

Beispiel 1: Lösung

[1] Hamiltonoperator:

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

[2a] CG-Koeffizienten:

$$\begin{aligned} \langle 1, 2-s; 1, s | 22 \rangle &= 1 & \dots & s=1 \\ \langle 1, 2-s; 1, s | 22 \rangle &= 0 & \dots & s=0, -1 \\ \langle 1, 1-s; 1, s | 21 \rangle &= \frac{1}{\sqrt{2}} & \dots & s=0, 1 \\ \langle 1, 1-s; 1, s | 21 \rangle &= 0 & \dots & s=-1 \\ \langle 1, -s; 1, s | 20 \rangle &= \frac{1}{\sqrt{6}} & \dots & s=\pm 1 \\ \langle 1, -s; 1, s | 20 \rangle &= \frac{2}{\sqrt{6}} & \dots & s=0 \\ \langle 1, -1-s; 1, s | 2-1 \rangle &= \frac{1}{\sqrt{2}} & \dots & s=0, -1 \\ \langle 1, -1-s; 1, s | 2-1 \rangle &= 0 & \dots & s=1 \\ \langle 1, -2-s; 1, s | 2-2 \rangle &= 1 & \dots & s=-1 \\ \langle 1, -2-s; 1, s | 2-2 \rangle &= 0 & \dots & s=0, 1 \\ \langle 1, -s; 1, s | 00 \rangle &= \frac{1}{\sqrt{3}} & \dots & s=\pm 1 \\ \langle 1, -s; 1, s | 00 \rangle &= -\frac{1}{\sqrt{3}} & \dots & s=0 \end{aligned}$$

[2b] Gesamtdrehimpuls-Basis:

$$\begin{aligned} |(11)SM\rangle &= \sum_{s=-1}^{+1} \langle 1, M-s; 1, s | SM \rangle |1, M-s; 1, s\rangle \\ |(11)22\rangle &= |11; 11\rangle \\ |(11)21\rangle &= \frac{1}{\sqrt{2}}(|11; 10\rangle + |10; 11\rangle) \\ |(11)20\rangle &= \frac{1}{\sqrt{6}}(|1-1; 11\rangle + 2|10; 10\rangle + |11; 1-1\rangle) \\ |(11)2-1\rangle &= \frac{1}{\sqrt{2}}(|1-1; 10\rangle + |10; 1-1\rangle) \\ |(11)2-2\rangle &= |1-1; 1-1\rangle \\ |(11)1M\rangle &= \dots \text{ (siehe Beispiel 2)} \\ |(11)00\rangle &= \frac{1}{\sqrt{3}}(|1-1; 11\rangle - |10; 10\rangle + |11; 1-1\rangle) \end{aligned}$$

[3a] EW-Gleichung:

$$\mathbf{H} | (11)SM \rangle = E_{SM} | (11)SM \rangle$$

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

[3b] EWe, EVen, Entartung:

EWe	EVen	Entartung
$E_{00} = -4$	$ (11)00 \rangle$	1
$E_{10} = -2$	$ (11)10 \rangle$	1
$E_{11}=E_{1-1} = -1$	$ (11)11 \rangle, (11)1-1 \rangle$	2
$E_{20} = +2$	$ (11)20 \rangle$	1
$E_{21}=E_{2-1} = +3$	$ (11)21 \rangle, (11)2-1 \rangle$	2
$E_{22}=E_{2-2} = +6$	$ (11)22 \rangle, (11)2-2 \rangle$	2

[4] Wahrscheinlichkeit $(+\hbar, -\hbar)$:

$$\begin{aligned} \mathbf{Q}_{+\hbar, -\hbar} &= |1, +1\rangle^{(1)} \langle 1, +1| \otimes |1, -1\rangle^{(2)} \langle 1, -1| \\ W &= \langle (11)00 | \mathbf{Q}_{+\hbar, -\hbar} | (11)00 \rangle = \frac{1}{3} \end{aligned}$$

Beispiel 2: Lösung

[1] Hamiltonoperator H_0 :

$$H_0 = \frac{1}{\hbar^4} (\mathbf{S}_z)^4 + \frac{1}{\hbar^2} \{ \mathbf{S}^2 - (\mathbf{S}^{(1)})^2 - (\mathbf{S}^{(2)})^2 \}$$

[2a] CG-Koeffizienten:

$$\begin{aligned} \langle 1, 1-s; 1, s | 11 \rangle &= -\frac{1}{\sqrt{2}} \quad \dots \quad s=1 \\ \langle 1, 1-s; 1, s | 11 \rangle &= +\frac{1}{\sqrt{2}} \quad \dots \quad s=0 \\ \langle 1, 1-s; 1, s | 11 \rangle &= 0 \quad \dots \quad s=-1 \\ \\ \langle 1, -s; 1, s | 10 \rangle &= -\frac{1}{\sqrt{2}} \quad \dots \quad s=1 \\ \langle 1, -s; 1, s | 10 \rangle &= 0 \quad \dots \quad s=0 \\ \langle 1, -s; 1, s | 10 \rangle &= +\frac{1}{\sqrt{2}} \quad \dots \quad s=-1 \\ \\ \langle 1, -1-s; 1, s | 1-1 \rangle &= 0 \quad \dots \quad s=1 \\ \langle 1, -1-s; 1, s | 1-1 \rangle &= -\frac{1}{\sqrt{2}} \quad \dots \quad s=0 \\ \langle 1, -1-s; 1, s | 1-1 \rangle &= +\frac{1}{\sqrt{2}} \quad \dots \quad s=-1 \end{aligned}$$

[2b] Gesamtdrehimpuls-Basis:

$$\begin{aligned} |(11)SM\rangle &= \sum_{s=-1}^{+1} \langle 1, M-s; 1, s | SM \rangle |1, M-s; 1, s\rangle \\ |(11)11\rangle &= \frac{1}{\sqrt{2}} (-|10; 11\rangle + |11; 10\rangle) \\ |(11)10\rangle &= \frac{1}{\sqrt{2}} (-|1-1; 11\rangle + |11; 1-1\rangle) \\ |(11)1-1\rangle &= \frac{1}{\sqrt{2}} (-|1-1; 10\rangle + |10; 1-1\rangle) \\ \\ |(11)00\rangle &= \dots \quad (\text{siehe Beispiel 1}) \\ \\ |(11)2M\rangle &= \dots \quad (\text{siehe Beispiel 1}) \end{aligned}$$

[3a] EW-Gleichung für H_0 :

$$\begin{aligned} H_0 | (11)SM \rangle &= E_{SM}^{(0)} | (11)SM \rangle \\ E_{SM}^{(0)} &= S(S+1) + M^2 - 4 \end{aligned}$$

[3b] EWe, EVen, Entartung:

EWe	EVen	Entartung
$E_{00}^{(0)} = -4$	$ (11)00 \rangle$	1
$E_{10}^{(0)} = -2$	$ (11)10 \rangle$	1
$E_{11}^{(0)} = E_{1-1}^{(0)} = -1$	$ (11)11 \rangle, (11)1-1 \rangle$	2
$E_{20}^{(0)} = +2$	$ (11)20 \rangle$	1
$E_{21}^{(0)} = E_{2-1}^{(0)} = +3$	$ (11)21 \rangle, (11)2-1 \rangle$	2
$E_{22}^{(0)} = E_{2-2}^{(0)} = +18$	$ (11)22 \rangle, (11)2-2 \rangle$	2

[4] Energiekorrektur $\varepsilon_{\min}^{(1)}(\xi)$:

$$\begin{aligned} \mathbf{W} | 1, r; 1, s \rangle &= r s | 1, r; 1s \rangle \\ \mathbf{W} | (11)00 \rangle &= -\frac{1}{\sqrt{3}} (| 1-1; 11 \rangle + | 11; 1-1 \rangle) \\ \varepsilon_{\min}^{(1)}(\xi) &= -\frac{2\xi}{3} \end{aligned}$$

[5] Energiekorrekturen $\varepsilon_{\max, \ell}^{(1)}(\xi)$:

$$\begin{aligned} \mathbf{W} | (11)22 \rangle &= | 11; 11 \rangle = | (11)22 \rangle \\ \mathbf{W} | (11)2-2 \rangle &= | 1-1; 1-1 \rangle = | (11)2-2 \rangle \\ \varepsilon_{\max, \ell}^{(1)}(\xi) &= \xi \quad \ell = 1, 2 \end{aligned}$$

Beachte: Keine Aufhebung der Entartung des EW's $E_{\max}^{(0)}$