Beispiel 1:

(1)

$$\begin{aligned} &\text{Bereich 1+4:} \quad (\partial_x^2 + k^2)u(x) = 0 \qquad k = \sqrt{\tfrac{2m}{\hbar^2}E} \\ &\text{Bereich 2:} \quad (\partial_x^2 + K^2)u(x) = 0 \qquad K = \sqrt{\tfrac{2m}{\hbar^2}(E - V_0)} \\ &\text{Bereich 3:} \quad (\partial_x^2 + Q^2)u(x) = 0 \qquad Q = \sqrt{\tfrac{2m}{\hbar^2}(E + 4V_0)} \end{aligned}$$

(2)

$$\begin{aligned} &\text{Bereich 1+4:} \quad k = \sqrt{\tfrac{2m}{\hbar^2}(\tfrac{4}{3}V_0)} \\ &\text{Bereich 2:} \quad K = \sqrt{\tfrac{2m}{\hbar^2}(\tfrac{1}{3}V_0)} = \tfrac{k}{2} \\ &\text{Bereich 3:} \quad Q = \sqrt{\tfrac{2m}{\hbar^2}(\tfrac{16}{3}V_0)} = 2k \end{aligned}$$

(3)

$$\mathbf{Q}(-a) = \frac{1}{2}\begin{bmatrix} (1+\frac{K}{k})e^{i(K-k)(-a)} & (1-\frac{K}{k})e^{-i(K+k)(-a)} \\ (1-\frac{K}{k})e^{i(K+k)(-a)} & (1+\frac{K}{k})e^{-i(K-k)(-a)} \end{bmatrix} = \frac{1}{4}\begin{bmatrix} 3e^{i\frac{ka}{2}} & e^{i\frac{3ka}{2}} \\ e^{-i\frac{3ka}{2}} & 3e^{-i\frac{ka}{2}} \end{bmatrix}$$

$$\mathbf{Q}(0) = \frac{1}{2}\begin{bmatrix} 1+\frac{Q}{K} & 1-\frac{Q}{K} \\ 1-\frac{Q}{K} & 1+\frac{Q}{K} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 5 & -3 \\ -3 & 5 \end{bmatrix}$$

$$\mathbf{Q}(a) = \frac{1}{2}\begin{bmatrix} (1+\frac{k}{Q})e^{i(k-Q)a} & (1-\frac{k}{Q})e^{-i(k+Q)a} \\ (1-\frac{k}{Q})e^{i(k+Q)a} & (1+\frac{k}{Q})e^{-i(k-Q)a} \end{bmatrix} = \frac{1}{4}\begin{bmatrix} 3e^{-ika} & e^{-i3ka} \\ e^{i3ka} & 3e^{ika} \end{bmatrix}$$

(4) $ka = \pi$:

$$\mathbf{Q}(-a) = \frac{i}{4}\begin{bmatrix} 3 & -1 \\ 1 & -3 \end{bmatrix}$$

$$\mathbf{Q}(0) = \frac{1}{2}\begin{bmatrix} 5 & -3 \\ -3 & 5 \end{bmatrix}$$

$$\mathbf{Q}(a) = \frac{1}{4}\begin{bmatrix} -3 & -1 \\ -1 & -3 \end{bmatrix}$$

$$\mathbf{M}(-a,0,a) = \mathbf{Q}(-a)\,\mathbf{Q}(0)\,\mathbf{Q}(a) = \frac{i}{4}\begin{bmatrix} -5 & 3 \\ -3 & 5 \end{bmatrix}$$

(5) $A_1 = 1\,,\, B_4 = 0$:

$$\begin{bmatrix} 1 \\ B_1 \end{bmatrix} = \frac{i}{4}\begin{bmatrix} -5 & 3 \\ -3 & 5 \end{bmatrix}\begin{bmatrix} A_4 \\ 0 \end{bmatrix} = \begin{bmatrix} -\frac{5i}{4}A_4 \\ -\frac{3i}{4}A_4 \end{bmatrix}$$

$$A_4 = i\tfrac{4}{5} \; ; \; B_1 = \tfrac{3}{5}$$

$$|\,B_1\,|^2 + |\,A_4\,|^2 = \tfrac{9}{25} + \tfrac{16}{25} = 1$$

Beispiel 2:

(1) $\mathbf{H} \;=\; 8\hbar\,\mathbf{S}_z + 4\big(\vec{\mathbf{S}}^2 - (\vec{\mathbf{S}}^{(1)})^2 - (\vec{\mathbf{S}}^{(2)})^2\big)$

$\vec{\mathbf{S}} \;=\; \vec{\mathbf{S}}^{(1)} + \vec{\mathbf{S}}^{(2)} \;;\; 2\,\vec{\mathbf{S}}^{(1)} \cdot \vec{\mathbf{S}}^{(2)} \;=\; \vec{\mathbf{S}}^2 - (\vec{\mathbf{S}}^{(1)})^2 - (\vec{\mathbf{S}}^{(2)})^2$

(2a) $\big\{\,\big|\,m,s\big\rangle : m = \pm\frac{1}{2},\pm\frac{3}{2} \;;\; s = \pm\frac{1}{2}\big\} \longrightarrow \big\{\,\big|\,(\frac{3}{2}\frac{1}{2})SM\big\rangle : S = 1,2 \;;\; -S \le M \le +S\big\}$

Kurzschreibweise: $\big|\,(\frac{3}{2}\frac{1}{2})SM\big\rangle \;=\; \big|\,SM\big\rangle$

$\big|\,SM\big\rangle \;=\; \sum_{s=\pm\frac{1}{2}} \big\langle\frac{3}{3}, M-s; \frac{1}{2}, s\,\big|\,SM\big\rangle\;\big|\,M-s,s\big\rangle$

(a) Δ–Ungleichung: $|\frac{3}{2}-\frac{1}{2}| \le S \le \frac{3}{2}+\frac{1}{2} \Longleftrightarrow S \;=\; 1,2$

(b) Summen–Regel: $M \;=\; m+s$

EW–Gleichung: $\mathbf{H}\,\big|\,SM\big\rangle \;=\; \hbar^2\big(8M + 4\big\{S(S+1) - \frac{3}{2}\cdot\frac{5}{2} - \frac{1}{2}\cdot\frac{3}{2}\big\}\big)\,\big|\,SM\big\rangle$

EWe: $E_{SM} \;=\; \hbar^2\big(8M + 4S(S+1) - 18\big)$

EVen: $\big|\,SM\big\rangle \;=\; \big|\,(\frac{3}{2}\frac{1}{2})SM\big\rangle \;;\; S = 1,2 \;;\; -S \le M \le +S$

$$E_{1M} \;=\; \hbar^2(8M-10) \;=\; \hbar^2\left\{\begin{array}{rcl} -2 & \ldots & M=1 \\ -10 & \ldots & M=0 \\ -18 & \ldots & M=-1 \end{array}\right.$$

$$E_{2M} \;=\; \hbar^2(8M+6) \;=\; \hbar^2\left\{\begin{array}{rcl} 22 & \ldots & M=2 \\ 14 & \ldots & M=1 \\ 6 & \ldots & M=0 \\ -2 & \ldots & M=-1 \\ -10 & \ldots & M=-2 \end{array}\right.$$

Zusammenfassung:
$E_{1,0} = E_{2,-2} = -10\hbar^2 \Longrightarrow$ **Entartung = 2**
$E_{1,1} = E_{2,-1} = -2\hbar^2 \Longrightarrow$ **Entartung = 2**
$E_{1,-1} \;;\; E_{2,0} \;;\; E_{2,1} \;;\; E_{2,2} \Longrightarrow$ **Entartung = 1**

(2b) CG–Koeffizienten: $j \;=\; \frac{3}{2}$

$$\big\langle\tfrac{3}{2}, M\mp\tfrac{1}{2}; \tfrac{1}{2}, \pm\tfrac{1}{2}\,\big|\,2,M\big\rangle \;=\; \sqrt{\tfrac{2\pm M}{4}} \qquad \ldots \quad M = 0,\pm1,\pm2$$

$$\big\langle\tfrac{3}{2}, M\mp\tfrac{1}{2}; \tfrac{1}{2}, \pm\tfrac{1}{2}\,\big|\,1,M\big\rangle \;=\; (-1)^{\frac{1}{2}\pm\frac{1}{2}}\sqrt{\tfrac{2\mp M}{4}} \qquad \ldots \quad M = 0,\pm1$$

Fall: $S=1$ $\quad \big|\,1M\big\rangle \;=\; \sum_s \big\langle\frac{3}{3}, M-s; \frac{1}{2}, s\,\big|\,1M\big\rangle\;\big|\,M-s,s\big\rangle$

$$\big|\,11\big\rangle \;=\; -\tfrac{1}{2}\,\big|\,\tfrac{1}{2},\tfrac{1}{2}\big\rangle + \tfrac{\sqrt{3}}{2}\,\big|\,\tfrac{3}{2},-\tfrac{1}{2}\big\rangle$$

$$\big|\,10\big\rangle \;=\; -\tfrac{1}{\sqrt{2}}\,\big|\,-\tfrac{1}{2},\tfrac{1}{2}\big\rangle + \tfrac{1}{\sqrt{2}}\,\big|\,\tfrac{1}{2},-\tfrac{1}{2}\big\rangle$$

$$\big|\,1-1\big\rangle \;=\; -\tfrac{\sqrt{3}}{2}\,\big|\,-\tfrac{3}{2},\tfrac{1}{2}\big\rangle + \tfrac{1}{2}\,\big|\,-\tfrac{1}{2},-\tfrac{1}{2}\big\rangle$$

(2b) **Fall: $S = 2$**

$$\big|\, 2M \big\rangle \;=\; \textstyle\sum_s \big\langle \tfrac{3}{3}, M-s; \tfrac{1}{2}, s \,\big|\, 2M \big\rangle \,\big|\, M-s, s \big\rangle$$

$$\begin{aligned}
\big|\, 22 \big\rangle &= \big|\, \tfrac{3}{2}, \tfrac{1}{2} \big\rangle \\
\big|\, 21 \big\rangle &= \tfrac{\sqrt{3}}{2} \big|\, \tfrac{1}{2}, \tfrac{1}{2} \big\rangle + \tfrac{1}{2} \big|\, \tfrac{3}{2}, -\tfrac{1}{2} \big\rangle \\
\big|\, 20 \big\rangle &= \tfrac{1}{\sqrt{2}} \big|\, -\tfrac{1}{2}, \tfrac{1}{2} \big\rangle + \tfrac{1}{\sqrt{2}} \big|\, \tfrac{1}{2}, -\tfrac{1}{2} \big\rangle \\
\big|\, 2-1 \big\rangle &= \tfrac{1}{2} \big|\, -\tfrac{3}{2}, \tfrac{1}{2} \big\rangle + \tfrac{\sqrt{3}}{2} \big|\, -\tfrac{1}{2}, -\tfrac{1}{2} \big\rangle \\
\big|\, 2-2 \big\rangle &= \big|\, -\tfrac{3}{2}, -\tfrac{1}{2} \big\rangle
\end{aligned}$$

(3)

$$\begin{array}{lcll}
E_0 & = & -18\hbar^2 & \big|\, 1, -1 \big\rangle \\
E_1 & = & -10\hbar^2 & \big|\, 1, 0 \big\rangle \;;\; \big|\, 2, -2 \big\rangle \\
E_2 & = & -2\hbar^2 & \big|\, 1, 1 \big\rangle \;;\; \big|\, 2, -1 \big\rangle \\
E_3 & = & +6\hbar^2 & \big|\, 2, 0 \big\rangle \\
E_4 & = & +14\hbar^2 & \big|\, 2, 1 \big\rangle \\
E_5 & = & +22\hbar^2 & \big|\, 2, 2 \big\rangle
\end{array}$$

(4) **Wahrscheinlichkeit:** $\mathsf{Q} \;=\; \mathsf{Q}_1 + \mathsf{Q}_2$

$$\mathsf{Q}_1 \;=\; \big|\, \tfrac{3}{2}, -\tfrac{3}{2} \big\rangle \big\langle \tfrac{3}{2}, -\tfrac{3}{2} \,\big| \otimes \mathbf{1}^{(2)}$$

$$\mathsf{Q}_2 \;=\; \mathbf{1}^{(1)} \otimes \big|\, \tfrac{1}{2}, -\tfrac{1}{2} \big\rangle \big\langle \tfrac{1}{2}, -\tfrac{1}{2} \,\big|$$

Grundzustand: $\big|\, z_0 \big\rangle \;=\; \big|\, (\tfrac{3}{2}\tfrac{1}{2})1, -1 \big\rangle \;=\; \big|\, 1, -1 \big\rangle$

$$\begin{aligned}
\mathsf{Q}_1 \big|\, z_0 \big\rangle &= -\tfrac{\sqrt{3}}{2} \big|\, -\tfrac{3}{2}, \tfrac{1}{2} \big\rangle \Longrightarrow \big\langle z_0 \,\big|\, \mathsf{Q}_1 \,\big|\, z_0 \big\rangle = \tfrac{3}{4} \\
\mathsf{Q}_2 \big|\, z_0 \big\rangle &= \tfrac{1}{2} \big|\, -\tfrac{1}{2}, -\tfrac{1}{2} \big\rangle \Longrightarrow \big\langle z_0 \,\big|\, \mathsf{Q}_2 \,\big|\, z_0 \big\rangle = \tfrac{1}{4} \\
W &= \big\langle z_0 \,\big|\, \mathsf{Q} \,\big|\, z_0 \big\rangle = 1
\end{aligned}$$

(5) **Erwartungswert:** $\big\langle z_0 \,\big|\, \mathbf{S}(\underline{e}) \,\big|\, z_0 \big\rangle$

$$\mathbf{S}(\underline{e}) \;=\; \tfrac{1}{\sqrt{2}} \big(\mathbf{S}_x - \mathbf{S}_z \big)$$

$$\mathbf{S}_x \;=\; \tfrac{1}{2} \big(\mathbf{S}_+ + \mathbf{S}_- \big)$$

$$\mathbf{S}_x \big|\, z_0 \big\rangle \;=\; \tfrac{\hbar}{\sqrt{2}} \big|\, 1, 0 \big\rangle \Longrightarrow \big\langle z_0 \,\big|\, \mathbf{S}_x \,\big|\, z_0 \big\rangle \;=\; 0$$

$$\mathbf{S}_z \big|\, z_0 \big\rangle \;=\; -\hbar \big|\, z_0 \big\rangle \Longrightarrow \big\langle z_0 \,\big|\, \mathbf{S}(\underline{e}) \,\big|\, z_0 \big\rangle \;=\; \tfrac{\hbar}{\sqrt{2}}$$