Small perturbations to "easy" Hamiltonian

old hopefully easy to get solution

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

Now our Hamiltonian get changed

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

notice Ψ ("flat palms" on psi)

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

new solution

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

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

We can hope that $\Psi_n \simeq \psi_n^{(0)}$ more precizely

$$\Psi_n = \psi_n^{(0)} + \underbrace{\lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \lambda^3 \Psi_n^{(3)} + \dots}_{} \qquad (**)$$

corrections to unperturbed solutions

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

$$\boxed{\text{small 'o' notation} \Leftrightarrow \frac{\tilde{o}(\lambda)}{\lambda} \xrightarrow[\lambda \to 0]{} 0}$$

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

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

$$= \Big(E_n^{(0)} + \underbrace{\lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \tilde{o}(\lambda^2)}_{\text{energy correction}}\Big)\left(|\Psi_n^{(0)}\rangle + \lambda|\Psi_n^{(1)}\rangle + \lambda^2|\Psi_n^{(2)}\rangle + \bar{o}(\lambda^2)\right)$$

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

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

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

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

Now let's look at

$$\hat{H}|\psi\rangle = (\hat{H}_0 + \lambda\hat{H}_1)\left(|\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \tilde{o}(\lambda^2)\right)$$

$$= H_0|\psi_n^{(0)}\rangle + \lambda\hat{H}_0|\psi_n^{(1)}\rangle + \lambda^2\hat{H}_0|\psi_n^{(2)}\rangle + \hat{H}_0\,\tilde{o}(\lambda^2)$$

$$+ \lambda\hat{H}_1|\psi_n^{(0)}\rangle + \lambda^2\hat{H}_1|\psi_n^{(1)}\rangle + \lambda^3\hat{H}_1|\psi_n^{(2)}\rangle + \lambda\hat{H}_1\,\tilde{o}(\lambda^2)$$

for any λ

λ^0 : $= \Rightarrow \boxed{\hat{H}_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle}$ 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 $\langle\psi_n^{(0)}|$

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

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

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

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

1st order energy correction

a careful eye would notice that energy correction is λE_1 but at this point we say $\lambda H_1 \to H_1$ 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 $k \neq n$

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

$$E_k^{(0)} \underline{\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle} + \langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle = E_n^{(0)} \underline{\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle} + E_n^{(1)} \underbrace{\langle \psi_k^{(0)} | \psi_n^{(0)} \rangle}_{= \delta_{kn}} \to 0$$

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

What for are those c_{kn} ?
Will see in a moment. But first recall that

$$\sum_k |\psi_k^{(0)}\rangle\langle\psi_k^{(0)}| = \hat{1}$$

since they are the complete set of states of $\hat{H}_0$ 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

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

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

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

Now we will use orthonormality property

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

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

$$\langle \psi_n | \psi_n \rangle = (1 + \lambda A^*)(1 + \lambda A) \, 1$$

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

$$+ \; \bar{o}(\lambda)$$

$$= (1 + \lambda A^*)(1 + \lambda A) + \bar{o}(\lambda) =$$

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

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

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

$$\left(1+\lambda i|a|\right)|\psi_n^{(0)}\rangle \underset{\text{for } \lambda \ll 1}{\approx} e^{i|a|\lambda}|\psi_n^{(0)}\rangle$$

a phase factor which we will set to '0' for convinience

Putting all together: 1st order correction

$$\boxed{\begin{aligned} \psi_n &= \psi_n^{(0)} + \sum_{k=n} c_{kn}\,\psi_k^{(0)} \\ c_{kn} &= \frac{\langle \psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} \end{aligned}}$$

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 $c_{kn} \ll 1$