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S. No.	Date	Title	Page No.	Teacher's Sign / Remarks
Books				
	1 →	Modern Quantum Mechanics. – J. J. Sakurai		
	2 →	Introduction of Quantum mechanics David J. Griffiths.		
	3 →	Principles of Q.M – R. Shankar		
	4 →	Quantum Mechanics E. Merzbacher		

Quantum II

$\Rightarrow \quad H = \frac{-\hbar^2}{2m} \nabla^2 + V(\vec{x})$

$$i\hbar \frac{\partial \psi}{\partial t}(t,\vec{x}) = \frac{-\hbar^2}{2m} \nabla^2 \psi(t,x) + V(\vec{x}) \psi(t,\vec{x})$$

$$\psi(\vec{x},t) \sim \int d^3p \cdot e^{i\frac{\vec{p}}{\hbar}\vec{x}} \phi(\vec{p},t)$$

probability $\rightarrow$ $\rho d^3x = |\psi(t,\vec{x})|^2 d^3x$

$$e^{-i\frac{E}{\hbar}t} \psi(0,\vec{x}) = \psi(t,\vec{x})$$

☆

$$\underbrace{\langle \vec{x} | \psi(t) \rangle}_{\psi(\vec{x},t)} = \langle x | e^{-i\frac{Ht}{\hbar}} | \psi \rangle_0 = \langle \vec{x} | e^{-i\frac{Ht}{\hbar}} \sum_n c_n |n\rangle$$

$$\phi(\vec{p},t) \langle O \rangle = \int \psi_N^* O \psi_N d^3x$$

$$\langle k | \psi \rangle = \phi_k(t)$$

☆

$$\Rightarrow \langle \vec{x} | \sum_n c_n e^{-i\frac{E_n t}{\hbar}} | n \rangle$$

$$= \sum_n c_n e^{-i\frac{E_n t}{\hbar}} \psi_{E_n}(\vec{x})$$

$$E\varphi_E(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\varphi_E(\vec{x}) + V(\vec{x})\varphi_E(\vec{x})$$

$$\langle \vec{x}' | \varphi \rangle = \langle \vec{x}' | \sum C_n | n \rangle$$

$$\varphi(x') = \sum_n C_n \varphi_n(\vec{x}')$$

→ **Bound state** $E < V$

$$\lim_{|\vec{x}| \to \infty} \varphi(\vec{x}, t) \to 0$$

III) Time independent perturbation theory (Non-degenerate)

$$H = \underbrace{H_0}_{\text{unperturbed Hamiltonian}} + \lambda V \to \text{perturbation}$$

$$\{|n^0\rangle\} \longrightarrow \{E_n^0\}$$

✓

$$H|n\rangle = E_n|n\rangle$$

$$(H_0 + \lambda V)|n\rangle = E_n|n\rangle$$

$$|n\rangle = |n^0\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots$$

$$\lambda \longrightarrow 1$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots$$

$$E_n - E_n^0 = \Delta_n = \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \cdots$$

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

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

$$= \phi_n(\Delta_n - \lambda V)|n\rangle$$

$$\frac{1}{H_0 - E_n}|n^{(0)}\rangle = \frac{1}{E_n^0 - E_n^0}|n^{(0)}\rangle$$

$$= \frac{1}{-E_n^{(0)}\left(1 - \frac{H_0}{E_n^{(0)}}\right)} = -\frac{1}{E_n^0}\left(1 + \frac{H_0}{E_n^0} + (\ )^2 \cdots\right)|n^0\rangle$$

$$\langle n^0|(\Delta_n - \lambda V)|n\rangle = 0$$

$$\sum_n |n^0\rangle\langle n^0| = 1$$

$$\phi_n = 1 - |n^0\rangle\langle n^0| = \sum_{k \neq n} |k^0\rangle\langle k^0|$$

$$\phi_n |m^0\rangle = \sum_{k \neq n} |k^0\rangle\langle k^0|m^0\rangle$$

$$\langle n^{(0)}| \frac{1}{H_0 - E_n^0} \phi_n (\Delta_n - \lambda V)|n\rangle$$

$$\lambda \longrightarrow 0$$

$$|n\rangle \rightarrow |n^{(0)}\rangle$$

$$E_n \longrightarrow E_n^{(0)}$$

$$|n\rangle = C_n(\lambda)\,|n^{(0)}\rangle + \frac{1}{E_n^0 - H_0} \phi_n^0 (\lambda V - \Delta_n)|n\rangle$$

$$\lambda \longrightarrow 0 \qquad C_n(\lambda \to 0) \Rightarrow 1$$

$$\langle n^0|n\rangle = C_n(\lambda) + \langle n^0| \frac{1}{E_n^0 - H_0} \phi_n (\lambda V - \Delta_n)|n\rangle$$

$$\frac{1}{0} \times 0 \times 0 = 0$$

$$= C_n(\lambda)$$

$$= 1$$

$$|n\rangle = C_n(\lambda)\left[|n^{(0)}\rangle + \frac{1}{C_n(\lambda)\,(E_n^0 - H_0)} \phi_n (\lambda V - \Delta_n)|n\rangle\right]$$

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$$|n\rangle = \cancel{C_n(\lambda)}\,|n^0\rangle + \frac{1}{E_n^0 - H_0}\,\phi_n\,(\lambda V - \Delta_n)|n\rangle \rightarrow (1)$$

$$C_n(\lambda) = \langle n^0 | n\rangle = 1$$

$$\Delta_n = ?$$

$$\langle n^0 | (\lambda V - \Delta_n)|n\rangle = 0$$

$$\Rightarrow \Delta_n = \lambda \langle n^0 | V | n\rangle$$

Satisfied for $\forall$ orders of λ

$$|n\rangle = |n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \ldots$$

$$\Delta_n = \lambda \Delta_n^1 + \lambda^2 \Delta_n^2 + \ldots$$

$$\lambda \Delta_n^1 + \lambda^2 \Delta_n^2 + \ldots = \lambda \langle n^0 | V \left(|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n\right.$$

$$O(\lambda) = \Delta_n^1 = \langle n^0 | V | n^0\rangle$$

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

$$O(\lambda^3) = \Delta_n^3 = \langle n^{(0)} | V | n^{(2)}\rangle$$

Solving Equation ④

$$\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \dots = |n^{(0)}\rangle + \frac{1}{E_n^{(0)} - H_0}\phi_n$$

$$\left\{\lambda V - \left(\lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + \dots\right)\right\}\left(|n^0\rangle + \lambda|n^1\rangle + \lambda^2|n^2\rangle + \dots\right)$$

$$(\lambda^1) = \frac{1}{E_n^0 - H_0}\phi_n\left(V - \Delta_n^{(1)}\right)|n^{(0)}\rangle = \frac{1}{E_n^0 - H_0}\phi_n V|n^0\rangle$$

$$(\lambda^2) = \frac{1}{E_n^0 - H_0}\phi_n\left(V - \Delta_n^{(1)}\right)|n^1\rangle$$

$$= \langle n^{(0)}|V\frac{1}{E_n^0 - H_0}\phi_n V|n^{(0)}\rangle$$

$$= \langle n^0|V\phi_n\frac{1}{E_n^0 - H_0}\phi_n V|n^0\rangle$$

$$\sum_{k(k\neq n)}|k^0\rangle\langle k^0| \qquad \sum_{l(l\neq n)}|l^{(0)}\rangle\langle l^{(0)}|$$

$$= \sum_{\substack{k,l \\ (k,l\neq n)}}\langle n^{(0)}|V|k^0\rangle\underbrace{\langle k^0|\frac{1}{E_n^0 - H_0}|l^0\rangle}\langle l^{(0)}|V|n^{(0)}\rangle$$

$$\frac{1}{E_n^0 - E_l^0}\langle k^0|l^0\rangle$$

$$\frac{1}{\dots^0 - \dots^0}\delta_{kl}$$

Identity

$$\phi_n \frac{1}{E_n^0 - H_0} \phi_n = \frac{1}{E_n^0 - H_0} \phi_n = \phi_n$$

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$$A|a\rangle = a'|a\rangle \qquad A^{-1}A = 1$$

$$A^{-1}A|a\rangle = |a\rangle \Rightarrow A^{-1} a'|a\rangle = |a\rangle$$

$$= A^{-1}|a\rangle = \frac{1}{a'}|a\rangle$$

$$= \sum_{k \neq n} \frac{\langle n^{(0)}|v|k^0\rangle \langle k^0|v|n^0\rangle}{E_n^0 - E_k^0}$$

$$\sum_{k (k \neq n)} \frac{|\langle n^0|v|k^0\rangle|^2}{E_n^0 - E_k^0} \equiv \sum_{k(\neq n)} \frac{|V_{nk}|^2}{E_n^0 - E_k^0}$$

$$\Rightarrow \Delta_n = E_n - E_n^0 = \lambda V_{nn} + \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|^2}{E_n^0 - E_k^0} + \cdots$$

$$\{ V_{nk} = \langle n^0|v|k^0\rangle \}$$

$$\Rightarrow |n^{(1)}\rangle = \frac{1}{E_n^{(0)} - H_0} \phi_n V |n^{(0)}\rangle$$

$$\sum_{k(\neq n)} |k^0\rangle\langle k^0|$$

$$= \sum_{k(\neq n)} \frac{1}{E_n^0 - E_k^0} |k^0\rangle \langle k^0|v|n^0\rangle$$

$$|n\rangle = |n^{(0)}\rangle + \lambda \sum_{k(\neq n)} |k^0\rangle \frac{V_{kn}}{E_n^0 - E_k^0} +$$

$$\lambda^2 \left[\sum_{\substack{k(\neq n)\\ l(\neq n)}} \frac{|k^0\rangle V_{kl} V_{ln}}{(E_n^0 - E_k^0)(E_n^0 - E_l^0)} - \sum_{k(\neq n)} \frac{|k^{(0)}\rangle V_{nn} V_{kn}}{(E_n^0 - E_k^0)^2} \right.$$

$$+ \cdots$$

$$|n\rangle_N = Z_n^{1/2} |n\rangle$$

normalised

$${}_N\langle n|n\rangle_N = 1 = Z_n \langle n|n\rangle \Rightarrow Z_n = \frac{1}{\langle n|n\rangle}$$

$$\langle n^0|n\rangle_N = Z_n^{1/2} \langle n^0|n\rangle = Z_n^{1/2}$$

$$Z_n^{-1} = \langle n|n\rangle = \left(\langle n^0| + \lambda\langle n^1| + \lambda^2\langle n^2| + \cdots\right)\left(\cdots\right)$$

$$Z_n = 1 + \lambda^2 \sum_{k(\neq n)} \frac{|V_{kn}|^2}{E_n^0 - E_k^0} + \cdots$$

$$|n\rangle_N = Z_n^{1/2}\,|n\rangle \qquad Z_n^{-1} = \langle n|n\rangle$$

$$= \left(\langle n^{(0)}| + \lambda\langle n^1| + \lambda^2\langle n^2| + \cdots\right)\left(|n^0\rangle + \lambda|n^1\rangle + \lambda^2|n^2\rangle + \cdots\right)$$

$$= 1 + \lambda\left(\underbrace{\langle n^0|n^1\rangle}_{=0} + \underbrace{\langle n^1|n^0\rangle}_{=0}\right) + \lambda^2\left(\underbrace{\langle n^2|n^0\rangle}_{=0} + \langle n^1|n^1\rangle + \underbrace{\langle n^0|n^2\rangle}_{=0}\right) + \cdots$$

$$= 1 + \lambda^2\langle n^1|n^1\rangle + \cdots$$

$$\cancel{Z_n^{-1} = 1 + \lambda^2 \sum_{k(\neq n)} \frac{|k^0\rangle V_{nk} V_{nk}^*}{E_n^0 - E_k^0}}$$

$$Z_n^{-1} = 1 + \lambda^2 \sum_{\substack{k(\neq n)\\ l(\neq n)}} \frac{\langle l^0|k^0\rangle V_{nk} V_{nl}^*}{(E_n^0 - E_k^0)(E_n^0 - E_l^0)} + \cdots$$

$$= 1 + \lambda^2 \sum_{k\neq n} \frac{V_{nk} V_{nk}^*}{(E_n^0 - E_k^0)^2} + \cdots$$

$$Z_n^{-1} = 1 + \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|^2}{(E_n^0 - E_k^0)^2} + \cdots$$

$$\Rightarrow Z_n = 1 - \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|^2}{(E_n^0 - E_k^0)^2} + \cdots$$

$$Z_n = \langle n^0 | n \rangle_N \qquad \boxed{\Delta_n = E_n - E_n^0}$$

$$\Delta_n = \lambda V_{nn} + \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|^2}{E_n^0 - E_k^0}$$

$$\frac{\partial E_n}{\partial E_n^0} = 1 - \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|^2}{(E_n^0 - E_k^0)^2} + \ldots$$

$$\frac{\partial E_n}{\partial E_n^0} = Z_n \quad \forall \lambda$$

Day

→ 1D harmonic oscillator

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

$$E_n^{(0)} = \left(n + \frac{1}{2}\right) \hbar\omega \;, \quad n = 0, 1, 2, 3 \ldots$$

$$\{ |n^{(0)}\rangle \} \qquad \underset{\text{perturbed potential}}{V} = -e|\underset{\text{electric field}}{\vec{E}}|x \qquad e < 0$$

$$V = \frac{1}{2} m \omega^2 x^2 \, \varepsilon \qquad \varepsilon <<< 1$$

$\delta_{nk} = 0$
is different

$V_{nk} = \langle n^0 | V | k^0 \rangle$

$$|0\rangle = |0\rangle + \lambda \sum_{k \neq 0} |k^0\rangle \frac{V_{k0}}{\epsilon_0^0 - \epsilon_k^0} + \ldots$$

$$\Delta_0 = \lambda V_{00} + \lambda^2 \sum_{k(\neq 0)} \frac{|V_{k0}|^2}{\epsilon_n^0 - \epsilon_k^0} +$$

$$V_{nk} = \langle n^0 | V | k^0 \rangle = \frac{1}{2} m\omega^2 \epsilon \langle n^0 | x^2 | k^0 \rangle$$

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right) \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right)$$

$$x^2 = \left(\sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \right)^2 = \frac{\hbar}{2m\omega} (a + a^\dagger)(a + a^\dagger)$$

$$= \frac{\hbar}{2m\omega} \left(a^2 + aa^\dagger + a^\dagger a + {a^\dagger}^2 \right)$$

$$a |n^{0}\rangle = \sqrt{n} |n^0 - 1\rangle$$

$$a^\dagger |n^0\rangle = \sqrt{n+1} |n^{0} + 1\rangle$$

Ans $V_{nk} = \frac{\epsilon \hbar \omega}{4} \Big[\sqrt{k(k-1)}\, \delta_{n,k-2} + \sqrt{(k+1)(k+2)}\, \delta_{n,k+2} + k\delta_{nk} + (k+1)\delta_{nk} \Big]$

$$V_{01} = 0$$

$$V_{20} = \frac{\epsilon \hbar \omega}{4} \left[\sqrt{2} \right]$$

$\epsilon_0^\circ = \frac{1}{2}\hbar\omega$ $\quad$ $\epsilon_2^\circ = \frac{5}{2}\hbar\omega$

$$|0\rangle = |0^\circ\rangle + \lambda |2^\circ\rangle \frac{\epsilon \hbar\omega\sqrt{2}}{4(-2\hbar\omega)}$$

$$V_{00} = \frac{\epsilon\hbar\omega}{4}$$

$$\Delta_0 = \hbar\omega\left(\frac{\epsilon}{4} - \frac{\epsilon^2}{16} + \cdots\right)$$

$$|0\rangle = |0^\circ\rangle - \frac{\epsilon}{4\sqrt{2}}|2^{(0)}\rangle + \cdots$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2(1+\epsilon)x^2$$

$$= \frac{p^2}{2m} + \frac{1}{2}mW^2x^2$$

$$\psi_0(x) = \langle x|0^\circ\rangle = \frac{1}{\pi^{1/4}\sqrt{x_0}} e^{-\frac{x^2}{2x_0^2}}$$

$$\rightarrow \frac{1}{\pi^{1/4}\sqrt{x}}(1+\epsilon)^{1/8} e^{\frac{-x^2}{2x_0^2}(1+\epsilon)^2}$$

$$\left(x_0 = \sqrt{\frac{\hbar}{m\omega}}\right)$$

$\downarrow$ new

$$\sqrt{\frac{\hbar}{m\omega}}(1+\epsilon)^{-1/4}$$

$$\parallel$$

$$x_0(1+\epsilon)^{-1/4}$$

$$\psi_0(x) \longrightarrow \frac{1}{\pi^{1/4}\sqrt{x_0}}\left(1+\frac{\epsilon}{8}\right) e^{-\frac{x^2}{2x_0^2}\left(1+\frac{\epsilon}{2}\right)} \quad (\text{up to } O(\epsilon))$$

$$= \frac{1}{\pi^{1/4}\sqrt{x_0}} e^{-\frac{x^2}{2x_0^2}}\left[1-\frac{x^2}{4x_0^2}\epsilon+\frac{\epsilon}{8}\right]+ \cdots$$

$$H = \langle x|0^\circ\rangle + \frac{\epsilon\, e^{-x^2/2x_0^2}}{\pi^{1/4}\sqrt{x_0}}\left(\frac{1}{8}-\frac{x^2}{4x_0^2}\right)$$

$$\cancel{H} = \langle x|2^\circ\rangle = \frac{1}{2\sqrt{2}}\frac{1}{\pi^{1/4}\sqrt{x_0}} e^{-\frac{x^2}{2x_0^2}}\left[-2+4\left(\frac{x}{x_0}\right)^2\right]$$

$$H = \langle x|0^\circ\rangle - \frac{\epsilon}{4\sqrt{2}}\langle x|2^\circ\rangle + \cdots$$

Quadratic Stark effect :

$$H_0 = \frac{\vec{P}^2}{2m} + V_0(r)$$

$$[\Pi, H_0] = 0$$

$\uparrow$ parity operator

Degeneracy $\quad E_n^{(0)} \sim \frac{1}{n^2}$

$n = 1, 2, 3 \ldots$

$$\psi_{n\ell m}(\vec{x}) = \langle \vec{x}|n\ell m\rangle \qquad \vec{L}^2,\ L_z$$

$\langle \vec{x}|100\rangle \rightarrow \psi_{100}(x) \rightarrow$ Non-degenerate classmate

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H atom is kept in a constant $\vec{E} = |\vec{E}|\hat{z}$

$$H = H_0 + \lambda V \qquad V = -e|\vec{E}|z$$

$$\Delta_n = \cancel{\lambda V_{nn}} + \lambda^2 \sum_{n(\neq k)} \frac{|V_{nk}|^2}{E_n^0 - E_k^0} + \text{---}$$

$$V_{nk} = \langle n^{(0)} | V | k^{(0)} \rangle$$

$$V = -e|\vec{E}|z$$

$$V_{nk} = -e|\vec{E}| \langle n^{(0)} | z | k^{(0)} \rangle$$

$n=1 \rightarrow$ ground state

ψ_{100} is simultaneous eigenstate of Π and H_0 as this state is non-degenerate.

$V_{nn} \Rightarrow \langle n | z | n \rangle_0 = 0$ parity selection rule

↳ ground state

$$= \int d^3x \langle n | \vec{x} \rangle \langle \vec{x} | z | n \rangle$$

$$\stackrel{?}{=} \int d^3x\, \psi^*_{100}(\vec{x})\, z \langle \vec{x} | n \rangle$$

$\psi_{100}(x)$

2nd term

$V_{12}, V_{13}, \text{---}$

$$V_{1k} = -e|\vec{E}| \langle 100 | z | k(\neq n) lm \rangle$$

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$$\sum_{k(\neq 1)} \frac{|V_{1k}|^2}{E_1^0 - E_k^0}$$

$$\sum_{k(\neq 1)} |V_{1k}|^2 = \sum_{k(\neq 1)} \left| \langle 1^{(0)} | V | k^{(0)} \rangle \right|^2$$

$$= \sum_{k(\neq 1)} \langle 1^{(0)} | V | k^{(0)} \rangle \langle k^{(0)} | V | 1^{(0)} \rangle$$

~~taking (k=1)~~

$$= \sum_{k} \langle 1^0 | V^2 | 1^0 \rangle = e^2 |\vec{E}|^2 \langle z^2 \rangle_{100}$$

$$\Downarrow$$

$$\frac{e^2 |\vec{E}|^2 \langle r^2 \rangle_{100}}{3}$$

$$\langle x^2 \rangle_{100} = \langle y^2 \rangle_{100} = \langle z^2 \rangle_{100}$$

$$\langle r^2 \rangle_{100} = 3 \langle z^2 \rangle_{100}$$

Ans $3a_0^2$

$$\sum_{k(\neq 1)} \frac{|V_{1k}|^2}{E_1^0 - E_k^0}$$

$$\sum_{k(\neq 1)} |V_{1k}|^2 = \sum_{k(\neq 1)} |\langle 1^{(0)}|V|k^{(0)}\rangle|^2$$

$$= \sum_{k(\neq 1)} \langle 1^{(0)}|V|k^{(0)}\rangle \langle k^{(0)}|V|1^{(0)}\rangle$$

~~taking (k=1)~~

$$= \sum_{k} \langle 1^0|V^2|1^0\rangle = e^2|\vec{E}|^2\langle z^2\rangle_{100}$$

$$\Downarrow$$

$$\frac{e^2|\vec{E}|^2\langle r^2\rangle_{100}}{3}$$

$$\langle x^2\rangle_{100} = \langle y^2\rangle_{100} = \langle z^2\rangle_{100}$$

$$\langle r^2\rangle_{100} = 3\langle z^2\rangle_{100}$$

Ans $3a_0^2$

$$\Delta_0 = e^2|\vec{E}|^2 \sum_{j(\neq 0)} \frac{|z_{0j}|^2}{E_0^{(0)} - E_j^{(0)}} + \cdots$$

$$\sum_{j(\neq 0)} |z_{0j}|^2 = a_0^2$$

$$E_0^0 \leq E_j^{(0)}$$

$n=1$ $\quad$ $n=2$

$$\Rightarrow -E_0^{(0)} + E_j^{(0)} \geq -E^{(0)} + E^{(0)}$$

$$\frac{3e^2}{8a_0}$$

$$\left(E_n^0 = -\frac{e^2}{2a_0 n^2}\right)$$

$n = 1, 2, 3, \ldots$

$$\sum_{k(\neq 1)} \frac{|V_{k1}|^2}{E_1^0 - E_k^0}$$

$$\sum_{k(\neq 1)} |V_{k1}|^2 = \sum_{k(\neq 1)} |\langle 1 | V | k \rangle|^2$$

$$= \sum_{k(\neq 1)} \langle 1 | V | k \rangle \langle k | V | 1 \rangle$$

taking $k=1$

$$= \sum_k \langle 1 | V^2 | 1 \rangle = e^2 |E|^2 \langle z^2 \rangle_{100}$$

$$\frac{e^2 |E|^2 \langle r^2 \rangle_{100}}{3}$$

$$\langle x^2 \rangle_{100} = \langle y^2 \rangle_{100} = \langle z^2 \rangle_{100}$$

$$\langle r^2 \rangle_{100} = 3 \langle z^2 \rangle_{100}$$

$3a_0^2$

$$\Delta_0 = e^2 |E|^2 \sum_{j(\neq 0)} \frac{|z_{0j}|^2}{E_0^{(0)} - E_j^{(0)}} + \cdots$$

$$\sum_{j(\neq 0)} |z_{0j}|^2 = a_0^2$$

$$E_0^0 \leq E_j^{(0)}$$

$$-E_0^{(0)} + E_j^{(0)} \geq -E_0^{(0)} + E_1^{(0)}$$

$$\frac{3e^2}{8a_0} \qquad E_n^0 = -\frac{e^2}{2a_0 n^2}$$

$$\frac{1}{\epsilon_j^0 - \epsilon_0^{(0)}} \le \frac{4}{3}\frac{2a_0}{e^2} \quad \text{valid for each } j$$

→ Polarisability :

Energy $\simeq -e|\vec{E}|z$

$\simeq -d|\vec{E}|$

$$\alpha = \frac{-2}{|\vec{E}|^2} \Delta_n$$

$$\alpha = \frac{d}{|\vec{E}|} \qquad d = \frac{\text{Energy}}{|\vec{E}|} = \frac{\epsilon_n^0 + \ldots}{|\vec{E}|}$$

$$d = \frac{\partial\,\text{Energy}}{\partial|\vec{E}|} = \frac{d\Delta_n}{\partial|\vec{E}|}$$

$$\alpha = -\frac{1}{|\vec{E}|}\frac{\partial \Delta_n}{\partial|\vec{E}|}$$

$$\partial(\Delta_n) = -\alpha|\vec{E}|\,\partial|\vec{E}|$$

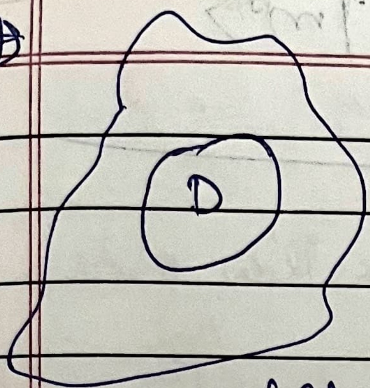
$$\Delta_n = -\frac{\alpha|\vec{E}|^2}{2}$$

$$\Rightarrow \alpha = \frac{-2}{|\vec{E}|^2}\Delta_0 = 2e^2 \sum_{(j\neq 0)} \frac{|z_{0j}|^2}{\epsilon_j^0 - \epsilon_0^0}$$

$$\alpha < 2e^2 \times a_0^2 \times \frac{4}{3}\frac{2a_0}{e^2}$$

$$\Rightarrow \alpha < \frac{16}{3}a_0^3 \simeq 5.3a_0^3$$

#



$$H_0|m^\circ\rangle = \epsilon_0^D|m^\circ\rangle$$

$$m = 1, 2, \ldots g$$

$$H_0|M_i\rangle = H_0 \sum_{m \in D} C_m |m^\circ\rangle$$

g-fold degeneracy $\quad = \epsilon_0^{(D)}|M_i\rangle$

$$\langle M_i|M_j\rangle = \delta_{ij}$$

H_0 is diagonal in $\{|M_i\rangle\}$

2) Non - Degenerate

$$\Delta_n = \lambda V_{nn} + \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|^2}{\epsilon_n^\circ - \epsilon_k^\circ} + \ldots$$

$$|n\rangle = |n^\circ\rangle + \lambda \sum_{k(\neq n)} |k^\circ\rangle \frac{V_{kn}}{\epsilon_n^\circ - \epsilon_k^\circ} + \ldots$$

$\Rightarrow V_{kn} = 0$ (for degenerate case)

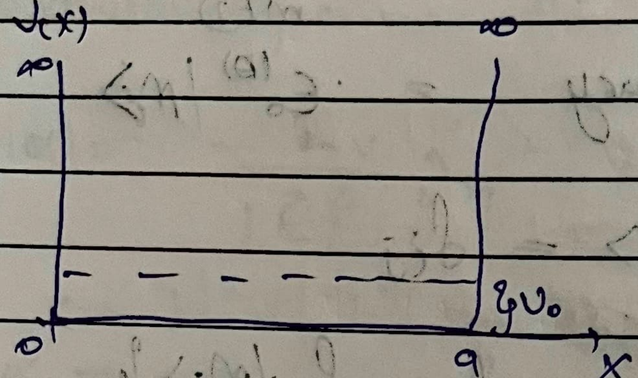
$$\{|m^\circ\rangle\} \xrightarrow[V]{\text{under perturbation}} \{|l\rangle\} \xrightarrow{\lambda \to 0} \{|l^\circ\rangle\}$$

choose a particular linear combination of $\{|m^\circ\rangle\} \in D$ such that V is diagonalized

$$|l^0\rangle = \sum_{m\in D} \langle m^0|l^0\rangle |m^0\rangle$$

Tutorial

Q.4



$$\Delta_n = \lambda V_{nn} + \lambda^2 \sum_{k(\neq n)} \frac{|V_{nk}|}{\epsilon_n^0 -}$$

$\lambda \to 1$

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \equiv \langle x|n^{(0)}\rangle$$

$$\epsilon_{(n)}^{0} = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3 \ldots$$

$V = V_0$

$$V_{nn} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$$= \int dx \, \langle n^0|x\rangle \langle x|V|n^0\rangle$$

$\left\{ \int dx \, |x\rangle\langle x| = \mathbb{1} \right\}$

$$\int dx \, \psi_n^*(x) \, V_0 \, \langle x|n^0\rangle$$

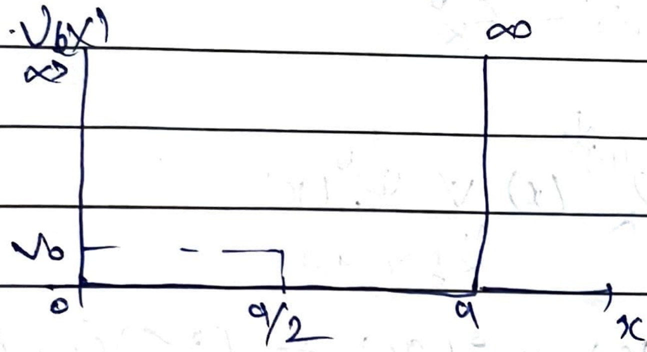
$$\Rightarrow \int dx \, \psi_n^{*(0)}(x) \, V_0 \, \psi_n^0(x)$$

$$= V_0 \langle n^0|n^0\rangle = V_0 \qquad \{\Delta_n = V_0\}$$

$$\{ V_{nk} = \langle n^0|V_0|k^0\rangle = V_0 \langle n^0|k^0\rangle$$

$$|n\rangle = |n^{(0)}\rangle + \lambda \sum_{k(\neq n)} \frac{V_{kn}}{E_n^0 - E_k^0} \qquad V_{kn} = 0$$

states will remain same.

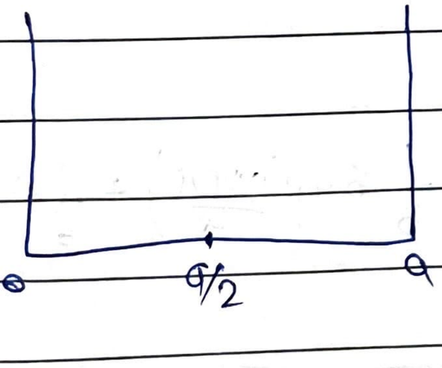


$$V_{nn} = \langle n^0|V|n^0\rangle = \int_0^{a/2} dx\, \psi_n^{0*}(x)\, V_0\, \psi_n^0(x)$$

$$= \lambda V_0 \left(\frac{2}{a}\right) \int_0^{a/2} dx\, \sin^2\left(\frac{n\pi x}{a}\right)$$

$$= \frac{V_0}{2}$$

$$V_{nk} = V_0 \left(\frac{2}{a}\right) \cdot \int_0^{a/2} dx\, \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{k\pi x}{a}\right)$$



$$V_{nn} = \int dx\, \psi_n^{(0)*}(x)\, V(x)\, \psi_n^{(0)}(x)$$

$$= \int dx\, |\psi_n^{(0)}(x)|^2\, \alpha\, \delta(x - a/2)$$

$$= \alpha\, |\psi_n^{(0)}(a/2)|^2$$

$$= \frac{2\alpha}{a} \sin^2\left(\frac{n\pi}{2}\right) = \begin{cases} 0 & n \text{ is even } 2, 4, 6 \\ \frac{2\alpha}{a} & \text{if } n \text{ is odd } 1, 3, 5 \end{cases}$$

even vanishing wavefunction itself vanishes.

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$$\psi_1'(x) = \langle x | 1^{(1)} \rangle = \sum_{K(\neq 1)} \frac{\langle x | K^0 \rangle V_{K1}}{E_1^0 - E_K^0}$$

$$= \sum_{K(\neq 1)} \frac{\psi_K^{(0)}(x)\, V_{K1}}{E_1^0 - E_K^0}$$

$$V_{K1} = \int dx\, \psi_K^{(0)*}(x)\, \underset{\alpha\delta(x-a/2)}{V}\, \psi_1^0(x)$$

$$= \alpha\, \psi_K^0(a/2)\, \psi_1^0(a/2) = \left(\frac{2\alpha}{a}\right) \sin\left(\frac{K\pi}{2}\right) \sin\left(\frac{\pi}{2}\right)$$

$$= \frac{2\alpha}{a} (-1)^K \quad \text{for } K = 2n+1$$

$(n = 1, 2, 3 \ldots)$

$$\frac{2\alpha}{a} \sqrt{\frac{2}{a}} \left[\frac{-\sin\left(\frac{3\pi x}{a}\right)}{E_1^0 - E_3^0} + \frac{\sin(5\pi x/a)}{E_1^0 - E_5^0} + \frac{-\sin\left(\frac{7\pi x}{a}\right)}{E_1^0 - E_7^0} \ldots \right.$$

$$E_n^0 = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$\frac{m\alpha}{\pi^2 \hbar^2} \sqrt{\frac{a}{2}} \left[\sin\left(\frac{3\pi x}{a}\right) - \frac{1}{3} \sin\left(\frac{5\pi x}{a}\right) + \frac{1}{6} \sin\left(\frac{7\pi x}{a}\right) \right.$$

$V = bx$

$\{|m^{(0)}\rangle\} : g$ $\quad \{H_0 = H_0 + \lambda V\}$

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

perturbed states $\{|l\rangle\} \xrightarrow{\lambda \to 0} \{|l^{(0)}\rangle\}$ $\quad H|l\rangle = E_l|l\rangle$

$E_l = E_D^{0} + \Delta_l$

$|l^{(0)}\rangle = \sum_{m \in D} \langle m^{(0)}|l^{(0)}\rangle |m^{0}\rangle$

$\Rightarrow P_0 = \sum_{m \in D} |m^{(0)}\rangle\langle m^{(0)}|$ $\quad P_1 = 1 - P_0$

$P_0 = \sum_{m \in D} H_0|m^0\rangle\langle m^0| = E_D^{(0)} P_0$

$\underbrace{(E_l - H)}_{}\underbrace{|l\rangle}_{P_0+P_1} = 0$

$|l^{(0)}\rangle = \sum_{m \in D} \langle m^0|l^{(0)}\rangle |l^0\rangle \to (1)$

$\Rightarrow (E - H_0 - \lambda V) P_0|l\rangle + (E - H_0 - \lambda V) P_1|l\rangle = 0$

$(E - E_D^{0} - \lambda V) P_0|l\rangle + (E - H_0 - \lambda V) P_1|l\rangle = 0 \to (2)$

$\Rightarrow P_0 \times (2).$ $\quad P_0 H_0 P_1 = E_D^{0} P_0 P_1 = 0$

$(E P_0 - E_D^{(0)} P_0 - \lambda V P_0)|l\rangle - \lambda P_0 V P_1|l\rangle = 0 \to (3)$

$\Rightarrow P_1 \times (2)$

$-\lambda P_1 V P_0|l\rangle + (E - H_0 - \lambda P_1 V P_1) P_1|l\rangle = 0 \to (4)$

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$$\Rightarrow P_1|l\rangle = P_1 \frac{1}{E - H_0 - \lambda P_1 V P_1} \lambda P_1 V P_0 |l\rangle \Rightarrow ⑤$$

$$|l\rangle = |l^{(0)}\rangle + \lambda |l^{(1)}\rangle + \lambda^2 |l^{(2)}\rangle \cdots$$

$$E = E_D^0 + \lambda \Delta_l^1 + \cdots$$

$$P_1 \frac{\lambda}{E - H_0 + \lambda P_1 V P_1} = P_1 \frac{\lambda}{E_D^0 - H_0 + \lambda(\Delta_l^1 + P_1 V P_1 + \cdots)}$$

$$= \sum_{K \notin D} |K^0\rangle\langle K^0| \frac{\lambda}{E_D^0 - H_0 + \lambda(\Delta_l^1 + P_1 V P_1 + \cdots)}$$

$$= \sum_{K \notin D} |K^{(0)}\rangle\langle K^0| \frac{\lambda}{E_D^{(0)} - E_K^{(0)} + \lambda(\Delta_l + P_1 V P_1 - \cdots)}$$

$$= \sum_{K \notin D} |K^{(0)}\rangle\langle K^{(0)}| \frac{\lambda}{E_D^{(0)} - E_K^{(0)}} \left[1 + \frac{\lambda(\Delta_l^1 + P_1 V P_1 - \cdots)}{E_D^{(0)} - E_K^{(0)}} \right.$$

$$= \sum_{K \notin D} |K^{(0)}\rangle\langle K^{(0)}| \frac{\lambda}{E_D^{(0)} - E_K^{(0)}} + \cancel{O(\lambda^2)}\, P_1 V P_0 (|l^{(0)}\rangle + \lambda |l^{(1)}\rangle + \lambda^2 |l^{(2)}\rangle$$

$$O(\lambda^1) = P_1 |l^1\rangle = \sum_{K \notin D} \frac{1}{E_D^0 - E_K^0} |K^0\rangle\langle K^0| P_1 V P_0 |l^{(0)}\rangle$$

$$\sum_{K \notin D} \frac{1}{E_D^0 - E_K^0} |K^0\rangle \underbrace{\langle K^0| V |l^{(0)}\rangle}_{V_{Kl}}$$

$$(E - E_D^{0} - \lambda P_0 V)\, P_0|l\rangle - \lambda P_0 V P_1|l\rangle = 0 \quad (3)$$

$$-\lambda P_1 V P_0|l\rangle + (E - H_0 - \lambda P_1 V P_1)\, P_1|l\rangle = 0 \rightarrow (4)$$

$$P_1|l^{(1)}\rangle = \sum_{k \notin D}' \frac{|k^{(0)}\rangle}{E_D^{(0)} - E_k^{(0)}} V_{kl} \rightarrow (6)$$

$$P_1|l\rangle = P_1 \frac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0|l\rangle \longrightarrow (5)$$

$$|l^{(1)}\rangle = P_0|l^{(1)}\rangle + P_1|l^{(1)}\rangle$$

$\Rightarrow$ Substitute (5) in (3)

$$\Rightarrow \underbrace{(E - E_D^{(0)}}_{\lambda \Delta_l^{(1)} + \lambda^2 \Delta_l^{(2)} + \dots} - \lambda P_0 V P_0)\, \underbrace{P_0|l\rangle}_{|l^{0}\rangle + \lambda|l^{(1)}\rangle + \lambda^2|l^{(2)}\rangle + \dots} - \lambda^2 P_0 V P_1 \frac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0|l\rangle = 0$$

$$O(\lambda^1): (\Delta_l^{1} - P_0 V P_0)(P_0|l^{(0)}\rangle) = 0$$

$$\Rightarrow \underbrace{(P_0 V P_0)}_{X} \underbrace{(P_0|l^{(0)}\rangle)}_{|l^{(0)}\rangle} = \Delta_l^{(1)} \underbrace{(P_0|l^{(0)}\rangle)}_{|l^{(0)}\rangle}$$

$$X \underbrace{|l^{(0)}\rangle}_{\text{zeroth order perturbed state}} = \Delta_l^{(1)} |l^{(0)}\rangle$$

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$X = P_0 V P_0$

$$X P_0 |l^{(0)}\rangle = \Delta_l^{(1)} P_0 | l^{(0)}\rangle \quad (\in D)$$

$$\Rightarrow \sum_{m' \in D} X | m'^{(0)}\rangle \langle m'^{(0)} | P_0 | l^{(0)}\rangle = \Delta_l^{(1)} P_0 | l^{(0)}\rangle$$

$$\Rightarrow \sum_{m' \in D} \langle m^{(0)} | X | m'^{(0)}\rangle \langle m'^{(0)} | l^{(0)}\rangle = \Delta_l^{(1)} \langle m^{(0)} | l^{(0)}\rangle$$

$$\Rightarrow \sum_{m' \in D} X_{mm'} \langle m'^{(0)} | l^{(0)}\rangle = \Delta_l^{(1)} \langle m^{(0)} | l^{(0)}\rangle$$

$$\begin{pmatrix} X_{11} & X_{12} & \cdots \\ X_{21} & X_{22} & \cdots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \\ \\ \end{pmatrix} = \Delta_l^{(1)} \begin{pmatrix} \\ \\ \end{pmatrix}$$

$$\Rightarrow \langle l'^{(0)} | P_0 V P_0 | l^{(0)}\rangle = \langle l'^{(0)} | \Delta_l^{(1)} | l^{(0)}\rangle$$

$$\rightarrow \langle l'^{(0)} | V | l^{(0)}\rangle = \Delta_l^{(1)} \delta_{l'l}$$

Degenerate $\quad V_{ll'} = 0 \ (\text{if } l \neq l')$

$$\Rightarrow O(\lambda^2) = (\Delta_l^{(1)} - P_0 V P_0) P_0 | l^{(1)}\rangle = \cancel{(\Delta_l^{(2)} + P_0 \ldots)}$$

$$= \left[-\Delta_l^{(2)} + P_0 V P_1 \frac{1}{E_D^0 - H_0} P_1 V P_0 \right] P_0 | l^{(0)}\rangle$$

$$O(\lambda^1) = | l^{(0)}\rangle ; \quad \Delta_l^{(1)}$$

$| l^{(1)}\rangle$

$\Delta^{(1)}_{l_i} \neq \Delta^{(1)}_{l_j}$ for $i \neq j$

$|l^{(0)}\rangle + |l^{(1)}\rangle \simeq |l\rangle$ up to $O(\lambda)$ is non degenerate / Degenerate

$(x) \equiv O(\lambda)$ of non-degenerate case

$\Rightarrow (V - \Delta_n^{(1)})|n^{(0)}\rangle = (E_n^{(0)} - H_0)|n^{(1)}\rangle$

$\therefore |n^{(1)}\rangle = \sum_{k(\neq n)} \frac{|k^{(0)}\rangle V_{kn}}{E_n^{(0)} - E_k^{(0)}}$

$\Rightarrow \Delta_l^{(1)} \equiv E_n^{(0)}$

$P_0 V P_0 \equiv H_0$

$P_0 |l^{(0)}\rangle \equiv |n^{(0)}\rangle$

$V \equiv P_0 V P_1 \cdot \frac{1}{E_D^{(0)} - H_0} P_1 V P_0$

$\Delta_n^{(1)} \equiv \Delta_l^{(2)}$

$|n^{(0)}\rangle = P_0 |l_i^{(0)}\rangle$

$\Rightarrow (E - E_D^{(0)} - \lambda P_0 V P_0) P_0 |l\rangle - \lambda^2 P_0 V P_1 \frac{1}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0 |l\rangle$ (main)

$\Rightarrow O(\lambda^2) = \left(P_0 V P_1 \cdot \frac{1}{E_D^0 - H_0} P_1 V P_0 - \Delta_{l_i}^{(2)} \right] P_0 | l_i^{(0)}\rangle$

$= (\Delta_{l_i}^{(1)} - P_0 V P_0) \cdot P_0 |l_i^{(1)}\rangle$

$O(\lambda^1) : (V - \Delta_n^{(1)})|n^{(0)}\rangle = (E_n^{(0)} - H_0)|n^{(1)}\rangle$

$$|n^{(1)}\rangle = \lambda \sum_{k(\neq n)} |k^{(0)}\rangle \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}}$$

$$P_0|l_i^{(1)}\rangle = \lambda \sum_{j(\neq i)} \frac{|l_j^{(0)}\rangle \langle l_j| P_0 V P_1 \frac{1}{E_D^{(0)} - H_0} P_1 V P_0}{\Delta_{l_i}^{(1)} - \Delta_{l_j}^{(1)}}$$

$$\Rightarrow P_0|l_i^{(1)}\rangle = \lambda \sum_{j(\neq i)} \frac{|l_j^{(0)}\rangle \langle l_j^{(0)}| V P_1 \frac{1}{E_D^{0} - H_0} P_1 V |l_i^{(0)}\rangle}{\Delta_{l_i}^{(1)} - \Delta_{l_j}^{(1)}}$$

$$P_1 = \sum_{k \notin D} |k^{(0)}\rangle \langle k^0|$$

$P_1 V|l_i\rangle$

$$P_0|l_i^{(1)}\rangle = \lambda \sum_{j(\neq i)} \frac{|l_j^{(0)}\rangle}{\Delta_{l_i}^{(1)} - \Delta_{l_j}^{(1)}} \langle l_j^{(0)}| V \sum_{k \notin D} |k^0\rangle\langle k^0| \frac{1}{E_D^0 - H_0}$$

$E_D^0 - H_0 \Downarrow E_k^{(0)}$

$$= \lambda \sum_{j(\neq i)} \frac{|l_j^{(0)}\rangle}{\Delta_{l_i}^{(1)} - \Delta_{l_j}^{(1)}} \sum_{k \notin D} V_{l_j k} \frac{1}{E_D^{(0)} - E_k^{(0)}} V_{k l_i}$$

$$\Rightarrow P_0|l_i^{(1)}\rangle = \lambda \sum_{\substack{j(\neq i) \\ k \notin D}} \frac{|l_j^{(0)}\rangle V_{l_j k} V_{k l_i}}{(\Delta_{l_i}^{(1)} - \Delta_{l_j}^{(1)})(E_D^{(0)} - E_k^{(0)})}$$

$$|l_i^{(1)}\rangle = P_0|l_i^{(1)}\rangle + P_1|l_i^{(1)}\rangle$$

$$= \lambda \sum_{k \notin D} \frac{|k^{(0)}\rangle V_{k l_i}}{E_D^{(0)} - E_k^{(0)}} + (\quad)$$

Eqn (8) $\Rightarrow \langle l_i^{(0)}| (\epsilon - E_D^{(0)} - \lambda P_0 V) P_0 |l_i\rangle - \langle l_i^{0}| \lambda P_0 V P_1 |l_i\rangle = 0$

$$\Rightarrow \Delta_{l_i} \underbrace{\langle l_i^{(0)}|l_i\rangle}_{1} - \lambda \langle l_i^{(0)}| V P_0 |l_i\rangle = \lambda \langle l_i^{(0)}| V P_1 |l_i\rangle$$

$$\Rightarrow \Delta_{l_i} = \lambda \left(\langle l_i^{(0)}| V (P_0 + P_1) |l_i\rangle \right)$$

$$= \lambda \langle l_i^{(0)}| V |l_i\rangle$$

$$\Rightarrow \lambda \Delta_{l_i}^{(1)} + \lambda^2 \Delta_{l_i}^{(2)} + \ldots = \lambda \langle l_i^{(0)}| V \left(|l_i^{0}\rangle + \lambda |l_i^{(1)}\rangle + \ldots \right)$$

$$\Rightarrow \Delta_{l_i}^{(2)} = \langle l_i^{(0)}| V |l_i^{(1)}\rangle \qquad \langle l_i^{(0)}| V P_1 |l_i^{(1)}\rangle$$

$$= \langle l_i^{(0)}| V \left(P_0 |l_i^{(1)}\rangle + P_1 |l_i^{(1)}\rangle \right)$$

$$\langle l_i^{(0)}| P_0 V P_0 |l_i^{(1)}\rangle = \Delta_{l_i}^{(1)} \langle l_i^{(0)}| P_0 |l_i^{(1)}\rangle = 0$$

$$X |l_i^{(0)}\rangle \underset{V_{l_i k}}{=} \Delta_{l_i}^{(1)} |l_i^{(0)}\rangle$$

$$\Rightarrow = \sum_{K \notin D} \frac{\langle l_i^{(0)}| V |K^{(0)}\rangle V_{K l_i}}{G_D^{(0)} - G_K^{(0)}}$$

$$= \sum_{K \notin D} \frac{|V_{K l_i}|^2}{G_D^{(0)} - G_K^{(0)}}$$

$\Rightarrow E_n = -\frac{1}{n^2} \equiv E_0^{(0)} \quad n = 1, 2, 3 \ldots$

non-degenerate

$n=2: \{|2,1,1\rangle, |2,1,0\rangle, |2,1,-1\rangle\}$

$l = 1, 0 \rightarrow m=0 \quad |2,0,0\rangle$

$m = \pm 1, 0$

$|200\rangle \quad |210\rangle$

$V = -e|\vec{E}|z$

$$V = \begin{array}{c|cccc} & |200\rangle & |210\rangle & |211\rangle & |2,1,-1\rangle \\ \hline |2,0,0\rangle & 0 & \langle 200|V|210\rangle & 0 & 0 \\ |210\rangle & \langle 210|V|200\rangle & 0 & 0 & 0 \\ |211\rangle & 0 & 0 & 0 & 0 \\ |21-1\rangle & 0 & 0 & 0 & 0 \end{array}$$