Beispiel 1:

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(1) Matrixdarstellung von H:

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

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(2) Hermitizität von H:

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

($3a_1$) Säkulargleichung von $\tilde{\mathbf{H}}$:

$$\big(\lambda - (1+\sqrt{\tfrac{2}{3}})\big)\big\{(1-\lambda)^2 - \tfrac{2}{3}\big\} = 0$$

$$\big(\lambda - (1+\sqrt{\tfrac{2}{3}})\big)\big(\lambda - (1-\sqrt{\tfrac{2}{3}})\big)\big(\lambda - (1+\sqrt{\tfrac{2}{3}})\big) = 0$$

($3a_2$) Eigenwerte von H:

$$E_1 = \hbar\omega(1-\sqrt{\tfrac{2}{3}}) \qquad \mathrm{Ent}(E_1) = 1$$

$$E_2 = \hbar\omega(1+\sqrt{\tfrac{2}{3}}) \qquad \mathrm{Ent}(E_2) = 2$$

($3b_1$) Eigenvektor zu E_1:

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

($3b_2$) Eigenvektoren zu E_2:

$$\mathbf{u}_{21} = \tfrac{1}{\sqrt{2}}\big(\mathbf{e}_1 + \tfrac{1+i}{\sqrt{2}}\,\mathbf{e}_2\big)$$

$$\mathbf{u}_{22} = \mathbf{e}_3$$

Beachte: Einfachste Wahl !

(abgesehen von Phasenfaktoren **!**)

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(4) Ordnung $E_1 < E_2$:

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

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(5) Erwartungswert von H:

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

$$\mathbf{H} = \hbar\omega\,\tilde{\mathbf{H}}$$

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

$$\langle\mathbf{H}\rangle = \langle\tilde{\boldsymbol{\Phi}}\,,\mathbf{H}\tilde{\boldsymbol{\Phi}}\rangle = \hbar\omega\big(1+(\tfrac{2}{3})^{3/2}\big)$$

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(6) Wahrscheinlichkeit (E_2):

$$W_{E_2}(\tilde{\boldsymbol{\Phi}}) = \langle\tilde{\boldsymbol{\Phi}}, \mathsf{Q}_2\tilde{\boldsymbol{\Phi}}\rangle$$

$$\mathsf{Q}_2\tilde{\boldsymbol{\Phi}} = \langle\mathbf{u}_{21}\,,\tilde{\boldsymbol{\Phi}}\rangle\,\mathbf{u}_{21} + \langle\mathbf{u}_{22}\,,\tilde{\boldsymbol{\Phi}}\rangle\,\mathbf{u}_{22} = $$

$$= \tfrac{1-i}{2\sqrt{3}}\,\mathbf{u}_{21} + i\sqrt{\tfrac{2}{3}}\,\mathbf{u}_{22}$$

$$W_{E_2}(\tilde{\boldsymbol{\Phi}}) = \big(\tfrac{1-i}{2\sqrt{3}}\big)^*\big(\tfrac{1-i}{2\sqrt{3}}\big) + \big(i\sqrt{\tfrac{2}{3}}\big)^*\big(i\sqrt{\tfrac{2}{3}}\big) = \tfrac{5}{6}$$

Beispiel 2:

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

$$\mathbf{H}(\xi) = 3\hbar\omega\,\tilde{\mathbf{H}} + \hbar\omega\xi\,\tilde{\mathbf{W}} = \hbar\omega\,\tilde{\mathbf{H}}(\xi)$$

$$\tilde{\mathbf{H}}^{\{e\}}(\xi) = \begin{bmatrix} 12 & 0 & -9i \\ 0 & 9+3\xi & i\xi \\ 9i & -i\xi & 12+3\xi \end{bmatrix}$$

$$\tilde{\mathbf{H}}^{\{e\}} = \begin{bmatrix} 4 & 0 & -3i \\ 0 & 3 & 0 \\ 3i & 0 & 4 \end{bmatrix}$$

(2a$_1$) Säkulargleichung von $\tilde{\mathbf{H}}$:

$$(3-\lambda)\big\{(4-\lambda)^2 - 9\big\} = 0$$

$$(3-\lambda)(1-\lambda)(7-\lambda) = 0$$

(2a$_2$) Eigenwerte von $\mathbf{H}$:

$$E_1 = 3\hbar\omega \qquad \mathrm{Ent}(E_1) = 1$$

$$E_2 = 9\hbar\omega \qquad \mathrm{Ent}(E_2) = 1$$

$$E_3 = 21\hbar\omega \qquad \mathrm{Ent}(E_3) = 1$$

(2b$_1$) Eigenvektor zu E_1: $\quad \mathbf{u}_1 = \frac{1}{\sqrt{2}}\big(\mathbf{e}_1 - i\mathbf{e}_3\big)$

(2b$_2$) Eigenvektoren zu E_2: $\quad \mathbf{u}_2 = \mathbf{e}_2$

(2b$_3$) Eigenvektoren zu E_3: $\quad \mathbf{u}_3 = \frac{1}{\sqrt{2}}\big(\mathbf{e}_1 + i\mathbf{e}_3\big)$

Beachte: EVen eindeutig bis auf Phasenfaktoren !

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

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

$$\tilde{\mathbf{W}}\,\mathbf{e}_1 = 0$$

$$\tilde{\mathbf{W}}\,\mathbf{e}_2 = 3\,\mathbf{e}_2 - i\,\mathbf{e}_3$$

$$\tilde{\mathbf{W}}\,\mathbf{e}_3 = i\,\mathbf{e}_2 + 3\,\mathbf{e}_3$$

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

$$\mathbf{W}(\xi)\,\mathbf{u}_1 = \frac{\hbar\omega\xi}{\sqrt{2}}\,\big(\mathbf{e}_2 - 3i\,\mathbf{e}_3\big)$$

$$\varepsilon_1^{(1)}(\xi) = \frac{\hbar\omega\xi}{2}\,\big\langle(\mathbf{e}_1 - i\mathbf{e}_3)\,,\,(\mathbf{e}_2 - 3i\,\mathbf{e}_3)\big\rangle = \hbar\omega\xi\,\frac{3}{2}$$

Beispiel 2 (Fortsetzung):

(4a) Korrekturvektor $\boldsymbol{\chi}_1^{(1)}(\xi)$:

$$\boldsymbol{\chi}_1^{(1)}(\xi) = \frac{\langle \mathbf{u}_2 \,, \mathbf{W}(\xi)\, \mathbf{u}_1 \rangle}{E_1(0)-E_2(0)}\, \mathbf{u}_2 + \frac{\langle \mathbf{u}_3 \,, \mathbf{W}(\xi)\, \mathbf{u}_1 \rangle}{E_1(0)-E_3(0)}\, \mathbf{u}_3$$

$$E_1(0) - E_2(0) = -6\hbar\omega$$
$$E_1(0) - E_3(0) = -18\hbar\omega$$

$$\langle \mathbf{u}_2 \,, \mathbf{W}(\xi)\, \mathbf{u}_1 \rangle = \tfrac{\hbar\omega\xi}{\sqrt{2}} \langle \mathbf{e}_2 \,, (\mathbf{e}_2 - 3i\, \mathbf{e}_3) \rangle = + \tfrac{\hbar\omega\xi}{\sqrt{2}}$$
$$\langle \mathbf{u}_3 \,, \mathbf{W}(\xi)\, \mathbf{u}_1 \rangle = \tfrac{\hbar\omega\xi}{2} \langle (\mathbf{e}_1 + i\, \mathbf{e}_3) \,, (\mathbf{e}_2 - 3i\, \mathbf{e}_3) \rangle = - \tfrac{3\hbar\omega\xi}{2}$$

$$\boldsymbol{\chi}_1^{(1)}(\xi) = -\tfrac{\xi}{6\sqrt{2}}\, \mathbf{u}_2 + \tfrac{\xi}{12}\, \mathbf{u}_3 = \tfrac{\xi}{12\sqrt{2}} \big(\mathbf{e}_1 - 2\, \mathbf{e}_2 + i\, \mathbf{e}_3 \big)$$

(4b) Energiekorrektur $\varepsilon_1^{(2)}(\xi)$:

$$\varepsilon_1^{(2)}(\xi) = \langle \mathbf{u}_1 \,, \mathbf{W}(\xi)\, \boldsymbol{\chi}_1^{(1)}(\xi) \rangle = \hbar\omega\xi\, \langle \mathbf{u}_1 \,, \tilde{\mathbf{W}}\, \boldsymbol{\chi}_1^{(1)}(\xi) \rangle$$

$$\tilde{\mathbf{W}}\, \boldsymbol{\chi}_1^{(1)}(\xi) = \tfrac{\xi}{12\sqrt{2}}\, \tilde{\mathbf{W}}\, \big(\mathbf{e}_1 - 2\, \mathbf{e}_2 + i\, \mathbf{e}_3 \big)$$
$$= \tfrac{\xi}{12\sqrt{2}} \big(-2(3\, \mathbf{e}_2 - i\, \mathbf{e}_3) + i(i\, \mathbf{e}_2 + 3\, \mathbf{e}_3) \big)$$
$$= \tfrac{\xi}{12\sqrt{2}} \big(-7\, \mathbf{e}_2 + 5i\, \mathbf{e}_3 \big)$$

$$\varepsilon_1^{(2)}(\xi) = \tfrac{\hbar\omega\xi^2}{24} \langle (\mathbf{e}_1 - i\, \mathbf{e}_3) \,, (-7\, \mathbf{e}_2 + 5i\, \mathbf{e}_3) \rangle = -\tfrac{5\hbar\omega\xi^2}{24}$$

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(5) Erwartungswert von H:

$$\boldsymbol{\Phi}(a) \longmapsto \tilde{\boldsymbol{\Phi}} = \tfrac{1}{\sqrt{1+|a|^2}} \boldsymbol{\Phi} = \tfrac{1}{\sqrt{1+|a|^2}} \big(\mathbf{e}_2 + a\, \mathbf{e}_3 \big)$$
$$\mathbf{H} = 3\hbar\omega\, \tilde{\mathbf{H}}$$
$$\tilde{\mathbf{H}}\, \tilde{\boldsymbol{\Phi}} = \tfrac{1}{\sqrt{1+|a|^2}} \big(3\, \mathbf{e}_2 + a(-3i\, \mathbf{e}_1 + 4\, \mathbf{e}_3) \big)$$
$$\langle \mathbf{H}(a) \rangle = \langle \tilde{\boldsymbol{\Phi}}(a) \,, \mathbf{H}\tilde{\boldsymbol{\Phi}}(a) \rangle$$
$$= \tfrac{3\hbar\omega}{1+|a|^2} \langle (\mathbf{e}_2 + a\mathbf{e}_3) \,, \big(3\, \mathbf{e}_2 + a(-3i\, \mathbf{e}_1 + 4\, \mathbf{e}_3) \big) \rangle =$$
$$= 3\hbar\omega\, \tfrac{3+4\,|a|^2}{1+|a|^2}$$

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(6) Erwartungswert $9\hbar\omega$:

$$\langle \mathbf{H}(a) \rangle = 9\hbar\omega \iff a = 0$$
