Lecture #20

Time-independent perturbation theory

Most QM problems cannot be solved exactly
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need approximation methods!
⇓
one of them is time-independent perturbation theory ⟷ Rayleigh-Schrödinger theory

Consider a time-independent Hamiltonian

$$\underbrace{H_0}_{\substack{\uparrow \\ \text{unperturbed} \\ \text{Hamiltonian}}} + \lambda V \quad \text{with } V \leftarrow \text{perturbation}, \quad \lambda \leftarrow \text{real parameter from 0 to 1}$$

$H = H_0 + \lambda V$

$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$ ← known
⇓
How do the energy levels & states change under perturbation?
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$H|n\rangle = E_n |n\rangle$ — $|n\rangle$?, E_n ?

For now assume that the energy spectrum is non-degenerate (i.e. for each $E_n^{(0)}$ there is just one state $|n^{(0)}\rangle$)

Closure: $\sum_n |n^{(0)}\rangle\langle n^{(0)}| = 1$ → complete basis

Need to solve $\underbrace{H(\lambda)}_{H_0+\lambda V} |n\rangle_\lambda = E_n^{(\lambda)} |n\rangle_\lambda$ (2.1)

<u>Assume</u> $E_n^{(\lambda)}$ and $|n\rangle_\lambda$ can be expanded in powers of λ:

$$E_n^{(\lambda)} = E_n^{(0)} + \lambda E_n^{(1)} + \ldots + \lambda^k E_n^{(k)} + \ldots$$

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

Substitute these into Eq. (2.1) $\Rightarrow$ collect terms with equal powers of λ

λ^0: $\quad H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$ ← unperturbed case

λ^1: $\quad H_0 |n^{(1)}\rangle + V |n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle$

$$\Downarrow$$

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

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

$$\underbrace{\underbrace{\langle n^{(0)}| H_0}_{\langle n^{(0)}| E_n^{(0)}} - E_n^{(0)} |n^{(1)}\rangle}_{=0} = E_n^{(1)} \overbrace{\langle n^{(0)}|n^{(0)}\rangle}^{=1} - \langle n^{(0)}|V|n^{(0)}\rangle,$$

$\Rightarrow$

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

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

$\Downarrow$

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

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

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

$\Downarrow$

$$E_n^{(2)} = \langle n^{(0)} | V | \underbrace{n^{(1)} \rangle}_{?} - E_n^{(1)} \underbrace{\langle n^{(0)} | n^{(1)} \rangle}_{?} \tag{28.2}$$

$\Downarrow$

How do we normalize our states?

$\Downarrow$

<u>convention</u>: since $|n\rangle_\lambda$ is defined within a const. factor $\Rightarrow$ can choose the norm and the phase $\Rightarrow$ require that $|n\rangle_\lambda$ is normalized and choose the phase such that $\langle n^{(0)} | n \rangle_\lambda$ is real.

Then, to the 0^{th} order: $|n\rangle_{\lambda=0} = |n^{(0)}\rangle$

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

<u>1st order</u>: $\underset{\lambda=1}{\langle} n|n\rangle_{\lambda=1} = 1 \Rightarrow$

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

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

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

since we consider terms up to $\underline{\underline{\lambda}}$

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

since we required that $\langle n^{(0)}|n\rangle_\lambda$ is real

<u>2nd order</u>

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

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

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

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

$$= -\frac{1}{2}\langle n^{(1)}|n^{(1)}\rangle$$

Back to Eq. (2~~8~~.2):

$$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle - E_n^{(1)} \underbrace{\langle n^{(0)}|n^{(1)}\rangle}_{=0}, \text{ but}$$

what is $|n^{(1)}\rangle$?

$\Downarrow$

let's try a different approach: back to p. 3, 4

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

Take a state $|k^{(0)}\rangle$, so that $H_0|k^{(0)}\rangle = E_k^{(0)}|k^{(0)}\rangle$, $k \neq n$

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

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

$$\underbrace{\langle k^{(0)}|H_0}_{\langle k^{(0)}|E_k^{(0)}} - E_n^{(0)}|n^{(1)}\rangle = \langle k^{(0)}|E_n^{(1)} - V|n^{(0)}\rangle$$

$$(E_k^{(0)} - E_n^{(0)})\langle k^{(0)}|n^{(1)}\rangle = E_n^{(1)} \underbrace{\langle k^{(0)}|n^{(0)}\rangle}_{=0 \text{ (since } k\neq n)} - \langle k^{(0)}|V|n^{(0)}\rangle \Rightarrow$$

$$\underline{\langle k^{(0)}|n^{(1)}\rangle = \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}} \quad (n \neq k) \quad (2~~8~~.3)$$

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

How to extract $|n^{(1)}\rangle$ out of Eq. (2.3)? ⇒ (6)

Recall: $\sum_k |k^{(0)}\rangle\langle k^{(0)}| = 1$ ← closure

$$|n^{(1)}\rangle = \sum_k |k^{(0)}\rangle \underbrace{\langle k^{(0)}|n^{(1)}\rangle}_{\text{given by Eq. (2.3)}}$$

⇓

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

Back to Eq. (2.2) ⇒

$$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle = \sum_{k\neq n} \frac{|\overbrace{\langle k^{(0)}|V|n^{(0)}\rangle}^{V_{kn}}|^2}{E_n^{(0)}-E_k^{(0)}}$$

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

$$|n\rangle_\lambda = |n^{(0)}\rangle + \lambda \sum_{k\neq n}\frac{V_{kn}}{E_n^{(0)}-E_k^{(0)}}\,|k^{(0)}\rangle + \underset{\overset{\uparrow}{\text{HW}}\atop \overset{\shortparallel}{\lambda^2|n^{(2)}\rangle}}{\ldots}$$

Clearly, pert. theory is valid if $\left|\frac{V_{kn}}{E_n^{(0)}-E_k^{(0)}}\right|$ is "small".

Note: if $|n^{(0)}\rangle$ is a ground state ⇒ $E_n^{(2)}$ is negative ⇒ lowers the