Sakurai 5.1.1–4

Warm-up

$$H_0 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}, \quad V = \begin{pmatrix} 0 & \Omega & 0 \\ \Omega^* & \varepsilon & 0 \\ 0 & 0 & \delta \end{pmatrix} \qquad a < b < c$$

a) Find eigenvalues / eigenvecs of H_0

b) Find 1st & 2nd order shifts of E_2

→ a) eigenvalues of H_0: a, b, c

eigenvecs : $|1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |3^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

b) $$\Delta_2^{(1)} = \langle 0 \;\; 1 \;\; 0 \rangle \begin{pmatrix} 0 & \Omega & 0 \\ \Omega^* & \varepsilon & 0 \\ 0 & 0 & \delta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$= (0 \;\; 1 \;\; 0) \begin{pmatrix} \Omega \\ \varepsilon \\ 0 \end{pmatrix} = \varepsilon$$

$$\boxed{\Delta_2^{(1)} = \varepsilon}$$

$$\delta_2^{(2)} = \sum_{m=1,3} \frac{|V_{m2}|^2}{E_2^{(0)} - E_m^{(0)}} \qquad E_1^{(0)} = a$$

$$E_2^{(0)}$$

$$E_3^{(0)}$$

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

$$= \frac{1}{(b-a)} \left(\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \Omega & 0 \\ \Omega^* & \varepsilon & 0 \\ 0 & 0 & \delta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right)^2$$

$$+ \frac{1}{(b-c)} \left(\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \Omega & 0 \\ \Omega^* & \varepsilon & 0 \\ 0 & 0 & \delta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right)^2$$

$$= \frac{1}{(b-a)} \left(\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Omega \\ \varepsilon \\ 0 \end{pmatrix} \right)^2 + \frac{1}{(b-c)} \left(\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \Omega \\ \varepsilon \\ 0 \end{pmatrix} \right)^2$$

$$= \frac{1}{(b-a)} |\Omega|^2 + 0$$

$$\boxed{\Delta_2^{(2)} = \frac{|\Omega|^2}{(b-a)}}$$

(Ω could be complex $\Rightarrow |\Omega|^2 = \Omega^* \Omega$)

—x—x—x—

Review: Given $H = H_0 + V$

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$$

assume discrete and non-degenerate

(the states other than the one we are perturbing can be degenerate)

want to find $E_n, |n\rangle$, such that

$$H_\lambda |n\rangle = E_n |n\rangle$$
$$H_\lambda = H_0 + \lambda V$$

use:

$$E_n(\lambda) = E_n^{(0)} + \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \ldots$$
$$|n, \lambda\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \ldots$$

now we want to find: $\Delta_n^{(1)}, \Delta_n^{(2)}$ & $|n^{(1)}\rangle$

Normalization: let $\langle n^{(0)}|n\rangle = 1$ $\quad (\Rightarrow \langle n|n\rangle \neq 1)$

Consequence: $$1 = \langle n^{(0)}|n\rangle = \langle n^{(0)}|n^{(0)}\rangle + \lambda\langle n^{(0)}|n^{(1)}\rangle + \lambda^2\langle n^{(0)}|n^{(2)}\rangle + \dots$$

comparing the coefficients of powers of λ on L.H.S and R.H.S

$$\lambda^0 : \quad 1 = \langle n^{(0)}|n^{(0)}\rangle$$
$$0 = \langle n^{(0)}|n^{(1)}\rangle$$
$$0 = \langle n^{(0)}|n^{(2)}\rangle$$

$$\Rightarrow \boxed{\langle n^{(0)}|n^{(k)}\rangle = 0} \quad \text{for } k > 0$$

using time-independent S.E:

$$H_\lambda|n\rangle = E_n|n\rangle$$
$$(H_0 + \lambda V)|n\rangle = E_n|n\rangle = (E_n^{(0)} + \Delta_n)|n\rangle$$

$$\Rightarrow \underbrace{(E_n^{(0)} - H_0)}_{\text{unperturbed}}|n\rangle = \underbrace{(\lambda V - \Delta_n)}_{\text{perturbed}}|n\rangle \quad - (\ddot\smile)$$

apply $\langle n^{(0)}|$ to the equation

$$\underbrace{\langle n^{(0)}|E_n^{(0)} - H_0|n\rangle}_{=0} = \langle n^{(0)}|\lambda V|n\rangle - \Delta_n\langle n^{(0)}|n\rangle$$
$$= \lambda\langle n^{(0)}|V(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \dots)$$

$$\Rightarrow \Delta_n = \lambda\langle n^{(0)}|V|n\rangle$$
$$= \underbrace{\lambda\langle n^{(0)}|V|n^{(0)}\rangle}_{\Delta_n^{(1)}} + \lambda^2\langle n^{(0)}|V|n^{(1)}\rangle + \dots$$

$$\boxed{\begin{aligned}\Delta_n^{(1)} &= \langle n^{(0)} | V | n^{(0)} \rangle \\ &= V_{nn}\end{aligned}}$$

and $\Delta_n^{(2)} = \langle n^{(0)} | V | n^{(1)} \rangle$

using eqn (˙ᴗ˙) again & apply $\langle m^{(0)} | H_0$ to it, we have

assuming, $m \neq n$

$$\langle m^{(0)} | E_n^{(0)} - \underbrace{H_0}_{E_m^{(0)}} | n \rangle = \langle m^{(0)} | \lambda V - \Delta_n | n \rangle$$

$$\Rightarrow \langle m^{(0)} | E_n^{(0)} - E_m^{(0)} \left[|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \dots \right]$$

$$= \lambda \langle m^{(0)} | \left[V \; |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \dots \right]$$

$$- \Delta_n \langle m^{(0)} | \left(|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \dots \right)$$

$$\Rightarrow \lambda \langle m^{(0)} | n^{(1)} \rangle \left(E_n^{(0)} - E_m^{(0)} \right)$$

....

→ equation erased before I could write it down :C

$$\boxed{\langle m^{(0)} | n^{(1)} \rangle = \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}} \quad \text{for } m \neq n$$

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

using completeness:

$$|n^{(1)}\rangle = \sum_m |m^{(0)}\rangle\langle m^{(0)}|n^{(1)}\rangle$$

$$\boxed{|n^{(1)}\rangle = \sum_{m\neq n} |m^{(0)}\rangle \frac{V_{mn}}{E_n^{(0)}-E_m^{(0)}}}$$

$$\Delta_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle$$

$$\boxed{\Delta_n^{(2)} = \sum_{m\neq n} \frac{V_{nm}V_{mn}}{E_n^{(0)}-E_m^{(0)}} = \sum_{m\neq n} \frac{|V_{mn}|^2}{E_n^{(0)}-E_m^{(0)}}}$$