Wave function Renormalization

We have obtained the n-th eigenket of the perturbed Hamiltonian:

$$|n\rangle = |n^{(0)}\rangle + \lambda \sum_{k\neq n} |k^{(0)}\rangle \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$$
$$+ \lambda^2 \left[\sum_{k\neq n} \sum_{l\neq n} |k^{(0)}\rangle \frac{\langle k^{(0)}|V|l^{(0)}\rangle \langle l^{(0)}|V|n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})} - \sum_{k\neq n} |k^{(0)}\rangle \frac{\langle k^{(0)}|V|n^{(0)}\rangle \langle n^{(0)}|V|n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})^2} \right]$$
$$+ O(\lambda^3).$$

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

We call

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

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

Then $|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + O(\lambda^3)$

[illegible] $+\lambda^2|n^{(2)}\rangle+O(\lambda^3)$ / n-th

We define the renormalized eigenket

$$|n\rangle_R \equiv \sqrt{Z_n}\,|n\rangle$$

such that ${}_R\langle n|n\rangle_R = 1$.

Then ${}_R\langle n|n\rangle_R = Z_n\langle n|n\rangle$.

$$\therefore\ Z_n = 1/\langle n|n\rangle.$$

The square of the n-th eigenket is

$$\langle n|n\rangle = \langle n^{(0)}|n^{(0)}\rangle + \lambda\left(\langle n^{(0)}|n^{(1)}\rangle + \langle n^{(1)}|n^{(0)}\rangle\right) + \lambda^2\left(\langle n^{(0)}|n^{(2)}\rangle + \langle n^{(1)}|n^{(1)}\rangle + \langle n^{(2)}|n^{(0)}\rangle\right) + O(\lambda^3)$$

Because $|n^{(1)}\rangle = \sum_{k\neq n} |k^{(0)}\rangle \dfrac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$,

$\langle n^{(0)}|n^{(1)}\rangle = 0$. It is also true that $\langle n^{(0)}|n^{(2)}\rangle = 0$ and so on.

~~Therefore, the norm~~

[Note that in the beginning, we have chosen the normalization such that

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

Sure, $\langle n^{(0)}|n^{(0)}\rangle = 1$.]

Therefore,

$$\langle n|n\rangle = 1 + \lambda^2\langle n^{(1)}|n^{(1)}\rangle + O(\lambda^3).$$

The normalization deviates from 1 from order λ^2. There is no shift at order λ.

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

$$\langle n^{(1)}|n^{(1)}\rangle = \sum_{k\neq n}\sum_{l\neq n} \frac{V_{nk}\underbrace{\langle k^{(0)}|l^{(0)}\rangle}_{\delta_{kl}} V_{ln}}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})}$$

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

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

$$= Z_n^{-1}$$

$$\therefore \quad Z_n^{-1} = 1+\lambda^2\langle n^{(1)}|n^{(1)}\rangle + O(\lambda^3)$$

and $$Z_n = 1-\lambda^2\langle n^{(1)}|n^{(1)}\rangle + O(\lambda^3)$$

$$= 1-\lambda^2\sum_{k\neq n}\frac{|V_{nk}|^2}{(E_n^{(0)}-E_k^{(0)})^2} + O(\lambda^3).$$

The renormalization constant Z_n is similar order-λ^2 correction to the

to the 2nd order energy shift.

Recall that

$$\Delta_n = E_n - E_n^{(0)} = \lambda V_{nn} + \lambda^2 \sum_{k\neq n}\frac{|V_{kn}|^2}{E_n^{(0)}-E_k^{(0)}} + O(\lambda^3)$$

or $$E_n = E_n^{(0)} + \lambda V_{nn} + \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{E_n^{(0)}-E_k^{(0)}} + O(\lambda^3)$$

If we take the partial derivative of E_n w.r.t. $E_n^{(0)}$, then we find that

$$\frac{\partial E_n}{\partial E_n^{(0)}} = 1-\lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{E_n^{(0)}-E_k^{(0)}} + O(\lambda^3) = Z_n \quad !!!$$

Elementary Examples

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \quad \text{harmonic oscillator}$$

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

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

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

where $\omega' = \sqrt{1+\varepsilon}\,\omega$.

Therefore, the problem is exactly solvable!

$$E_n = \hbar\omega\sqrt{1+\varepsilon}\,(n+\tfrac{1}{2}),$$

$$|n\rangle = \frac{(a^+)^n}{\sqrt{n!}}|0\rangle, \quad \text{for } n=0,1,2,\cdots.$$

$$|0^{(0)}\rangle \to |0\rangle$$

order ε

$$|0\rangle = |0^{(0)}\rangle + \sum_{k\neq 0} |k^{(0)}\rangle \frac{V_{k0}}{E_0^{(0)} - E_k^{(0)}} + O(\varepsilon^2)$$

$$E_n = \frac{1}{2}\hbar\omega + \Delta_0$$

$$\Delta_0 = \underbrace{V_{00}}_{\text{order } \varepsilon} + \underbrace{\sum_{k\neq 0} \frac{|V_{k0}|^2}{E_0^{(0)} - E_k^{(0)}}}_{\text{order } \varepsilon^2} + O(\varepsilon^3)$$

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

$$= \frac{\hbar\omega}{2}\left(\frac{p^2}{m\hbar\omega} + \frac{m\omega}{\hbar}x^2\right) \qquad p = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$= \frac{\hbar\omega}{2}\left(\frac{m\omega}{\hbar}x^2 - \frac{\hbar}{m\omega}\frac{d}{dx^2}\right) \qquad p^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$= \frac{\hbar\omega}{2}\left(\xi^2 - \frac{d^2}{d\xi^2}\right)$$

We define

$$a \equiv \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\, x + i\sqrt{\frac{1}{m\hbar\omega}}\, p\right) = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$$

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\, x - i\frac{p}{\sqrt{m\hbar\omega}}\right) = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)$$

$$a^\dagger a = \frac{1}{2}\left(\xi - \frac{d}{d\xi}\right)\left(\xi + \frac{d}{d\xi}\right)$$

$$= \frac{1}{2}\left(\xi^2 - \frac{d^2}{d\xi^2} - 1\right)$$

Therefore,

$$\frac{1}{2}\left(\xi^2 - \frac{d^2}{d\xi^2}\right) = a^\dagger a + \frac{1}{2}$$

$$\therefore\ H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) = \hbar\omega\left(N + \frac{1}{2}\right)$$

$$N \equiv a^\dagger a = \frac{1}{2}\left(\xi^2 - \frac{d^2}{d\xi^2} - 1\right)$$

$$a a^\dagger = \frac{1}{2}\left(\quad \text{''} \quad + 1\right)$$

$$\therefore \quad [a, a^\dagger] = a a^\dagger - a^\dagger a = 1.$$

$$[N,a] = a^\dagger a a - a a^\dagger a$$
$$= [a^\dagger, a] a = -a$$
$$[N, a^\dagger] = a^\dagger a a^\dagger - a^\dagger a^\dagger a$$
$$= a^\dagger [a, a^\dagger] = a^\dagger .$$

$$\Rightarrow \quad N|n\rangle \equiv n|n\rangle$$
$$N(a|n\rangle) = \left[[N,a] + aN\right]|n\rangle$$
$$= (-a + an)|n\rangle$$
$$= (n-1)\, a|n\rangle$$
$$\Rightarrow \quad a^k|n\rangle \propto |n-k\rangle$$
$$N a^\dagger|n\rangle = \left[[N,a^\dagger] + a^\dagger N\right]|n\rangle$$
$$= (a^\dagger + n a^\dagger)|n\rangle$$
$$= (n+1)(a^\dagger|n\rangle)$$
$$\Rightarrow (a^\dagger)^k|n\rangle \propto |n+k\rangle.$$

We can show that

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

and $n = 0, 1, 2, \cdots$

$$E_n = \hbar\omega'(n+\tfrac{1}{2})$$
$$= \hbar\omega\sqrt{1+\varepsilon}\,(n+\tfrac{1}{2})$$

In the case of the ground state, $(n=0)$

$$E_n = \hbar\omega\sqrt{1+\varepsilon}\times\frac{1}{2}$$
$$= E_n^{(0)} + \Delta_n^{(1)} + \Delta_n^{(2)} + O(\varepsilon^3)$$

$$\sqrt{1+\varepsilon} = 1+\frac{1}{2}\varepsilon+\frac{\frac{1}{2}\left(-\frac{1}{2}\right)}{2}\varepsilon^2 + O(\varepsilon^3)$$
$$= 1+\frac{1}{2}\varepsilon-\frac{1}{8}\varepsilon^2+O(\varepsilon^3)$$

$$\Delta_n^{(1)} = \frac{1}{2}\hbar\omega\times\frac{1}{2}\varepsilon = \frac{1}{4}\hbar\omega\varepsilon$$

$$\Delta_n^{(2)} = \frac{1}{2}\hbar\omega\times\left(-\frac{1}{8}\varepsilon^2\right) = -\frac{1}{16}\hbar\omega\varepsilon^2$$

We want to check $\Delta_n^{(1)}$ and $\Delta_n^{(2)}$ by making use of the perturbation theory.

$$\Delta_0^{(1)} = V_{00} = \langle 0|\,\frac{1}{2}\varepsilon m\omega^2 x^2|0\rangle = \frac{1}{2}\varepsilon m\omega^2\langle 0|x^2|0\rangle$$

We need to evaluate the matrix-element $\langle 0|x^2|0\rangle$.

We recall that

$$a = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + i\frac{p}{\sqrt{m\hbar\omega}}\right)$$
$$a^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - i\frac{p}{\sqrt{m\hbar\omega}}\right)$$

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

Therefore, $\quad x^2 = \frac{2m\omega}{\hbar}(a+a^\dagger)^2.$

$$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|(a+a^\dagger)^2|0\rangle$$
$$= \frac{\hbar}{2m\omega}\langle 0|aa^\dagger|0\rangle,$$

where we have used

$$a|0\rangle = 0 \quad (\& \; a^2|0\rangle, \; a^\dagger a|0\rangle = 0)$$
$$(a^\dagger)^2|0\rangle \propto |2\rangle \quad \therefore \quad \langle 0|(a^\dagger)^2|0\rangle \propto \langle 0|2\rangle = 0$$

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle \Rightarrow \quad (a^\dagger)^n|0\rangle = \sqrt{n!}\,|n\rangle$$
$$a^\dagger|0\rangle = |1\rangle$$
$$\Rightarrow \quad \left|a^\dagger|0\rangle\right|^2 = \langle 0|aa^\dagger|0\rangle = \langle 1|1\rangle = 1.$$

$$\therefore \quad \langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}\langle 1|1\rangle = \frac{\hbar}{2m\omega}$$

$$\Rightarrow \Delta_0^{(1)} = V_{00} = \frac{1}{2}\varepsilon m\omega^2 \times \frac{\hbar}{2m\omega} = \frac{1}{4}\hbar\omega\,\varepsilon$$

This result agrees with the first-order energy shift that has been expanded from the exact solution.

Let us compute $\Delta_0^{(2)}$.

$$\Delta_0^{(2)} = \sum_{k\neq 0}\frac{|V_{0k}|^2}{E_0^{(0)}-E_k^{(0)}} = -\frac{1}{\hbar\omega}\sum_{k\neq 0}\frac{|V_{0k}|^2}{k}.$$

$$\left.\begin{aligned} E_k^{(0)} &= \hbar\omega\left(\tfrac{1}{2}+k\right) \\ E_0^{(0)} &= \hbar\omega\cdot\tfrac{1}{2} \end{aligned}\right\} \rightarrow \; E_0^{(0)}-E_k^{(0)} = -\hbar\omega k$$

$$V_{0k} = \langle 0|\frac{\varepsilon}{2}m\omega^2 x^2|k\rangle$$
$$= \frac{\varepsilon}{2}m\omega^2\frac{\hbar}{2m\omega}\langle 0|(a+a^\dagger)^2|k\rangle = \frac{\varepsilon}{4}\hbar\omega\langle 0|(a+a^\dagger)^2|k\rangle$$

$\langle 0|a^2|k\rangle \neq 0$ only if $k=2$
$\langle 0|aa^\dagger|k\rangle \neq 0$ only if $k=0$ (no need!)
$\langle 0|a^\dagger a|k\rangle = 0$ for all k
$\langle 0|(a^\dagger)^2|k\rangle = 0$ for all k.

Therefore, $\langle 0|a^2|2\rangle =$

$$\big|a|n\rangle\big|^2 = \langle n|a^\dagger a|n\rangle = \langle n|N|n\rangle$$
$$= n\langle n|n\rangle = n$$
$$\therefore\ a|n\rangle = \sqrt{n}\,|n-1\rangle$$
$$a^2|n\rangle = a(a|n\rangle)$$
$$= a(\sqrt{n}\,|n-1\rangle)$$
$$= \sqrt{n}\,(a|n-1\rangle)$$
$$= \sqrt{n(n-1)}\,|n-2\rangle$$
$$\therefore\ a^2|2\rangle = \sqrt{2\cdot 1}\,|0\rangle = \sqrt{2}\,|0\rangle$$

Therefore, $\langle 0|a^2|2\rangle = \sqrt{2}\langle 0|0\rangle = \sqrt{2}$.

From this, $V_{0k} = \frac{\varepsilon}{4}\hbar\omega\langle 0|a^2|k\rangle$
$(k\neq 0)$ $= \frac{\varepsilon}{4}\hbar\omega\sqrt{2}\,\delta_{k2} = \frac{\varepsilon}{2\sqrt{2}}\hbar\omega\,\delta_{k2}$

$$\Delta_0^{(2)} = -\frac{1}{\hbar\omega}\sum_{k\neq 0}\frac{|V_{0k}|^2}{k} = -\frac{1}{\hbar\omega}\times\frac{1}{2}\left(\frac{\varepsilon}{2\sqrt{2}}\hbar\omega\right)^2$$
$$= -\frac{\varepsilon^2}{16}\hbar\omega$$

$$\Rightarrow\ E_n = \frac{1}{2}\hbar\omega + \frac{\varepsilon}{4}\hbar\omega - \frac{\varepsilon^2}{16}\hbar\omega + O(\varepsilon^3)$$
$$= \frac{1}{2}\hbar\omega\left[1 + \frac{\varepsilon}{2} - \frac{\varepsilon^2}{8} + O(\varepsilon^3)\right].$$

Checked!