

Small perturbations to 'easy' Hamiltonian

$\hat{H}_0 |\psi_n^{(0)}\rangle = E_n^{(0)} |\psi_n^{(0)}\rangle$ let's say we know how to solve for $\psi_n^{(0)}, E_n^{(0)}$
old hopefully easy to get solution

Now our Hamiltonian get changed

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1 \quad (*)$$

what are the solutions $E_n |\psi_n\rangle$ which satisfy

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle$$

if $\lambda \hat{H}_1$ is small (we define what it means later)

We can hope that $\psi_n \approx \psi_n^{(0)}$ more precisely

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \lambda^3 \psi_n^{(3)} + \dots \quad (**)$$

corrections to unperturbed solutions

$$\Psi_n = \Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \tilde{o}(\lambda^2)$$

small 'o' notation $\Leftrightarrow \frac{\tilde{o}(\lambda)}{\lambda} \xrightarrow{\lambda \rightarrow 0} 0$

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle$$

$$\hat{H} (|\Psi_n^{(0)}\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \tilde{o}(\lambda^2)) = E_n |\Psi_n\rangle =$$

$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \tilde{o}(\lambda^2)) (|\Psi_n^{(0)}\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \tilde{o}(\lambda^2))$$

$$= E_n^{(0)} |\Psi_n^{(0)}\rangle + \lambda E_n^{(0)} |\Psi_n^{(1)}\rangle + \lambda^2 E_n^{(0)} |\Psi_n^{(2)}\rangle + E_n^{(0)} \tilde{o}(\lambda^2)$$

$$+ \lambda E_n^{(1)} |\Psi_n^{(0)}\rangle + \lambda^2 E_n^{(1)} |\Psi_n^{(1)}\rangle + \lambda^3 E_n^{(1)} |\Psi_n^{(2)}\rangle + \lambda E_n^{(1)} \tilde{o}(\lambda^2)$$

$$+ \lambda^2 E_n^{(2)} |\Psi_n^{(0)}\rangle + \lambda^3 E_n^{(2)} |\Psi_n^{(1)}\rangle + \lambda^4 |\Psi_n^{(2)}\rangle + \lambda^2 E_n^{(2)} \tilde{o}(\lambda^2)$$

$$+ \tilde{o}(\lambda^2) \cdot |\Psi_n\rangle$$

Now let's look at

$$\begin{aligned} \hat{H}|\psi\rangle &= (\hat{H}_0 + \lambda\hat{H}_1)(|\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \tilde{o}(\lambda^3)) \\ &= \hat{H}_0|\psi_n^{(0)}\rangle + \lambda\hat{H}_0|\psi_n^{(1)}\rangle + \lambda^2\hat{H}_0|\psi_n^{(2)}\rangle + \hat{H}_0\tilde{o}(\lambda^3) \\ &+ \lambda\hat{H}_1|\psi_n^{(0)}\rangle + \lambda^2\hat{H}_1|\psi_n^{(1)}\rangle + \lambda^3\hat{H}_1|\psi_n^{(2)}\rangle + \lambda\hat{H}_1\tilde{o}(\lambda^2) \end{aligned}$$

for any λ

λ^0

$$=$$

\Rightarrow

$$\hat{H}_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle$$

our starting point

λ^1

$$=$$

\Rightarrow

$$\hat{H}_0|\psi_n^{(1)}\rangle + \hat{H}_1|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}|\psi_n^{(0)}\rangle$$

λ^2

$$=$$

\Rightarrow

$$\hat{H}_0|\psi_n^{(2)}\rangle + \hat{H}_1|\psi_n^{(1)}\rangle = E_n^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)}|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle$$

1st order correction

term, let's surround it with bra $\langle \Psi_n^{(0)} |$

$$\langle \Psi_n^{(0)} | \hat{H}_0 | \Psi_n^{(1)} \rangle + \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle = E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle + E_n^{(1)} \langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle$$

$$\langle \Psi_n^{(0)} | \hat{H}_0 | \Psi_n^{(1)} \rangle + \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle = E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle + E_n^{(1)} \langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle$$

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

$$\cancel{E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle} + \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle = \cancel{E_n^{(0)} \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle} + E_n^{(1)} \underbrace{\langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle}_{=1}$$

$$E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle$$

1st order energy correction

a careful eye would notice that energy correction is λE_1 but at this point we say $\lambda H_1 \rightarrow H_1$ is true perturbation

Next (in difficulty level) we would like to find what is $\psi_n^{(1)}$.

Let's surround with "bra" $\langle \psi_k^{(0)} |$ where $k \neq n$

$$\langle \psi_k^{(0)} | \hat{H}_0 | \psi_n^{(1)} \rangle + \hat{H}_1 | \psi_n^{(0)} \rangle = E_n^{(0)} | \psi_n^{(1)} \rangle + E_n^{(1)} | \psi_n^{(0)} \rangle$$

$$E_k^{(0)} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle = E_n^{(0)} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle + E_n^{(1)} \langle \psi_k^{(0)} | \psi_n^{(0)} \rangle$$

$\delta_{kn} \rightarrow 0$

$$\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle = \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} = C_{kn}$$

What for are those c_{kn} ?

Will see in a moment. But first recall that

$$\sum_k |\psi_k^{(0)}\rangle \langle \psi_k^{(0)}| = \hat{1} \quad \text{since they are the complete set of states of } \hat{H}_0 \text{ operator}$$

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

$$\hat{1} |\psi_n\rangle = \sum_k |\psi_k^{(0)}\rangle \underbrace{\langle \psi_k^{(0)} | \psi_n^{(0)} \rangle}_{\delta_{kn}} + \lambda \sum_k |\psi_k^{(0)}\rangle \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$$

split in $k \neq n$ and n

$$= |\psi_n^{(0)}\rangle + \lambda \sum_{k \neq n} |\psi_k^{(0)}\rangle \underbrace{\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle}_{= c_{kn}}$$

$$+ \lambda |\psi_n^{(0)}\rangle \underbrace{\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle}_{\text{tricky } \dots, \text{ we will call it } A_n}$$

$$|\psi_n\rangle = (1 + \lambda A) |\psi_n^{(0)}\rangle + \lambda \sum_{k \neq n} c_{kn} |\psi_k^{(0)}\rangle + \mathcal{O}(\lambda^2)$$

Now we will use orthonormality property

$$\langle \psi_n | \psi_n \rangle = 1$$

keeping terms $\sim \lambda$, and dropping $\sim \lambda^2 \dots$

$$\begin{aligned} \langle \psi_n | \psi_n \rangle &= (1 + \lambda A^*) (1 + \lambda A) \downarrow \\ &+ \lambda \langle \psi_n^{(0)} | \sum_{k \neq n} c_{kn} \psi_k^{(0)} \rangle + \text{c.c.} \\ &+ \bar{o}(\lambda) \end{aligned}$$

Note: A blue arrow points from the sum term to 0, indicating it is zero.

$$\begin{aligned} &= (1 + \lambda A^*) (1 + \lambda A) + \bar{o}(\lambda) = \\ &= 1 + \lambda A^* + \lambda A + \lambda^2 A^* A + \bar{o}(\lambda) \end{aligned}$$

Note: A blue circle highlights the term $\lambda^2 A^ A$, and a blue arrow points from it to the $\bar{o}(\lambda)$ term in the next line.*

$$\Rightarrow \lambda(A^* + A) = 0$$

$$\Rightarrow \boxed{A = i|a|}$$

$$(1 + \lambda i|\lambda|) |\Psi_n^{(0)}\rangle \approx \text{for } \lambda \ll 1$$

$e^{i|\lambda|\lambda} |\Psi_n^{(0)}\rangle$
 a phase factor
 which we will set
 to '0' for convenience

Putting all together: 1st order correction

$$\Psi_n = \Psi_n^{(0)} + \sum_{k \neq n} C_{kn} \Psi_k^{(0)}$$

$$C_{kn} = \frac{\langle \Psi_k^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$$

Where did
 the λ go
 from eq ~~**~~ ?
 recall that
 we had $\lambda \hat{H}_1$ and
 λC_{kn}

so we absorbed λ
 into \hat{H}_1 .

So it is a bit weird: we needed λ to set
 correction equations but not for the final answer.

Finally, \hat{H}_1 is perturbative if $C_{kn} \ll 1$