5i \end{bmatrix} \begin{bmatrix} A_4 \\ B_4 \end{bmatrix}$

[5,1] Berechnung: B_1, A_4 $A_1 = 1$ und $B_4 = 0$
 $\begin{bmatrix} 1 \\ B_1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} -5i & +3i \\ -3i & +5i \end{bmatrix} \begin{bmatrix} A_4 \\ 0 \end{bmatrix} \implies A_4 = \frac{4i}{5} \text{ und } B_1 = \frac{3}{5}$

[5,2] Unitarität: $|B_1|^2 + |A_4|^2 = 1$

[5,3] Streumatrix $\mathbf{S}$: $A_1 = 1$ und $B_4 = 0$
Ansatz: $\mathbf{S} = \begin{bmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{bmatrix}$ mit $|\alpha|^2 + |\beta|^2 = 1$
 $\begin{bmatrix} B_1 \\ A_4 \end{bmatrix} = \mathbf{S} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \implies \alpha = B_1 = \frac{3}{5}, \beta = A_4 = \frac{4i}{5}$