Lecture #9

Time-indep. perturb. theory (cont.)

Recall: $\hat{H} = \hat{H}_0 + \lambda \hat{H}'$

$\hat{H}_0$ ← unperturbed; $\hat{H}'$ ← perturbation

we know: $\hat{H}_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$

need: $\hat{H}|n\rangle_\lambda = E_n^{(\lambda)} |n\rangle_\lambda$ ← ? ?

$$E_n^{(\lambda)} = E_n^{(0)} + \lambda \underbrace{E_n^{(1)}}_{= \langle n^{(0)} | \hat{H}' | n^{(0)} \rangle} + \ldots$$

$$|n\rangle_\lambda = |n^{(0)}\rangle + \lambda \underbrace{|n^{(1)}\rangle}_{= ?} + \ldots$$

? ← find the 1st-order correction to the state!

- How do we normalize the state?

$\langle n^{(0)} | n^{(0)} \rangle = 1$ but what is $\langle n^{(1)} | n^{(1)} \rangle$, $\langle n^{(0)} | n^{(1)} \rangle$? ....?

Convention:

require that $|n\rangle_\lambda$ is normalized

& $\langle n^{(0)} | n \rangle_\lambda$ is real

So; 1st order: $\underset{\lambda \Rightarrow \text{1st order}}{\langle n|} \underset{\lambda \Rightarrow \text{1st order}}{|n\rangle} = 1 \Rightarrow$

$$|n\rangle_{\lambda = \text{1st order}} = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle$$

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

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

$$+ \lambda \langle n^{(1)} | n^{(0)} \rangle + \underbrace{\lambda^2 \langle n^{(1)} | n^{(1)} \rangle}$$

discard since this is the next order

$$\Downarrow$$

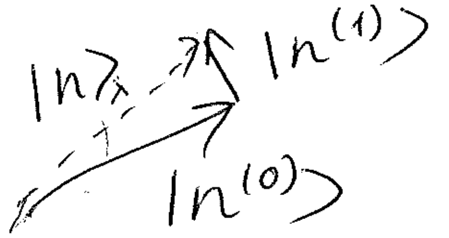
$$\langle n^{(0)} | n^{(1)} \rangle + \langle n^{(1)} | n^{(0)} \rangle = 0 \Rightarrow \langle n^{(0)} | n^{(1)} \rangle = -\underbrace{\langle n^{(1)} | n^{(0)} \rangle}$$

real by convention $(a = -a^* = -a)$

if $a = -a$ $\Rightarrow a = 0 \Rightarrow$

real number

so $\underbrace{\langle n^{(0)} | n^{(1)} \rangle}_{} = 0$!



So, the 1st order correction is orthogonal to the unperturbed state!

Now let's find $|n^{(1)}\rangle$:

Back to Schrödinger equation, collecting terms with λ^1: (see lecture #8)

$$\lambda^1: \quad (\hat{H}_0 - E_n^{(0)}) |n^{(1)}\rangle = (E_n^{(1)} - \hat{H}') |n^{(0)}\rangle$$

multiply by $\langle k^{(0)}|$ where $k \neq n \Rightarrow$

(recall that to find $E_n^{(1)}$ we multiplied by $\langle n^{(0)}|$)

$$\langle k^{(0)} | \hat{H}_0 - E_n^{(0)} | n^{(1)} \rangle = \langle k^{(0)} | E_n^{(1)} - \hat{H}' | n^{(0)} \rangle$$ 3

$$\langle k^{(0)} | \hat{H}_0 = \langle k^{(0)} | E_k^{(0)}$$

$$\langle k^{(0)} | E_k^{(0)} - E_n^{(0)} | n^{(1)} \rangle = E_n^{(1)} \underbrace{\langle k^{(0)} | n^{(0)} \rangle}_{= \delta_{kn}} -$$

$$- \langle k^{(0)} | \hat{H}' | n^{(0)} \rangle ;$$

$$\left(E_k^{(0)} - E_n^{(0)}\right) \langle k^{(0)} | n^{(1)} \rangle \underset{k \neq n}{=} - \langle k^{(0)} | \hat{H}' | n^{(0)} \rangle$$

$$\underset{(n \neq k)}{\langle k^{(0)} | n^{(1)} \rangle} = \frac{\langle k^{(0)} | \hat{H}' | n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} = \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}}$$

if $n = k \Rightarrow \langle n^{(0)} | n^{(1)} \rangle = 0$ (page 2)

How do you get $|n^{(1)}\rangle$ from $\langle k^{(0)} | n^{(1)} \rangle$?

Recall that any state can be presented as a superposition of basis states:

$$|n^{(1)}\rangle = \sum_m c_m |m^{(0)}\rangle \quad \text{where } c_m = \langle m^{(0)} | n^{(1)} \rangle$$

sum over <u>all</u> states

remember that unperturbed states form a complete & orthonormal basis!

these include n & $k \neq n$

the state for which we are looking for corrections

all others

So, $|n^{(1)}\rangle = \underbrace{\langle n^{(0)}|n^{(1)}\rangle}_{=0} |n^{(0)}\rangle$

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

$$= \sum_{k \neq n} \underbrace{\langle k^{(0)}|n^{(1)}\rangle}_{\frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}}} |k^{(0)}\rangle$$

Next target: if $E_n^{(1)} = 0 \Rightarrow$ need $E_n^{(2)}$!

2nd-order energy correction,

Back to Schrödinger equation

λ^2: $\hat{H}_0 |n^{(2)}\rangle + \hat{H}' |n^{(1)}\rangle =$

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

$\Downarrow$

$(\hat{H}_0 - E_n^{(0)}) |n^{(2)}\rangle = (E_n^{(1)} - \hat{H}') |n^{(1)}\rangle +$

$+ E_n^{(2)} |n^{(0)}\rangle$

multiply by $\langle n^{(0)}|$:

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$$\langle n^{(0)}|\hat{H}_0 - E_n^{(0)}|n^{(2)}\rangle = 0 =$$

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

$$= \langle n^{(0)}|E_n^{(1)} - \hat{H}'|n^{(1)}\rangle + E_n^{(2)} \cdot \underbrace{\langle n^{(0)}|n^{(0)}\rangle}_{=1}$$

$$\Downarrow$$

$$E_n^{(2)} = \langle n^{(0)}|\hat{H}'|n^{(1)}\rangle - E_n^{(1)} \underbrace{\langle n^{(0)}|n^{(1)}\rangle}_{=0}$$

(from page 2)

we know that

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

Then,

$$E_n^{(2)} = \sum_{k\neq n} \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} \underbrace{\langle n^{(0)}|\hat{H}'|k^{(0)}\rangle}_{=H'_{nk}} =$$

$$= \sum_{k\neq n} \frac{|H'_{kn}|^2}{E_n^{(0)} - E_k^{(0)}} \Leftarrow$$ 2nd order energy correction

Example A simple harmonic oscillator with charge q is subjected to electric field $\mathcal{E}$ along x-axis. Find the energy shift to the lowest order.

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So: $H_0 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$; $E_n^{(0)} = \hbar\omega(n+\frac{1}{2})$

Perturbation: force $= q\mathcal{E}$; $H' = -q\mathcal{E}x$

$$E_n^{(1)} = \langle n^{(0)} | (-q\mathcal{E}\underset{\sqrt{\frac{\hbar}{2m\omega}}(a^+ + a)}{x}) | n^{(0)} \rangle = 0$$

recall:
$a^+|n\rangle = \sqrt{n+1}|n+1\rangle$
$a|n\rangle = \sqrt{n}|n-1\rangle$

$\Downarrow$

need $E_n^{(2)}$!

$\Downarrow$

$$E_n^{(2)} = \sum_{k\neq n} \frac{|H'_{kn}|^2}{E_n^{(0)} - E_k^{(0)}} = ?$$

- $E_n^{(0)} - E_k^{(0)} = \hbar\omega(n^{(0)} + \frac{1}{2} - k^{(0)} - \frac{1}{2}) =$
  $= \hbar\omega(n^{(0)} - k^{(0)})$

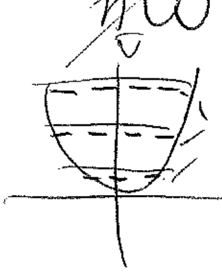
- $H'_{kn} = ?$

$$\langle k^{(0)} | (-q\mathcal{E}x) | n^{(0)} \rangle = -q\mathcal{E} \langle k^{(0)} | a^+ + a | n^{(0)} \rangle \cdot \sqrt{\frac{\hbar}{2m\omega}} = -q\mathcal{E}\sqrt{\frac{\hbar}{2m\omega}} \left(\langle k^{(0)} | n^{(0)}+1 \rangle \cdot \sqrt{n^{(0)}+1} + \langle k^{(0)} | n^{(0)}-1 \rangle \cdot \sqrt{n^{(0)}} \right) = -q\mathcal{E}\sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n^{(0)}+1}\, \delta_{k^{(0)}, n^{(0)}+1} + \sqrt{n^{(0)}}\, \delta_{k^{(0)}, n^{(0)}-1} \right)$$

So only two terms survive in the $\sum_{k \neq n}$ sum! $\rightarrow$ with $k^{(0)} = n^{(0)} \pm 1$

$$E_n^{(2)} = \frac{|H'_{n^{(0)}+1,\, n^{(0)}}|^2}{\hbar\omega(n^{(0)} - (n^{(0)}+1))} + \frac{|H'_{n^{(0)}-1,\, n^{(0)}}|^2}{\hbar\omega(n^{(0)} - (n^{(0)}-1))} =$$

$$= \frac{(q\mathcal{E})^2}{\hbar\omega} \cdot \frac{\hbar}{2m\omega} \underbrace{\left[\frac{n^{(0)}+1}{-1} + \frac{n^{(0)}}{+1}\right]}_{= -n^{(0)} - 1 + n^{(0)} = -1} = \underbrace{-\frac{(q\mathcal{E})^2}{2m\omega^2}}$$



with E-field on

Same correction to any E_n!

Let's also find the first-order correction to a state $|n^{(0)}\rangle$:

$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle = -(q\mathcal{E})\sqrt{\frac{\hbar}{2m\omega}} \cdot$$

$$\cdot \left(\frac{\sqrt{n^{(0)}+1}}{\hbar\omega(n^{(0)} - (n^{(0)}+1))} |n^{(0)}+1\rangle + \frac{\sqrt{n^{(0)}}}{\hbar\omega(n^{(0)} - (n^{(0)}-1))} |n^{(0)}-1\rangle \right)$$

$$= -q\mathcal{E}\sqrt{\frac{\hbar}{2m\omega}} \cdot \frac{1}{\hbar\omega}\left(-\sqrt{n^{(0)}+1}\,|n^{(0)}+1\rangle + \sqrt{n^{(0)}}\,|n^{(0)}-1\rangle\right)$$

Altogether:

$$E_n^{(\lambda)} = E_n^{(0)} + \lambda \underbrace{\langle n^{(0)} | \hat{H}' | n^{(0)} \rangle}_{= H'_{nn}} + \lambda^2 \sum_{k \neq n} \frac{|H'_{kn}|^2}{E_n^{(0)} - E_k^{(0)}} + \ldots$$

$$|n\rangle_\lambda = |n^{(0)}\rangle + \lambda \sum_{k \neq n} \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle + \ldots$$

Perturbation theory is valid if each order is a smaller correction than the previous order

$\Downarrow$

$$\left| \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} \right| \ll 1$$

$\Rightarrow$ note if states are degenerate $\Rightarrow$ $E_n^{(0)} = E_k^{(0)}$ $\Rightarrow$ this approach is not valid $\Rightarrow$ need to develop a new strategy for degenerate states!