Problem 6.2. A system with Hilbert space $\mathbb{C}^3$ has Hamiltonian given by

$$H = H_0 + H_{\mathrm{I}}\,, \quad H_0 = \epsilon \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad H_{\mathrm{I}} = a \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad 0 < a \ll \epsilon\,.$$

Find the exact eigenvalues and eigenvectors. Use first-order perturbation theory to determine the energy levels. Compare the approximate results with the exact expressions.

Solution. The exact eigenvalues and eigenvetors are

$$E_1 = \epsilon\,, \qquad |1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

$$E_2 = -\epsilon + a\,, \qquad |2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix},$$

$$E_3 = -\epsilon - a\,, \qquad |3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}.$$

The eigenstates and eigenvalues of the unperturbed Hamiltonian are

$$E_1^{(0)} = \epsilon\,, \ \text{non-degenerate}, \qquad |1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

$$E_2^{(0)} = -\epsilon\,, \ \text{degeneracy} = 2, \qquad |21^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |22^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Using perturbation theory for nondegenerate states, we obtain that the first-order correction to $E_1^{(0)}$ vanishes,

$$E_1^{(1)} = \langle 1^{(0)} | H_{\mathrm{I}} | 1^{(0)} \rangle = 0\,.$$

Hence we must resort to order two. The second-order correction is in turn given by

$$E_1^{(2)} = \frac{\left|\langle 21^{(0)} | H_{\mathrm{I}} | 1^{(0)} \rangle\right|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{\left|\langle 22^{(0)} | H_{\mathrm{I}} | 1^{(0)} \rangle\right|^2}{E_1^{(0)} - E_2^{(0)}}\,.$$

Using that

$$\langle 21^{(0)} | H_{\mathrm{I}} | 1^{(0)} \rangle = \langle 22^{(0)} | H_{\mathrm{I}} | 1^{(0)} \rangle = 0$$

we conclude that

$$E_1^{(2)} = 0\,.$$

More generally, since H_{I} does not connect $|1^{(0)}\rangle$ with $|21^{(0)}\rangle\,, |22^{(0)}\rangle$, the energy $E_1^{(0)}$ and the state $|1^{(0)}\rangle$ remain unchanged to all orders in perturbation theory.

To find the first-order correction $E_2^{(1)}$ to $E_2^{(0)}$, we must use perturbation theory for degenerate states. This amounts to finding the eigenvalues of the matrix

$$\tilde{H}_{\mathrm{I}} = \begin{pmatrix} \langle 21^{(0)}|H_{\mathrm{I}}|21^{(0)}\rangle & \langle 21^{(0)}|H_{\mathrm{I}}|22^{(0)}\rangle \\ \langle 22^{(0)}|H_{\mathrm{I}}|21^{(0)}\rangle & \langle 22^{(0)}|H_{\mathrm{I}}|22^{(0)}\rangle \end{pmatrix} = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix} .$$

This matrix has two simple eigenvalues,

$$E_{2-}^{(1)} = -a, \qquad E_{2+}^{(1)} = a \,,$$

with eigenvectors

$$|2-^{(0)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}, \qquad |2+^{(0)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} .$$

In the basis $\{|2-^{(0)}\rangle, |2+^{(0)}\rangle\}$ the perturbation H_{I} is diagonal. This is the basis that in the lectures we have been calling $\{|\varphi_\alpha^{(0)}\rangle\}$.

Putting everything together we conclude that

$$E_1^{(0)} = \epsilon \;\; \text{remains unchanged to all orders}\,,$$

$$E_2^{(0)} = -\epsilon \;\; \text{splits to first order in} - \epsilon \pm a$$

which agree with the exact eigenenergies.