2019 Modern - A4 [(QM)

Problem A4: Consider the Hamiltonian $H = H_0 + H'$ for a 3-state system where

$$H_0 = \begin{pmatrix} \frac{1}{2}\hbar\omega_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2}\hbar\omega_0 \end{pmatrix} \qquad H' = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2}\hbar\omega_1 & 0 \\ \frac{\sqrt{3}}{2}\hbar\omega_1 & \frac{1}{2}\hbar\omega_1 & \frac{\sqrt{3}}{2}\hbar\omega_1 \\ 0 & \frac{\sqrt{3}}{2}\hbar\omega_1 & 0 \end{pmatrix}.$$

where H' is considered the perturbation.

a. Find the first-order corrections to the energies of all three eigenstates?
b. Assume the zeroth-order eigenstates are $|1^{(0)}\rangle$, $|2^{(0)}\rangle$, and $|3^{(0)}\rangle$, find the first-order corrections to the eigenstate vectors.
c. Find the second-order corrections to the energies of all three eigenstates.

a) Since H_0 is diagonal its eigenvectors are:

$$\boxed{|1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |3^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}$$

Energy eigenvalues:

$$E_1^{(0)} = \frac{1}{2}\hbar\omega_0 \quad E_2^{(0)} = 0 \quad E_3^{(0)} = -\frac{\hbar\omega_0}{2}.$$

The 1st order correction is given

by (Griffiths, Intro to Quantum Mechanics 1st ed. Sect. 6.1 Eq. 6.9)

$$E_n^{(1)} = \langle n^{(0)} | H' | n^{(0)} \rangle$$

This is just the diagonal elements of H' in our basis:

$$\boxed{E_n^{(1)} = (H')_{nn}}$$

$$\boxed{E_1^{(1)} = 0, \quad E_2^{(1)} = \frac{1}{2}\hbar\omega_1, \quad E_3^{(1)} = 0}$$

b) $$|n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle m^{(0)} | H' | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle$$

Note: $\langle m^{(0)} | H' | n^{(0)} \rangle = H'_{mn}$

So,

$$|1^{(1)}\rangle = \frac{H'_{12}}{E_1^{(0)} - E_2^{(0)}} |2^{(0)}\rangle + \frac{H'_{13}}{E_1^{(0)} - E_3^{(0)}} |3^{(0)}\rangle$$

$$= \frac{\frac{\sqrt{3}}{2} \hbar\omega_1}{\frac{1}{2}\hbar\omega_0 - 0} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + 0 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\boxed{|1^{(1)}\rangle = \sqrt{3}\,\frac{\omega_1}{\omega_0} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}$$

Since we're using perturbation theory, presumably $\omega_1 \ll \omega_0 \rightarrow \frac{\omega_0}{\omega_1} \ll 1$

$$|2^{(1)}\rangle = \frac{H_{21}}{E_2^{(0)} - E_1^{(0)}} |1^{(0)}\rangle + \frac{H_{23}}{E_2^{(0)} - E_3^{(0)}} |3^{(0)}\rangle$$

$$\frac{\frac{\sqrt{3}}{2}\hbar\omega_1}{0 - \frac{1}{2}\hbar\omega_0} |1^{(0)}\rangle + \frac{\sqrt{3}/2\,\hbar\omega_1}{\frac{1}{2}\hbar\omega_0} |3^{(0)}\rangle$$

$$\boxed{|2^{(1)}\rangle = \begin{pmatrix} -\sqrt{3}\,\omega_1/\omega_0 \\ 0 \\ \sqrt{3}\,\frac{\omega_1}{\omega_0} \end{pmatrix}}$$

$$|3^{(1)}\rangle = \frac{H_{31}\,|1^{(0)}\rangle}{E_3^{(0)} - E_1^{(0)}} + \frac{H_{32}}{E_3^{(0)} - E_2^{(0)}} |2^{(0)}\rangle$$

$$= 0 + \frac{\frac{\sqrt{3}}{2}\hbar\omega_1}{-\frac{1}{2}\hbar\omega_0} |2^{(0)}\rangle$$

$$\boxed{|3^{(1)}\rangle = \begin{pmatrix} 0 \\ -\sqrt{3}\,\frac{\omega_1}{\omega_0} \\ 0 \end{pmatrix}}$$

c) $$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m^{(0)} | H' | n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$E_1^{(2)} = \frac{|H'_{21}|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{|H'_{31}|^2}{E_1^{(0)} - E_3^{(0)}}$$

$$= \frac{|\frac{\sqrt{3}}{2} \hbar \omega_1|^2}{1/2 \hbar \omega_0} + 0$$

$$= \frac{\frac{3}{4} \hbar^2 \omega_1^2}{1/2 \hbar \omega_0} = \frac{3}{2} \hbar \frac{\omega_1^2}{\omega_0}$$

$$\Rightarrow \boxed{E_1^{(2)} = \frac{3}{2} \hbar \omega_0 \left(\frac{\omega_1}{\omega_0}\right)^2}$$

Note

$$E_1 = E_1^{(0)} + E_1^{(1)} + E_1^{(2)} + \cdots$$

$$= \frac{1}{2}\hbar\omega_0 + 0 + \frac{3}{2}\hbar\omega_0 \left(\frac{\omega_1}{\omega_0}\right)^2 + \cdots$$

$$= \frac{1}{2}\hbar\omega_0 \left[1 + 3\left(\frac{\omega_1}{\omega_0}\right)^2 + \cdots \right]$$

Here $\varepsilon = \frac{\omega_1}{\omega_0}$ is our dimensionless expansion parameter.

$$E_2^{(2)} = \frac{|H'_{12}|^2}{E_2^{(0)} - E_1^{(0)}} + \frac{|H'_{32}|^2}{E_2^{(0)} - E_3^{(0)}}$$

$$= \frac{\left|\frac{\sqrt{3}}{2}\hbar\omega_1\right|^2}{0 - \frac{1}{2}\hbar\omega_0} + \frac{\left|\frac{\sqrt{3}}{2}\hbar\omega_1\right|^2}{0 - \left(-\frac{1}{2}\hbar\omega_0\right)}$$

$$= -\frac{\frac{3}{4}\hbar^2\omega_1^2}{\frac{1}{2}\hbar\omega_0} + \frac{\frac{3}{4}\hbar^2\omega_1^2}{\frac{1}{2}\hbar\omega_0}$$

$$\Rightarrow \quad \boxed{E_2^{(2)} = 0}$$

$$E_2 = E_2^{(0)} + E_2^{(1)} + E_2^{(2)} + \dots$$

$$E_2 = 0 + \frac{1}{2}\hbar\omega_1 + \dots$$

$$E_2 = \frac{1}{2}\hbar\omega_0\left(\frac{\omega_1}{\omega_0}\right) + \dots$$

Now,

$$E_3^{(2)} = \frac{|H'_{13}|^2}{E_3^{(0)} - E_1^{(0)}} + \frac{|H'_{23}|^2}{E_3^{(0)} - E_2^{(0)}}$$

$$= 0 + \frac{\left|\frac{\sqrt{3}}{2}\hbar\omega_1\right|^2}{-\frac{1}{2}\hbar\omega_0}$$

$$= -\frac{\frac{3}{4}\hbar^2\omega_1^2}{\frac{1}{2}\hbar\omega_0} = -\frac{3}{2}\hbar\frac{\omega_1^2}{\omega_0}$$

$$\Rightarrow \boxed{E_3^{(2)} = -\frac{3}{2}\hbar\omega_0\left(\frac{\omega_1}{\omega_0}\right)^2}$$

And

$$E_3 = -\frac{1}{2}\hbar\omega_0 - \frac{3}{2}\hbar\omega_0\left(\frac{\omega_1}{\omega_0}\right)^2 + \dots$$

$$E_3 = -\frac{1}{2}\hbar\omega_0\left[1 + 3\left(\frac{\omega_1}{\omega_0}\right)^2 + \dots\right]$$