Iterative process - time indep. perturbation theory

(Raleigh - Schrödinger pert. th.)



$$(H_0 + \lambda V)|n\rangle_\lambda = E_n^{(\lambda)} |n\rangle_\lambda$$

$$= (E_n^{(0)} + \lambda \Delta E_n^{(\lambda)})|n\rangle_\lambda$$

$$\therefore (H_0 - E_n^{(0)})|n\rangle_\lambda = \lambda(\Delta E_n^{(\lambda)} - V)|n\rangle_\lambda$$

$\langle n^{(0)}| \times$

$$0 = \lambda \Delta E_n^{(\lambda)} \langle n^{(0)}|n\rangle_\lambda - \lambda \langle n^{(0)}|V|n\rangle_\lambda$$

Now let $\Delta E_n^{(\lambda)} = E_n^{(1)} + \lambda E_n^{(2)} \dots$

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

Then the original eqn. is

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

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

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

$\underline{(\lambda^2)}$ $$H_0 |n^{(2)}\rangle + V|n^{(1)}\rangle = E_n^{(0)}|n^{(2)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle$$

$$(H_0 - E_n^{(0)})|n^{(2)}\rangle = E_n^{(2)}|n^{(0)}\rangle + (E_n^{(1)} - V)|n^{(1)}\rangle$$

$$\langle n^{(0)}| \times \qquad 0 = E_n^{(2)} + (E_n^{(1)} \cancel{\langle n^{(0)}|n^{(1)}\rangle} \to 0) - \langle n^{(0)}|V|n^{(1)}\rangle$$

Now recall as per Fredholm Thm. we have chosen $\langle n^{(0)}|n^{(j)}\rangle = 0$ for $j > 0$

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

We can that at order $p$, the terms $\lambda^p$

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

$$\cdots\cdots E_n^{(j)} |n^{(p-j)}\rangle \cdots$$

$$+ E_n^{(p)} |n^{(0)}\rangle$$



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

$$+ \sum_{j=2}^{p} E_n^{(j)} |n^{(p-j)}\rangle$$

$$\langle n^{(0)}| \times \qquad 0 = -\langle n^{(0)}| V | n^{(p-1)}\rangle + E_n^{(p)}$$

$$\boxed{E_n^{(p)} = \langle n^{(0)}| V | n^{(p-1)}\rangle}$$

Thus we need $|n\rangle_\lambda$ correct to order $p+1$ to be able to calculate $E_n$ correct to order $p$.

Return to $\lambda^1$ equation:

$$|n^{(1)}\rangle = \left[\frac{\mathbb{1} - |n^{(0)}\rangle\langle n^{(0)}|}{H_0 - E_n^{(0)}}\right](E_n^{(1)} - V)\,|n^{(0)}\rangle$$

[Now $\left(\mathbb{1} - |n^{(0)}\rangle\langle n^{(0)}|\right)\left(|n^{(0)}\rangle\right)$

$$= \left(\sum_k |k^{(0)}\rangle\langle k^{(0)}| - |n^{(0)}\rangle\langle n^{(0)}|\right)|n^{(0)}\rangle$$

$$= \sum_k \delta_{kn}\,|k^{(0)}\rangle - |n^{(0)}\rangle = 0$$ ]

$$|n^{(1)}\rangle = -\left[\frac{\mathbb{1} - |n^{(0)}\rangle\langle n^{(0)}|}{H_0 - E_n^{(0)}}\right] \underbrace{\sum_k |k^{(0)}\rangle\langle k^{(0)}|V|n^{(0)}\rangle}$$

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

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

Next, go to the equation

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

$$\therefore E_n^{(2)} = \langle n^0 | V \sum{}' \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle = \sum{}' \frac{V_{nk} V_{kn}}{E_n^{(0)} - E_k^{(0)}}$$

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Thus $$\boxed{E_n^{(2)} = \sum_k{}' \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}}}$$

## Normalization ?

Let to order $N$

$$|n\rangle_N = Z_N^{1/2} \underbrace{|n\rangle_\lambda}_{|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \ldots}$$

$\langle n^{(0)}| \times$

$$\langle n^{(0)}|n\rangle_N = Z_N^{1/2}$$

by hypothesis $\langle n^{(0)}|n^{(j)}\rangle = 0$, $j \neq 0$

$$Z_N \, {}_\lambda\langle n|n\rangle_\lambda = Z_N\left(\langle n^{(0)}|n^{(0)}\rangle + \lambda^2 \langle n^{(1)}|n^{(1)}\rangle + O(\lambda^4)\right)$$