Beispiel 1:

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(1) Matrixdarstellung von H:

$$\mathbf{H}^{\{e\}} = \frac{\hbar\omega}{3}\begin{bmatrix} 0 & 1-2i & 0 \\ 1+2i & 0 & 2i \\ 0 & -2i & 0 \end{bmatrix}$$

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(2) Hermitizität von H:

$$\mathbf{H}^{\{e\}\dagger} = \frac{\hbar\omega}{3}\begin{bmatrix} 0 & 1+2i & 0 \\ 1-2i & 0 & -2i \\ 0 & 2i & 0 \end{bmatrix} = \mathbf{H}^{\{e\}}$$

(3a$_1$) Säkulargleichung von $\tilde{\mathbf{H}}$:

$$(-\lambda)\big(\lambda^2-4\big) - (1-2i)(-\lambda)(1+2i) = 0$$
$$\lambda(\lambda-3)(\lambda+3) = 0$$

(3a$_2$) Eigenwerte von H:

$$E_1 = -\hbar\omega \qquad \mathrm{Ent}(E_1) = 1$$
$$E_2 = 0 \qquad \mathrm{Ent}(E_2) = 1$$
$$E_3 = +\hbar\omega \qquad \mathrm{Ent}(E_3) = 1$$

(3b$_1$) Eigenvektor zu E_1:

$$\mathbf{u}_1 = \tfrac{1}{3\sqrt{2}}\big((2+i)\,\mathbf{e}_1 - 3i\,\mathbf{e}_2 + 2\,\mathbf{e}_3\big)$$

(3b$_2$) Eigenvektor zu E_2:

$$\mathbf{u}_2 = \tfrac{1}{3\sqrt{5}}\big((4+2i)\,\mathbf{e}_1 - 5\,\mathbf{e}_3\big)$$

(3b$_3$) Eigenvektor zu E_3:

$$\mathbf{u}_3 = \tfrac{1}{3\sqrt{2}}\big((2+i)\,\mathbf{e}_1 + 3i\,\mathbf{e}_2 + 2\,\mathbf{e}_3\big)$$

Beachte: EVen eindeutig bis auf Phasenfaktoren !

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(4) Ordnung $E_1 < E_2 < E_3$:

Bereits in **(3)** berücksichtigt (sonst umordnen **!**)

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(5) Matrixdarstellung von H:

$$\mathbf{H}^{\{u\}} = \hbar\omega\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & +1 \end{bmatrix}$$

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(6) Matrixdarstellung von $\mathbf{U}(t)$:

$$\mathbf{U}(t)^{\{u\}} = \begin{bmatrix} e^{+i\omega t} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\omega t} \end{bmatrix}$$

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(7) Erwartungswert von H:

$$\boldsymbol{\Phi}(0) = 2\,\mathbf{u}_1 + (1-2i)\,\mathbf{u}_2 \quad\Longrightarrow$$
$$\tilde{\boldsymbol{\Phi}}(0) = \tfrac{1}{3}\big(2\,\mathbf{u}_1 + (1-2i)\,\mathbf{u}_2\big)$$
$$\mathbf{H}\,\tilde{\boldsymbol{\Phi}}(0) = \tfrac{2}{3}\,\mathbf{H}\,\mathbf{u}_1 + \tfrac{1-2i}{3}\,\mathbf{H}\,\mathbf{u}_2 = -\tfrac{2\hbar\omega}{3}\,\mathbf{u}_1$$

$$\big\langle \tilde{\boldsymbol{\Phi}}(0)\,,\mathbf{H}\,\tilde{\boldsymbol{\Phi}}(0)\big\rangle = -\tfrac{4\hbar\omega}{9}$$

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(8) Wahrscheinlichkeit (E_1):

$$W_{E_1}(\tilde{\boldsymbol{\Phi}}(t)) = \big\langle \tilde{\boldsymbol{\Phi}}(t)\,,\mathsf{Q}_1\tilde{\boldsymbol{\Phi}}(t)\big\rangle$$
$$\tilde{\boldsymbol{\Phi}}(t) = \mathbf{U}(t)\,\tilde{\boldsymbol{\Phi}}(0) = \tfrac{2}{3}e^{+i\omega t}\,\mathbf{u}_1 + \tfrac{1-2i}{3}\,\mathbf{u}_2$$
$$\mathsf{Q}_1\tilde{\boldsymbol{\Phi}}(t) = \big\langle \mathbf{u}_1\,,\tilde{\boldsymbol{\Phi}}(t)\big\rangle\,\mathbf{u}_1 = \tfrac{2}{3}e^{+i\omega t}\,\mathbf{u}_1$$

$$W_{E_1}(\tilde{\boldsymbol{\Phi}}(t)) = \tfrac{4}{9}$$

Beispiel 2:

(1) Matrixdarstellung von $\mathbf{H}(\xi)$:

$$\mathbf{H}(\xi) = \hbar\omega\,\big(\tilde{\mathbf{H}} + \xi\,\tilde{\mathbf{W}}\big) = \hbar\omega\,\tilde{\mathbf{H}}(\xi)$$

$$\tilde{\mathbf{H}}^{\{e\}}(\xi) = \begin{bmatrix} \xi & 2-i & i\xi\sqrt{2} \\ 2+i & 2\xi & -2i \\ -i\xi\sqrt{2} & 2i & -\xi \end{bmatrix} = \tilde{\mathbf{H}}^{\{e\}} + \xi\,\tilde{\mathbf{W}}^{\{e\}}$$

$$\tilde{\mathbf{H}}^{\{e\}} = \begin{bmatrix} 0 & 2-i & 0 \\ 2+i & 0 & -2i \\ 0 & 2i & 0 \end{bmatrix} \quad , \quad \tilde{\mathbf{W}}^{\{e\}} = \begin{bmatrix} 1 & 0 & i\sqrt{2} \\ 0 & 2 & 0 \\ -i\sqrt{2} & 0 & -1 \end{bmatrix}$$

($2a_1$) Säkulargleichung von $\tilde{\mathbf{H}}$:

$$\lambda(\lambda-3)(\lambda+3) = 0$$

($2a_2$) Eigenwerte von $\mathbf{H}$:

$$\begin{aligned} E_1 &= -3\hbar\omega & \qquad \mathrm{Ent}(E_1) &= 1 \\ E_2 &= 0 & \mathrm{Ent}(E_2) &= 1 \\ E_3 &= +3\hbar\omega & \mathrm{Ent}(E_3) &= 1 \end{aligned}$$

($2b_1$) Eigenvektor zu E_1:

$$\mathbf{u}_1 = \tfrac{1}{3\sqrt{2}}\big((-1-2i)\,\mathbf{e}_1 + 3i\,\mathbf{e}_2 + 2\,\mathbf{e}_3\big)$$

($2b_2$) Eigenvektor zu E_2:

$$\mathbf{u}_2 = \tfrac{1}{3\sqrt{5}}\big((2+4i)\,\mathbf{e}_1 + 5\,\mathbf{e}_3\big)$$

($2b_3$) Eigenvektor zu E_3:

$$\mathbf{u}_3 = \tfrac{1}{3\sqrt{2}}\big((-1-2i)\,\mathbf{e}_1 - 3i\,\mathbf{e}_2 + 2\,\mathbf{e}_3\big)$$

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(3) Energiekorrektur $\varepsilon_1^{(1)}(\xi)$:

$$\varepsilon_1^{(1)}(\xi) = \big\langle \mathbf{u}_1\,,\,\mathbf{W}(\xi)\,\mathbf{u}_1 \big\rangle = \hbar\omega\xi\,\big\langle \mathbf{u}_1\,,\,\tilde{\mathbf{W}}\,\mathbf{u}_1 \big\rangle$$

$$\begin{aligned} \tilde{\mathbf{W}}\,\mathbf{e}_1 &= \mathbf{e}_1 - \sqrt{2}i\,\mathbf{e}_3 \\ \tilde{\mathbf{W}}\,\mathbf{e}_2 &= 2\,\mathbf{e}_2 \\ \tilde{\mathbf{W}}\,\mathbf{e}_3 &= \sqrt{2}i\,\mathbf{e}_1 - \mathbf{e}_3 \end{aligned}$$

$$\begin{aligned} \tilde{\mathbf{W}}\,\mathbf{u}_1 &= \tfrac{1}{3\sqrt{2}}\Big\{(-1-2i)(\mathbf{e}_1 - \sqrt{2}i\,\mathbf{e}_3) + 6i\,\mathbf{e}_2 + 2(\sqrt{2}i\,\mathbf{e}_1 - \mathbf{e}_3)\Big\} \\ &= (-1+2i(\sqrt{2}-1))\,\mathbf{e}_1 + 6i\,\mathbf{e}_2 + (-2(1+\sqrt{2})+i\sqrt{2})\,\mathbf{e}_3 \end{aligned}$$

$$\begin{aligned} \big\langle \mathbf{u}_1\,,\,\tilde{\mathbf{W}}\,\mathbf{u}_1 \big\rangle &= \tfrac{1}{18}\Big\{(-1+2i)[-1+2i(\sqrt{2}-1)] + 18 + 2[-2(1+\sqrt{2})+i\sqrt{2}]\Big\} \\ &= \tfrac{19-8\sqrt{2}}{18} \end{aligned}$$

$$\varepsilon_1^{(1)}(\xi) = \hbar\omega\xi\,\tfrac{19-8\sqrt{2}}{18}$$

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(4) Erwartungswert von $\mathbf{H}$:

$$\mathbf{\Phi} \longmapsto \tilde{\mathbf{\Phi}} = \tfrac{1}{2}\big(\mathbf{e}_2 + \sqrt{3}\,\mathbf{e}_3\big)$$

$$\begin{aligned} \mathbf{H}(\xi)\,\mathbf{e}_2 &= \hbar\omega\big\{(2-i)\,\mathbf{e}_1 + 2\xi\,\mathbf{e}_2 + 2i\,\mathbf{e}_3\big\} \\ \mathbf{H}(\xi)\,\mathbf{e}_3 &= \hbar\omega\big\{i\sqrt{2}\xi\,\mathbf{e}_1 - 2i\,\mathbf{e}_2 - \xi\,\mathbf{e}_3\big\} \end{aligned}$$

$$\begin{aligned} \mathbf{H}(\xi)\,\tilde{\mathbf{\Phi}} &= \tfrac{1}{2}\,\mathbf{H}(\xi)\,\mathbf{e}_2 + \tfrac{\sqrt{3}}{2}\,\mathbf{H}(\xi)\,\mathbf{e}_3 \\ &= \tfrac{\hbar\omega}{2}\Big\{[2+i(\sqrt{6}\xi-1)]\,\mathbf{e}_1 + 2(\xi-\sqrt{3}i)\,\mathbf{e}_2 + (2i-\sqrt{3}\xi)\,\mathbf{e}_3\Big\} \end{aligned}$$

$$\big\langle \tilde{\mathbf{\Phi}}\,,\,\mathbf{H}(\xi)\tilde{\mathbf{\Phi}} \big\rangle = -\tfrac{\hbar\omega}{4}\xi \quad \longmapsto_{\xi=\frac{1}{2}} \quad \big\langle \mathbf{H}(\tfrac{1}{2}) \big\rangle = -\tfrac{\hbar\omega}{8}$$

Beispiel 3:

(1)

Bereich 1+3: $(\partial_x^2 + k^2)u(x) = 0 \qquad k = \sqrt{\frac{2m}{\hbar^2}E}$

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

(2)

Bereich 1+3: $k = \sqrt{\frac{2m}{\hbar^2}(\frac{1}{8}V_0)}$

Bereich 2: $K = \sqrt{\frac{2m}{\hbar^2}(\frac{9}{8}V_0)} = 3k$

(3)

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

$$\mathbf{Q}(a) = \frac{1}{2}\begin{bmatrix} (1+\frac{k}{K})e^{i(k-K)a} & (1-\frac{k}{K})e^{-i(k+K)a} \\ (1-\frac{k}{K})e^{i(k+K)a} & (1+\frac{k}{K})e^{-i(k-K)a} \end{bmatrix} = \frac{1}{3}\begin{bmatrix} 2e^{-i2ka} & e^{-i4ka} \\ e^{i4ka} & 2e^{i2ka} \end{bmatrix}$$

(4a)

$$\mathbf{M}(0,a) = \mathbf{Q}(0)\,\mathbf{Q}(a) = \frac{1}{3}\begin{bmatrix} 4e^{-i2ka} - e^{i4ka} & 2(e^{-i4ka} - e^{i2ka}) \\ 2(e^{i4ka} - e^{-i2ka}) & 4e^{i2ka} - e^{-i4ka} \end{bmatrix}$$

(4b) $ka = \frac{\pi}{4}$:

$$\mathbf{M}(0,a) = \frac{1}{3}\begin{bmatrix} 1-4i & -2(1+i) \\ -2(1-i) & 1+4i \end{bmatrix}$$

(5) $A_1 = 1\,,\, B_3 = 0$:

$$\begin{bmatrix} 1 \\ B_1 \end{bmatrix} = \frac{1}{3}\begin{bmatrix} 1-4i & -2(1+i) \\ -2(1-i) & 1+4i \end{bmatrix}\begin{bmatrix} A_3 \\ 0 \end{bmatrix}$$

$$A_3 = \frac{3(1+4i)}{17} \;;\; B_1 = \frac{(-2+2i)(1+4i)}{17}$$

$$|\,B_1\,|^2 + |\,A_3\,|^2 = \frac{8}{17} + \frac{9}{17} = 1$$

(6)

$$\mathbf{S}_{11} = \frac{(-2+2i)(1+4i)}{17}$$
$$\mathbf{S}_{12} = \frac{3(1+4i)}{17}$$
$$\mathbf{S}_{21} = \frac{3(1+4i)}{17}$$
$$\mathbf{S}_{22} = \frac{(2+2i)(1+4i)}{17}$$

$$\mathbf{S} = \frac{1+4i}{17}\begin{bmatrix} -2+2i & 3 \\ 3 & 2+2i \end{bmatrix}$$

$$\mathbf{S}\,\mathbf{S}^\dagger = \frac{1}{17}\begin{bmatrix} -2+2i & 3 \\ 3 & 2+2i \end{bmatrix}\begin{bmatrix} -2-2i & 3 \\ 3 & 2-2i \end{bmatrix} = \frac{1}{17}\begin{bmatrix} 17 & 0 \\ 0 & 17 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Beispiel 4:

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

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

(2) $\{\,|\,m,s\rangle : m = 0,\pm 1\ ;\ s = \pm\frac{1}{2}\} \longrightarrow \{\,|\,(1\frac{1}{2})SM\rangle : S = \frac{1}{2},\frac{3}{2}\ ;\ -S \le M \le +S\}$

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

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

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

(b) Summen–Regel: $M = m + s$

EW–Gleichung 1: $\vec{\mathbf{S}}^{(1)}\cdot\vec{\mathbf{S}}^{(2)}\,|\,SM\rangle = \frac{\hbar^2}{2}\big(S(S+1)-\frac{11}{4}\big)\,|\,SM\rangle$

EWe 1: $\hat{E}_S = \frac{\hbar^2}{2}\big(S(S+1)-\frac{11}{4}\big)$; Ent$(\hat{E}_S) = 2S+1$

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

$\vec{\mathbf{S}}^{(1)}\cdot\vec{\mathbf{S}}^{(2)}$ = **nicht–singulär**, weil beide **EWe** $\hat{E}_S \neq 0$ sind, daher $Det\{\,\vec{\mathbf{S}}^{(1)}\cdot\vec{\mathbf{S}}^{(2)}\} \neq 0$.

(3a) **Eigenwerte (samt Entartung) von H:**

EW–Gleichung 2: $\mathbf{H}\,|\,SM\rangle = \frac{2M}{S(S+1)-\frac{11}{4}}\,|\,SM\rangle$

EWe 2: $E_{SM} = \frac{8M}{4S(S+1)-11}$; Ent$(E_{SM}) = 1$

(3b) **CG–Koeffizienten:** $j = 1$

$\langle 1, M\mp\frac{1}{2}; \frac{1}{2}, \pm\frac{1}{2}\,|\,\frac{3}{2}, M\rangle = \sqrt{\frac{3\pm 2M}{6}}$ … $M = \pm\frac{1}{2},\pm\frac{3}{2}$

$\langle 1, M\mp\frac{1}{2}; \frac{1}{2}, \pm\frac{1}{2}\,|\,\frac{1}{2}, M\rangle = (-1)^{\frac{1}{2}\pm\frac{1}{2}}\sqrt{\frac{3\mp 2M}{6}}$ … $M = \pm\frac{1}{2}$

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

$$|\,\tfrac{1}{2}+\tfrac{1}{2}\rangle = -\sqrt{\tfrac{1}{3}}\,|\,0,\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|\,1,-\tfrac{1}{2}\rangle$$
$$|\,\tfrac{1}{2}-\tfrac{1}{2}\rangle = -\sqrt{\tfrac{2}{3}}\,|\,-1,\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|\,0,-\tfrac{1}{2}\rangle$$

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

$$|\,\tfrac{3}{2}+\tfrac{3}{2}\rangle = |\,1,\tfrac{1}{2}\rangle$$
$$|\,\tfrac{3}{2}+\tfrac{1}{2}\rangle = \sqrt{\tfrac{2}{3}}\,|\,0,\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|\,1,-\tfrac{1}{2}\rangle$$
$$|\,\tfrac{3}{2}-\tfrac{1}{2}\rangle = \sqrt{\tfrac{1}{3}}\,|\,-1,\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|\,0,-\tfrac{1}{2}\rangle$$
$$|\,\tfrac{3}{2}-\tfrac{3}{2}\rangle = |\,-1,-\tfrac{1}{2}\rangle$$

(4) **Eigenwerte & Eigenvektoren**

$$\begin{array}{lllll} E_1 & = & E_{\frac{3}{2},-\frac{3}{2}} & = & -3 & \quad \left|\tfrac{3}{2} - \tfrac{3}{2}\right\rangle \\ E_2 & = & E_{\frac{3}{2},-\frac{1}{2}} & = & -1 & \quad \left|\tfrac{3}{2} - \tfrac{1}{2}\right\rangle \\ E_3 & = & E_{\frac{1}{2},+\frac{1}{2}} & = & -\tfrac{1}{2} & \quad \left|\tfrac{1}{2} + \tfrac{1}{2}\right\rangle \\ E_4 & = & E_{\frac{1}{2},-\frac{1}{2}} & = & +\tfrac{1}{2} & \quad \left|\tfrac{1}{2} - \tfrac{1}{2}\right\rangle \\ E_5 & = & E_{\frac{3}{2},+\frac{1}{2}} & = & +1 & \quad \left|\tfrac{3}{2} + \tfrac{1}{2}\right\rangle \\ E_6 & = & E_{\frac{3}{2},+\frac{3}{2}} & = & +3 & \quad \left|\tfrac{3}{2} + \tfrac{3}{2}\right\rangle \end{array}$$

(5) **Wahrscheinlichkeit:** $\mathsf{Q} = \mathsf{Q}_1 \otimes \mathsf{Q}_2$

$$\mathsf{Q}_1 = \left|1,-1\right\rangle\left\langle 1,-1\right|$$

$$\mathsf{Q}_2 = \left|\tfrac{1}{2},+\tfrac{1}{2}\right\rangle\left\langle\tfrac{1}{2},+\tfrac{1}{2}\right|$$

1. angeregter Grundzustand: $\left|z\right\rangle = \left|\tfrac{3}{2} - \tfrac{1}{2}\right\rangle = \sqrt{\tfrac{1}{3}}\left|-1,\tfrac{1}{2}\right\rangle + \sqrt{\tfrac{2}{3}}\left|0,-\tfrac{1}{2}\right\rangle$

$$\mathsf{Q}\left|z\right\rangle = \sqrt{\tfrac{1}{3}}\left|-1,+\tfrac{1}{2}\right\rangle$$

$$W = \left\langle z\right|\mathsf{Q}\left|z\right\rangle = \tfrac{1}{3}$$

(6) **Erwartungswert:** $\left\langle \mathbf{S}_y\right\rangle = \left\langle \tilde{z}\right|\mathbf{S}_y\left|\tilde{z}\right\rangle$; $\mathbf{S}_y = \frac{1}{2i}(\mathbf{S}_+ - \mathbf{S}_-)$

Normierter Zustand: $\left|\tilde{z}\right\rangle = \frac{1}{2}\left\{\left|\tfrac{3}{2} + \tfrac{1}{2}\right\rangle - \sqrt{3}i\left|\tfrac{3}{2} - \tfrac{1}{2}\right\rangle\right\}$

$$\begin{aligned} \tfrac{1}{2i}(\mathbf{S}_+ - \mathbf{S}_-)\left|\tilde{z}\right\rangle &= \tfrac{1}{4i}(\mathbf{S}_+ - \mathbf{S}_-)\left|\left\{\left|\tfrac{3}{2} + \tfrac{1}{2}\right\rangle - \sqrt{3}i\left|\tfrac{3}{2} - \tfrac{1}{2}\right\rangle\right\}\right. \\ &= \tfrac{\hbar}{4}\left[-i\sqrt{3}\left|\tfrac{3}{2} + \tfrac{3}{2}\right\rangle - 2\sqrt{3}\left|\tfrac{3}{2} + \tfrac{1}{2}\right\rangle + 2i\left|\tfrac{3}{2} - \tfrac{1}{2}\right\rangle + 3\left|\tfrac{3}{2} - \tfrac{3}{2}\right\rangle\right] \end{aligned}$$

Erwartungswert: $\left\langle \mathbf{S}_y\right\rangle = \frac{\hbar}{8}\left\{-2\sqrt{3} - 2\sqrt{3}\right\} = -\frac{\hbar\sqrt{3}}{2}$