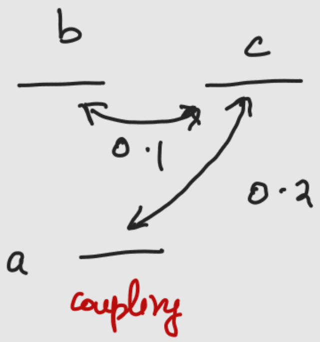
Quantum Mechanics 2- Sep 4

Today Degenerate P.T.
(Sakurai 5.2)

Example : Quantum Systems with 3 states

$$|a\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |b\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |c\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



$$H_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

$$V = \begin{pmatrix} 0 & 0 & 0.2 \\ 0 & 0 & 0.1 \\ 0.2 & 0.1 & 0 \end{pmatrix}$$

Q 1) Find eigenvalues, eigenvecs of H_0

$$\Rightarrow \quad E_1^{(0)} = 1 \rightarrow |1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |a\rangle$$

$$E_2^{(0)} = 2 \rightarrow |b\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |c\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

and any linear combination of $|b\rangle$ & $|c\rangle$

$$\Rightarrow |2^{(0)}\rangle = x|b\rangle + y|c\rangle$$

$$H_0 |2^{(0)}\rangle = H_0 (x|b\rangle + y|c\rangle) = 2|2^{(0)}\rangle$$

also, $|3^{(0)}\rangle = y|b\rangle - x|c\rangle$

⋮ ⋮

Q2 Find the 1st order energy shift of

a) $E_1^{(0)} = 1$

$\Rightarrow \quad \langle 1^{(0)} | V | 1^{(0)} \rangle = \boxed{0}$

b) $E_2^{(0)} = 2$, assuming $|2^{(0)}\rangle = |b\rangle$

$$\Delta_2^{(1)} = \langle b | V | b \rangle = \boxed{0}$$

c) $E_2^{(0)} = 2$, assuming $|2^{(0)}\rangle = \frac{1}{\sqrt{2}} |b\rangle + \frac{1}{\sqrt{2}} |c\rangle$

$\Delta_+^{(1)} = ?$

$$\Rightarrow \quad \frac{1}{\sqrt{2}} |b\rangle + \frac{1}{\sqrt{2}} |c\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

$$\Delta_+^{(1)} = \langle 2^{(0)} | V | 2^{(0)} \rangle$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0.2 \\ 0 & 0 & 0.1 \\ 0.2 & 0.1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0.2 \\ 0.1 \\ 0.1 \end{pmatrix}$$

$$= \frac{1}{2} (0.2) = 0.1$$

$$\boxed{\Delta_+^{(1)} = 0.1}$$

d) $E_3^{(0)} = 2$, assuming $|3^{(0)}\rangle = \frac{1}{\sqrt{2}} |b\rangle - \frac{1}{\sqrt{2}} |c\rangle$

$$\Delta_-^{(1)} = \frac{1}{2} \begin{pmatrix} 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} -0.2 \\ -0.1 \\ 0.1 \end{pmatrix}$$

$$\boxed{\Delta_-^{(1)} = -0.1}$$

Q Find 1^{st} order energy shift of $E_2^{(0)} = 2$ by directly solving

$$\det(H_0 + \underbrace{\lambda}_{\substack{\text{perturbation} \\ \text{theory lambda}}} V - E_2 I) = 0$$

$$E_2 = 2 + \lambda \Delta^{(1)} + O(\lambda^2)$$

$$0 = \begin{vmatrix} 1 - E_2 & 0 & 0.2\lambda \\ 0 & 2 - E_2 & 0.1\lambda \\ 0.2\lambda & 0.1\lambda & 2 - E_2 \end{vmatrix}$$

$$1 - E_2 = -1 - \lambda\Delta^{(1)} + O(\lambda^2)$$

$$2 - E_2 = -\lambda\Delta^{(1)} + O(\lambda^2)$$

$$\Rightarrow \quad 0 = \begin{vmatrix} -1-\lambda\Delta^{(1)}+O(\lambda^2) & 0 & 0.2\lambda \\ 0 & -\lambda\Delta^{(1)}+O(\lambda^2) & 0.1\lambda \\ 0.2\lambda & 0.1\lambda & -\lambda\Delta^{(1)}+O(\lambda^2) \end{vmatrix}$$

$$\Rightarrow \underbrace{\left(-1-\lambda\Delta^{(1)}+O(\lambda^2)\right)\begin{vmatrix} -\lambda\Delta^{(1)}+O(\lambda^2) & 0.1\lambda \\ 0.1\lambda & -\lambda\Delta^{(1)}+O(\lambda^2) \end{vmatrix}}_{O(\lambda^2)}$$

$$\underbrace{+\,0.2\lambda \begin{vmatrix} 0 & -\lambda\Delta^{(1)}+O(\lambda^2) \\ 0.2\lambda & 0.1\lambda \end{vmatrix}}_{O(\lambda^3)}$$

- order λ^2 terms

$$0 = (-1)\begin{vmatrix} -\Delta^{(1)} & 0.1 \\ 0.1 & -\Delta^{(1)} \end{vmatrix}$$

$$0 = (\Delta^{(1)})^2 - (0.1)^2$$

$$\Rightarrow \boxed{\Delta^{(1)} = \pm 0.1}$$ → same as two values found above using T.I.P.T

↳ eigenvalues of $\underbrace{\begin{pmatrix} 0 & 0.1 \\ 0.1 & 0 \end{pmatrix}}_{\text{submatrix of } V}$

$$\begin{array}{cccc} a & b & c & \\ \left(\begin{matrix} 0 \\ 0 \\ 0.2 \end{matrix}\right. & \begin{matrix} 0 \\ 0 \\ 0.1 \end{matrix} & \left.\begin{matrix} 0 \\ 0.1 \\ 0 \end{matrix}\right) & \begin{matrix} a \\ b \\ c \end{matrix} \end{array}$$

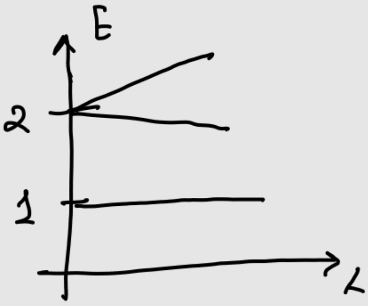
$$\begin{pmatrix} 0 & 0.1 \\ 0.1 & 0 \end{pmatrix} = \begin{pmatrix} \langle b|V|b\rangle & \langle b|V|c\rangle \\ \langle c|V|b\rangle & \langle c|V|c\rangle \end{pmatrix}$$

energies,

$$E_1 \cong 1$$

$$E_2 \cong 2 - 0.1 = 1.9$$

$$E \approx 2 + 0.1 = 2.1$$



eigenvectors

guess $\quad |2^{(0)}\rangle = \frac{1}{\sqrt{2}}|b\rangle - \frac{1}{\sqrt{2}}|c\rangle$ → gives the downward shift

$|3^{(0)}\rangle = \frac{1}{\sqrt{2}}|b\rangle + \frac{1}{\sqrt{2}}|c\rangle$ → gives the upward shift

* eigen vectors of

$$\begin{pmatrix} 0 & 0.1 \\ 0.1 & 0 \end{pmatrix} = 0.1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}}$$

$1/\sqrt{2}$ → coeff. of $|b\rangle$

$1/\sqrt{2}$ → coeff. of $|c\rangle$

$$\rightarrow \frac{1}{\sqrt{2}}|b\rangle + \frac{1}{\sqrt{2}}|c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

Degenerate Perturbation theory

- first-order energies
- zeroth-order energies

diagonalize the perturbation in the degenerate subspace.

i.e. find eigenvalues & vecs of

$$V_0 = \begin{pmatrix} \langle m_1^{(0)} | V | m_1^{(0)} \rangle & \cdots\cdots & \langle m_g^{(0)} | V | m_g^{(0)} \rangle \\ \\ \langle m_g^{(0)} | V | m_1^{(0)} \rangle & \cdots\cdots & \langle m_g^{(0)} | V | m_g^{(0)} \rangle \end{pmatrix}$$

where $|m_i^{(0)}\rangle$ for $i = 1$ to g is a basis for degenerate subspace:

$$H_0 |m_i^{(0)}\rangle = E_D^{(0)} |m_i^{(0)}\rangle$$

same energy

eigenvals of V_D are $\Delta_i^{(1)}$

eigenvecs $\begin{pmatrix} a_{i1} \\ \vdots \\ a_{ig} \end{pmatrix} \longrightarrow$ correct zeroth order states

$$\cancel{|l_i^{(0)}\rangle = \sum_{j=1}^{0} a_{ij} |m_j^{(0)}\rangle}$$

order of degeneracy

$$\boxed{|l_i^{(1)}\rangle = \sum_{j=1}^{g} a_{ij} |m_j^{(0)}\rangle}$$