Stationary State Perturbation Theory   chap. 11

$$H = H_0 + \lambda V$$

known Hamiltonian

perturbation (changes) with parameter λ

$H_0|n\rangle = \mathcal{E}_n|n\rangle$ $\langle n|n\rangle = 1$

state energy

(keep track of perturbation order

$$H|N\rangle = E_N|N\rangle \quad (1)$$

exact energy   exact wf

Assume that E_N & $|N\rangle$ are smoothly connected to H_0.

$H_0 \to H$
$\lambda\ 0 \to 1$

Adiabatic
Quantum Computing

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

$E_n^{(0)} = \mathcal{E}_n$ $E_n = \mathcal{E}_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots \quad (3)$

normalization convention

$\langle n|N\rangle = 1 \Rightarrow \langle N|N\rangle \neq 1$

$\langle n|N\rangle$ = $1 + \lambda\langle n|N^{(1)}\rangle + \lambda^2\langle n|N^{(2)}\rangle + \ldots \Rightarrow \boxed{\langle n|N^{(k)}\rangle = 0}$

all corrections to $|n\rangle$ must be orthogonal to $|n\rangle$

Sub (2) + (3) into 1

$$(H_0+\lambda V)\left\{\sum_{k=0}^{\infty} \lambda^k |N^{(k)}\rangle\right\} = \left(\sum_{i=0}^{\infty} \lambda^i E_N^{(i)}\right)\left(\sum_{l=0}^{\infty} \lambda^l |N^{(l)}\rangle\right)$$

$$H_0|n\rangle + \sum_{k=1}^{\infty} \lambda^k H_0|N^{(k)}\rangle + \underbrace{\sum_{k=0}^{\infty} \lambda^{k+1} V|N^{(k)}\rangle}_{\sum_{k=1}^{\infty} \lambda^k V|N^{(k-1)}\rangle}$$

$$= \sum_{i,l} \lambda^{(i+l)} E_N^{(i)}|N^{(l)}\rangle$$

$k = i+l$

$$\sum_{k=0}^{\infty}\left(\sum_{l=0}^{k} \lambda^k E_N^{(k-l)}|N^{(l)}\rangle\right)$$

For $k=1$

$$\cancel{H_0|n\rangle} + \lambda H_0|N^{(1)}\rangle + \lambda V|n\rangle = \cancel{\varepsilon_n|n\rangle} + \lambda E_N^{(1)}|N^{(0)}\rangle + \lambda E_N^{(0)}|N^{(1)}\rangle$$

$$H_0|N^{(1)}\rangle + V|n\rangle = E_N^{(1)}|n\rangle + \varepsilon_n|N^{(1)}\rangle$$

dot with $\langle n|$

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

$$E_N = \varepsilon_n + \lambda E_N^{(1)} = \varepsilon_n + \lambda\langle n|V|n\rangle$$

first order perturbation result

The $K^{\underline{th}}$ order perturbation:

$$H_0 |N^{(k)}\rangle + V|N^{(k-1)}\rangle$$
$$= E_N^{(k)}|N^{(0)}\rangle + E_N^{(k-1)}|N^{(1)}\rangle$$
$$+ \cdots \; E^0 |N^{(k)}\rangle$$

Dot it with $\langle n|$

$$\mathcal{E}_n \langle n\cancel{|N^{(k)}}\rangle + \langle n|V|N^{(k-1)}\rangle$$
$$= \langle n| E_N^{(k)} |n\rangle + \cdots \cancel{} \quad \cancel{\langle n|N^{(k)}\rangle = 0}$$

$k > 0$

$$\boxed{E_N^{(k)} = \langle n|V|N^{(k-1)}\rangle}$$

$E^{(k)}$ only needs $|N^{(k-1)}\rangle$

$\langle N^{(k-1)}|H|N^{(k-1)}\rangle \cong E_N^{2(k-1)}$

Can actually know $E^{2(k-1)}$ order

multiply by λ^k and sum

$$E_N - \mathcal{E}_n = \langle n|V|N\rangle$$

just a restatement of

$$H - H_0 = V$$

To compute $|N^{(k)}\rangle$ we expand in the original $|m\rangle$

$$|N^{(k)}\rangle = \sum_{m\neq n} |m\rangle\langle m|N^{(k)}\rangle$$

since $\langle n|N^{(k)}\rangle = 0$

To obtain $\langle m|N^{(k)}\rangle$ dot with $\langle m|$

$$\langle m|H_0|N^{(k)}\rangle + \langle m|V|N^{(k-1)}\rangle = \langle m|E_N^{(k)}|n\rangle + \langle m|E_N^{(k-1)}|N^{(1)}\rangle + \dots \langle m|\varepsilon_n|N^{(k)}\rangle$$

$$\varepsilon_m\langle m|N^{(k)}\rangle + \langle m|V|N^{(k-1)}\rangle = \varepsilon_n\langle m|N^{(k)}\rangle$$

$$\boxed{\langle m|N^{(k)}\rangle = \frac{1}{\varepsilon_n-\varepsilon_m}\Big(\langle m|V|N^{(k-1)}\rangle - E^{(1)}\langle m|N^{(k-1)}\rangle - E^{(2)}\langle m|N^{(k-2)}\rangle \cdots - E^{k-1}\langle m|N^{(1)}\rangle\Big)}$$

$|N^{(k)}\rangle$ depends on $|N^{(\ell)}\rangle$ for $\ell<k$

$$\langle m|N^{(1)}\rangle = \frac{1}{\varepsilon_n-\varepsilon_m}\Big(\langle m|V|n\rangle - E^{(1)}\underbrace{\langle m|n\rangle}_{=0}\Big)$$

$$\boxed{|N^{(1)}\rangle = \sum_{m\neq n}|m\rangle\frac{1}{\varepsilon_n-\varepsilon_m}\langle m|V|n\rangle}$$

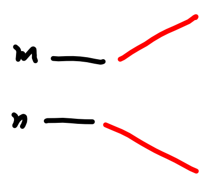
$$E^{(2)} = \langle n|V|N^{(1)}\rangle = \sum_{m\neq n}\frac{\langle n|V|m\rangle\langle m|V|n\rangle}{(\varepsilon_n-\varepsilon_m)} = \sum_{m\neq n}\frac{|\langle m|V|n\rangle|^2}{\varepsilon_n-\varepsilon_m}$$

1) If $n =$ g.s. the second order energy is always negative.

2) level repulsion: if $\varepsilon_n < \varepsilon_m$

$$E_N^{(2)} = \frac{|\ \ |^2}{\varepsilon_n-\varepsilon_m} < 0$$

$$E_M^{(2)} = \frac{|\ \ |^2}{\varepsilon_m-\varepsilon_n} > 0$$



Example 1) $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 - Fx$ $\qquad F = \lambda$

$\langle n|x|n\rangle = 0$ no first order correction

Second order $E_n^{(2)} = \sum_{m\neq n} \frac{|\langle m|V|n\rangle|^2}{\mathcal{E}_n - \mathcal{E}_m} = \sum_{m\neq n} F^2 \frac{|\langle m|x|n\rangle|^2}{(n-m)\hbar\omega}$

$\langle m|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{m\,n-1} + \sqrt{n+1}\,\delta_{m\,n+1}\right)$

$E_n^{(2)} = F^2 \frac{\hbar}{2m\omega}\left(\frac{n}{n-(n-1)} + \frac{n+1}{n-(n+1)}\right) = F^2\frac{\hbar}{2m\omega}\left(n + \frac{n+1}{-1}\right)\frac{1}{\hbar\omega}$

all levels are down shifted by $= -F^2 \frac{\cancel{\hbar}}{2m\omega}\frac{1}{\cancel{\hbar}\omega}$

a const amount

This is because

$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 - \frac{2Fx}{m\omega^2} + \left(\frac{F}{m\omega^2}\right)^2 - \left(\frac{F}{m\omega^2}\right)^2\right)$

$= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x - \frac{F}{m\omega^2}\right)^2 - \frac{1}{2}\cancel{m}\cancel{\omega^2}\frac{F^2}{m^{\cancel{2}}\omega^{\cancel{4}}\,2}$

Same

Example 2 : $\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}mb^2 x^2$

$$E = \hbar\sqrt{\omega^2 + b^2}\,(n+\tfrac{1}{2})$$

First order : $E^{(1)} = \frac{1}{2}mb^2 \langle n|x^2|n\rangle$

$$= \frac{1}{2}\cancel{m}b^2 \frac{\hbar}{\cancel{m}\omega}(n+\tfrac{1}{2})$$

$$= \frac{1}{2}\frac{b^2}{\omega^2}(n+\tfrac{1}{2})\hbar\omega$$

$\langle m|x^2|n\rangle$

$= \frac{\hbar}{m\omega}(n+\frac{1}{2})\delta_{mn}$

$+ \frac{1}{2}\frac{\hbar}{m\omega}\Big(\sqrt{n}\sqrt{n-1}\,\delta_{m\,n-2}$

$+ \sqrt{n+2}\sqrt{n+1}\,\delta_{m\,n+2}\Big)$

$$E = (n+\tfrac{1}{2})\hbar\omega\sqrt{1+\left(\tfrac{b^2}{\omega^2}\right)} = \left(1+\tfrac{1}{2}\tfrac{b^2}{\omega^2}\right)$$

$$= (n+\tfrac{1}{2})\hbar\omega + (n+\tfrac{1}{2})\hbar\omega\left(\tfrac{1}{2}\tfrac{b^2}{\omega^2}\right)$$

$\frac{\frac{1}{2}(\frac{1}{2}-1)}{2!}\left(\frac{b^2}{\omega^2}\right)^2 = -\frac{1}{8}\left(\frac{b^2}{\omega^2}\right)^2$

$$E^{(2)} = \sum_{m\neq n}\frac{\langle m|V|n\rangle^2}{\varepsilon_n - \varepsilon_m} = \left(\tfrac{1}{2}mb^2\right)^2\left(\tfrac{1}{2}\tfrac{\hbar}{m\omega}\right)^2\left\{\frac{n(n-1)}{\hbar\omega(2)} + \frac{(n+2)(n+1)}{\hbar\omega(-2)}\right\}$$

$$= \left(\tfrac{1}{4}\tfrac{b^2}{\omega^2}\hbar\omega\right)^2\frac{1}{2\hbar\omega}\left\{n(n-1)-(n+2)(n+1)\right\}$$

$\cancel{n^2} - n - \cancel{n^2} - 3n - 2$

$-(4n+2)$

$-4(n+\frac{1}{2})$

$$= \frac{1}{\cancel{16}_{\,8}}\left(\frac{b^2}{\omega^2}\right)^2\hbar\omega\,\frac{1}{\cancel{2}}\,(-\cancel{4}^{\,1})(n+\tfrac{1}{2})$$

$$= (n+\tfrac{1}{2})\hbar\omega\left[-\tfrac{1}{8}\left(\tfrac{b^2}{\omega^2}\right)^2\right]$$