Second Order Perturbation

$$\left.\begin{aligned} H &= H_0 + H' \\ H_0 U_n &= E_n U_n \\ H\psi_n &= W_n \psi_n \end{aligned}\right\} \quad H = H_0 + gH' \quad \left\{\begin{aligned} \psi_n &= \psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \cdots \\ W_n &= W_n^{(0)} + gW_n^{(1)} + g^2 W_n^{(2)} + \cdots \end{aligned}\right.$$

$$(H_0 + gH')(\psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \cdots) = (W_n^{(0)} + gW_n^{(1)} + g^2 W_n^{(2)} + \cdots)(\psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \cdots)$$

$$\Rightarrow \quad \begin{aligned} H_0\psi_n^{(0)} &= W_n^{(0)}\psi_n^{(0)} \\ H_0\psi_n^{(1)} + H'\psi_n^{(0)} &= W_n^{(0)}\psi_n^{(1)} + W_n^{(1)}\psi_n^{(0)} \\ H_0\psi_n^{(2)} + H'\psi_n^{(1)} &= W_n^{(0)}\psi_n^{(2)} + W_n^{(1)}\psi_n^{(1)} + W_n^{(2)}\psi_n^{(0)} \end{aligned}$$

Here $\psi_n^{(0)} = u_n$ & $W_n^{(0)} = E_n$

We expand $\psi_n^{(2)}$ as a linear combination of eigenfunctions of H_0 — second order correction

$$\Rightarrow \quad \psi_n^{(2)} = \sum_m a_m^{(2)} u_m$$

$$\Rightarrow \quad H_0 \sum_m a_m^{(2)} u_m + H' \sum_m a_m^{(1)} u_m = W_n^{(0)} \sum_m a_m u_m + W_n^{(1)} \sum_m a_m u_m + W_n^{(2)} u_n$$

Now multiply by u_k^* and then integrating

$$\sum a_m^{(2)} E_m \delta_{km} + \sum_m a_m^{(1)} H'_{km} = E_n \sum a_m^{(2)} \delta_{km} + H'_{nn} \sum a_m^{(1)} \delta_{km} + W_n^{(2)} \delta_{kn}$$

where $H'_{km} = \int u_k H' u_m \, d\tau$ and $W_n^{(1)} = H'_{nn} = \int u_n^* H' u_n \, d\tau$.

$$\Rightarrow \text{For } k = m \quad a_k^{(2)} E_k + \sum_m a_m^{(1)} H'_{km} = E_n a_k^{(2)} + H'_{nn} \sum_k a_k^{(1)} + W_n^{(2)} \delta_{kn}$$

$$\Rightarrow \quad a_k^{(2)}(E_n - E_k) + W_n^{(2)} \delta_{kn} = \sum_m a_m^{(1)} H'_{km} - a_k^{(1)} H'_{nn}$$

For $k = n$

$$W_n^{(2)} = \sum a_m^{(1)} H'_{nm} - a_n^{(1)} H'_{nn}$$

$$= \sum_{\substack{m \\ m \neq n}}' a_m^{(1)} H'_{nm}$$

We have not taken ~~n = m~~ $m = n$

$$a_k^{(1)} = \frac{H'_{kn}}{(E_n - E_k)}$$

$$\boxed{W_n^{(2)} = \sum_{\substack{m \\ m \neq n}}' \frac{|H'_{mn}|^2}{E_n - E_m}}$$

$$H'_{nm} = (H'_{mn})^* \quad k \neq n$$

Simple Harmonic Oscillator

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

$H|H'\rangle = H'|H'\rangle$ where $H' = E_n = (n+\frac{1}{2})\hbar\omega$ for $n = 0, 1, 2 \dots$

$$H|n\rangle = (n+\tfrac{1}{2})\hbar\omega|n\rangle$$

H – is Hermitial operator, all eigenvalues are real
Eigenkets belonging to different eigenvalues are orthogonal

$\langle m|n\rangle = 0$ if $m \neq n$

$\langle n|n\rangle = 1$ normalization

Any multiple of $|n\rangle$
$|p\rangle = c|n\rangle$ ✓
$H|p\rangle = (n+\frac{1}{2})\hbar\omega|p\rangle$

$$\Rightarrow \langle m|n\rangle = \delta_{mn} \begin{cases} =0 & m\neq n \\ =1 & m=n \end{cases}$$ – ~~Kronnike~~ Kronecker delta f^n.

$$H|n\rangle = (n+\tfrac{1}{2})\hbar\omega|n\rangle$$

$a = \dfrac{\mu\omega x + ip}{\sqrt{2\mu\hbar\omega}}$ if we take $H' = (n+\frac{1}{2})\hbar\omega$

$H\{a|n\rangle\} = (H' - \hbar\omega)\{a|n\rangle\}$ where $a|n\rangle \neq 0$

$= (n-\frac{1}{2})\hbar\omega\{a|n\rangle\}$

$$H|n-1\rangle = (n-\tfrac{1}{2})\hbar\omega|n-1\rangle$$

$|p\rangle = a|n\rangle = c_n|n-1\rangle$

$\langle p| = \langle n|\bar{a} = c_n^* \langle n-1|$

$\hbar\omega\langle p|p\rangle = \langle n|\hbar\omega\bar{a}a|n\rangle = \hbar\omega\langle n|\bar{a}a|n\rangle = \hbar\omega|c_n|^2\underbrace{\langle n-1|n}_{1}$

$= \langle n|H - \frac{1}{2}\hbar\omega|n\rangle$

$\Rightarrow \hbar\omega|c_n|^2 = \langle n|H|n\rangle - \frac{1}{2}\hbar\omega\langle n|n\rangle$

$= (n+\frac{1}{2})\hbar\omega\langle n|n\rangle - \frac{1}{2}\hbar\omega\langle n|n\rangle$

$\hbar\omega|c_n|^2 = n\hbar\omega \Rightarrow c_n = \sqrt{n}$

$$\Rightarrow a|n\rangle = \sqrt{n}\,|n-1\rangle$$

Simple Harmonic Oscillator

Dimensionless Complex Operator

$$a = \frac{1}{(2\mu\hbar\omega)^{1/2}}(\mu\omega x + ip)$$

where $\bar{x} = x$ and $\bar{p} = p$, and the adjoint of a

$$\bar{a} = \frac{1}{(2\mu\hbar\omega)^{1/2}}(\mu\omega x - ip)$$

$(xp - px) = [x, p] = i\hbar$

$$\Rightarrow \hbar\omega a\bar{a} = \frac{1}{2\mu}(\mu\omega x + ip)(\mu\omega x - ip)$$

$$= \frac{1}{2\mu}\left[\mu^2\omega^2 x^2 + p^2 - i\omega\mu(xp - px)\right]$$

$$= \frac{1}{2\mu}\left[\mu^2\omega^2 x^2 + p^2 + \hbar\omega\mu\right]$$

$$= \frac{1}{2}\mu\omega^2 x^2 + \frac{p^2}{2\mu} + \frac{1}{2}\hbar\omega$$

$$= \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2 + \frac{1}{2}\hbar\omega$$

$$\boxed{\begin{aligned}\hbar\omega a\bar{a} &= H + \tfrac{1}{2}\hbar\omega \\ \hbar\omega \bar{a} a &= H - \tfrac{1}{2}\hbar\omega\end{aligned}}$$

$\Rightarrow H = \frac{1}{2}\hbar\omega(\bar{a}a + a\bar{a})$

and $a\bar{a} - \bar{a}a = [a, \bar{a}] = 1$

$$\Rightarrow$$

$$\hbar\omega a\bar{a}a = Ha + \frac{1}{2}\hbar\omega a$$

$$\hbar\omega a\bar{a}a = aH - \frac{1}{2}\hbar\omega a$$

So $aH - Ha = [a, H] = \hbar\omega a$ and $[\bar{a}, H] = -\hbar\omega\bar{a}$

Eigen value Equation $H|H'\rangle = H'|H'\rangle$

$|H'\rangle$ is the Eigenket of the Operator H belonging to the eigenvalue H'. H — Operator and H' — a number

$$|p\rangle = a|H'\rangle \Rightarrow \langle p| = \langle H'|\bar{a}$$

$$\hbar\omega\langle p|p\rangle = \hbar\omega\langle H'|\bar{a}a|H'\rangle$$

$$\hbar\omega \langle p|p\rangle = \langle H'|H - \tfrac{1}{2}\hbar\omega|H'\rangle$$

$$= (H' - \tfrac{1}{2}\hbar\omega)\langle H'|H'\rangle$$

$\langle p|p\rangle$ and $\langle H'|H'\rangle$ are +ve numbers and therefore

$$H' \geq \tfrac{1}{2}\hbar\omega$$

and $H' = \frac{1}{2}\hbar\omega$ if and only if $|p\rangle = a|H'\rangle = 0$

or conversely $a|H'\rangle = 0$ then $H' = \frac{1}{2}\hbar\omega$

One can label eigen functions with the index n

$|n\rangle$ - Eigenfunctions corresponding to eigenvalue $(n+\frac{1}{2})\hbar\omega$

$$H|n\rangle = (n+\tfrac{1}{2})\hbar\omega|n\rangle \quad : \text{ for all } n = 0, 1, 2 \ldots$$

$|n\rangle$ - Eigen kets of Hermitian operator H

and therefore they must be orthogonal to each other

and we assume that the states $|n\rangle$ are normalized

$$\langle m|n\rangle = \delta_{mn}$$

Since $|0\rangle$ corresponds to $H' = \frac{1}{2}\hbar\omega$, we must have

$$a|0\rangle = 0$$

Now for $n = 1, 2, 3 \ldots$ $a|n\rangle$ is an eigenket of H belonging to the eigenvalue $(n-\frac{1}{2})\hbar\omega$

$\Delta x \cdot \Delta p$ for Harmonic Oscillator

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$$

where $\langle x\rangle = \langle n|x|n\rangle$, $\langle x^2\rangle = \langle n|x^2|n\rangle$

$\langle p\rangle = \langle n|p|n\rangle$, $\langle p^2\rangle = \langle n|p^2|n\rangle$

$$x = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\bar{a} + a)$$

$$p = i\left(\frac{\mu\hbar\omega}{2}\right)^{1/2}(\bar{a} - a)$$

$$\langle x\rangle = \langle n|x|n\rangle = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\langle n|\bar{a} + a|n\rangle$$

$$= \left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\left[\sqrt{n+1}\,\langle n|n+1\rangle + \sqrt{n}\,\langle n|n-1\rangle\right]$$

where we used $a|n\rangle = \sqrt{n}\,|n-1\rangle$

and $\bar{a}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$$\langle x\rangle = 0$$

$$\langle x^2\rangle = \langle n|x^2|n\rangle = \langle n|(\bar{a}+a)(\bar{a}+a)|n\rangle \times \left(\frac{\hbar}{2\mu\omega}\right)$$

$$= \frac{\hbar}{2\mu\omega}\langle n|\bar{a}\bar{a} + \bar{a}a + a\bar{a} + aa|n\rangle$$

$$= \frac{\hbar}{2\mu\omega}\left[0 + n + n+1 + 0\right]$$

$$= \frac{\hbar}{2\mu\omega}(2n+1) = \frac{\hbar}{\mu\omega}\left(n+\frac{1}{2}\right)$$

$\langle n|aa|n\rangle$

$|a\sqrt{n}\,|n-1\rangle$

$\langle n|a|n-1\rangle$

$\sqrt{n-1}\,\langle n|n-2\rangle$

Similarly $\langle p^2\rangle = \mu\omega\hbar\left(n+\frac{1}{2}\right)$ and $\langle p\rangle = 0$

$$\Delta x \cdot \Delta p = \left(n+\frac{1}{2}\right)\hbar$$