Time-independent perturbations

We are concerned with finding solutions for $\longrightarrow$ $\boxed{\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle}$

unfortunately there are not many hamiltonians where we can find close form solutions.

* square wells
* harmonic oscillator
* Coulomb potential

i.e. "important" ones

$\longrightarrow$ $\hat{H}_0, |\psi_n^{(0)}\rangle$ known solutions

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

Real world always perturbs them, i.e. modifyes $\longrightarrow$ $\hat{H}_0 + \lambda\hat{H}_1 = \hat{H}$

number $\ll 1$

perturbation

Since perturbation is small $(\sim\lambda)$ we hope that the original solutions are mostly as before but with small corrections $\sim \lambda, \lambda^2, \lambda^3, \ldots$

(think about Tyler expansion idea)

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

where

correction order

$$|\varphi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \lambda^3|\psi_n^{(3)}\rangle + \ldots$$

solution of $\hat{H}_0$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$$

corrections

Let's find general form of the 1st order corrections: $\lambda\psi_n^{(1)}$, $\lambda E_n^{(1)}$

$$(H_0+\lambda H_1)\left(|\psi_n^{(0)}\rangle+\lambda|\psi_n^{(1)}\rangle+\underbrace{\cancel{\lambda^2|\psi_n^{(2)}\rangle+\lambda^3|\psi_n^{(3)}\rangle+\dots}}_{\to 0}\right)=$$

we drop this as $\lambda\to 0$ since ⏟ is $\ll \lambda|\psi^{(1)}_n\rangle$

$$=\left(E_n^{(0)}+\lambda E_n^{(1)}+\underbrace{\cancel{\lambda^2E_n^{(2)}+\lambda^3E_n^{(3)}+\dots}}_{\to 0}\right)\left(|\psi_n^{(0)}\rangle+\lambda|\psi_n^{(1)}\rangle+\underbrace{\cancel{\lambda^2|\psi_n^{(2)}\rangle+\dots}}_{\to 0}\right)$$

$\Longrightarrow$

$$(H_0+\lambda H_1)\left(|\psi_n^{(0)}\rangle+\lambda|\psi^{(1)}\rangle\right)+\cancel{\lambda^2(\dots)}_{\to 0}=\left(E_n^{(0)}+\lambda E_n^{(1)}\right)\left(|\psi_n^{(0)}\rangle+\lambda|\psi_n^{(1)}\rangle\right)+\cancel{\lambda^2(\dots)}_{\to 0}$$

(*) $$\underline{H_0|\psi_n^{(0)}\rangle}+\lambda H_0|\psi^{(1)}\rangle+\lambda H_1|\psi_n^{(0)}\rangle+\cancel{\lambda^2H_1|\psi_1^{(1)}\rangle}_{\to 0}=$$

$$=\underline{E_n^{(0)}|\psi_n^{(0)}\rangle}+\lambda E^{(0)}|\psi_n^{(1)}\rangle+\lambda E_n^{(1)}|\psi_n^{(0)}\rangle+\cancel{\lambda^2E_n^{(1)}|\psi_n^{(1)}\rangle}_{\to 0}$$

unperturbed solution

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

First order correction

(*) $$\boxed{\begin{Bmatrix}\hat{H}_0|\psi_n^{(0)}\rangle\\ + \\ \lambda\left(\hat{H}_0|\psi_1^{(1)}\rangle+H_1|\psi_n^{(0)}\rangle\right)\end{Bmatrix}=\begin{Bmatrix}E_n^{(0)}|\psi_n^{(0)}\rangle\\ + \\ \lambda\left(E_n^{(0)}|\psi_n^{(1)}\rangle+E_n^{(1)}|\psi_n^{(0)}\rangle\right)\end{Bmatrix}}$$

same eq as (*) but decomposed to $\sim\lambda^0$ and $\sim\lambda^1$ terms

power

How to find $E_n^{(1)}$?

let's take eq. $(*)$ with 'bra' of $\psi_n^{(0)}$, i.e. $\langle \psi_n^{(0)} |$

$$\langle \psi_n^{(0)} | \, (*) \implies$$

$\langle \psi_n^{(0)} | E_n$, recall $H = H^\dagger$

$$\langle \psi_n^{(0)} | \underbrace{\hat{H}_0 \psi_n^{(0)}}_{E_n^{(0)}} \rangle + \lambda \Big(\underbrace{\langle \psi_n^{(0)} | \hat{H}_0}_{\langle \psi_n^{(0)} | E_n} | \psi_1^{(1)} \rangle + \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle \Big) =$$

// same

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

$$\lambda \Big(E_n^{(0)} \langle \psi_n^{(0)} | \psi_1^{(1)} \rangle + \langle \psi_n^{(0)} | H_1 | \psi_n^{(0)} \rangle \Big) =$$

// same

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

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

expectation value of $\hat{H}_1$ in the unperturbed state

1st order energy correction of 'nth' state

Now we are looking for the expression of $|\psi_n\rangle$, i.e. eigenstate of $\hat{H}$.

Again we take eq.(*) and wrap it, this time with $\langle \psi_k^{(0)} |$, where $k \neq n$

Recall: eigen solutions of $\hat{H}_0$ form orthonormal set: $\langle \psi_k^{(0)} | \psi_n^{(0)} \rangle = \delta_{kn}$

$\langle \psi_k^{(0)} | * \rangle \Rightarrow$

Note

$\langle \psi_k^{(0)} | H_0 | \psi_n^{(0)} \rangle =$
$= \langle \psi_k^{(0)} | E_n^{(0)} | \psi_n^{(0)} \rangle$
$= E_n \delta_{kn} = 0$, for $k \neq n$

simplifies too only λ containing term:

$E_k \langle \psi_k^{(0)} |$

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

$$= \langle \psi_k^{(0)} | E_n^{(0)} | \psi_n^{(1)} \rangle + \cancel{\langle \psi_k^{(0)} | E_n^{(1)} | \psi_n^{(0)} \rangle}$$

$E_n^{(1)} \langle \psi_k^{(0)} | \psi_n^{(0)} \rangle = E_n^{(1)} \delta_{kn} = 0, k \neq n$

just a number

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

$$\boxed{\underbrace{\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle}_{\text{just a number}} = \frac{\langle \psi_k^{(0)} | H_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} = C_{kn}} \quad (\ast\ast\ast)$$

We would like to express $\psi_n^{(1)}$ in the basis of old solutions $\psi_k^{(0)}$, to do so we will use the following property of a complete orthonormal set:

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

sum of all projections equal to vector itself

k ← all possible k

$\hat{1}$ ← unity operator

Now

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

$$| \psi_n^{(1)} \rangle = \underbrace{| \psi_n^{(0)} \rangle}_{\text{known}} \underbrace{\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle}_{\text{tricky}} + \sum_{k \neq n} \underbrace{| \psi_k^{(0)} \rangle}_{\text{known}} \underbrace{\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle}_{C_{kn}} \quad \left(\begin{matrix} \ast\ast \\ \ast\ast \end{matrix}\right)$$

Let's focus on the "tricky" part

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

recall the original construction

$\hat{H} = \hat{H}_0 + \hat{H}_1$ has eigen solution

$$\varphi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} \ldots$$

$$\langle \varphi_n | \varphi_n \rangle = 1 = \langle \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} \ldots | \psi_n^{(0)} + \lambda \psi_1^{(1)} + \hat{\lambda} \psi^{(2)} + \ldots \rangle$$

$$= \underbrace{\langle \psi_n^{(0)} | \psi_n^{(0)} \rangle}_{1 =} + \lambda \left(\langle \psi_n^{(1)} | \psi_n^{(0)} \rangle + \langle \psi_n^{(0)} | \psi_1^{(1)} \rangle \right) + O(\lambda^2)$$

other thing $\sim \lambda^2$ which we drop from the very beginning

$$1 = 1 + \lambda \left(\underbrace{\langle \psi_n^{(1)} | \psi_n^{(0)} \rangle + \langle \psi^{(0)} | \psi^{(1)} \rangle}_{\text{must be zero!}} \right)$$

if we call this number A than this is A^*

$A^* + A = 0 \Rightarrow A$ is imaginary

$A = ia$, where 'a' is real

Circling back to (**)

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

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

$$= \underbrace{|\psi_n^{(0)}\rangle + \lambda i a |\psi_n^{(0)}\rangle}_{|\psi_n^{(0)}\rangle (1 + \lambda i a) \approx e^{i\lambda a},\ \lambda \ll 1} + \lambda \sum_{k \neq n} C_{kn} |\psi_k^{(0)}\rangle$$

$$|\psi_n\rangle = e^{ia\lambda} |\psi_n^{(0)}\rangle + \lambda \sum_{k \neq n} C_{kn} |\psi_k^{(0)}\rangle$$

just a phase factor which we for convinience set to 1, i.e. $a = 0$

Note: making $a = 0$ also make sense since $|\psi_n\rangle$ already has $|\psi_n^{(0)}\rangle$

Finally

$$\boxed{|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{k \neq n} \frac{\langle \psi_k^{(0)} | H_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle}$$

Perturbed eigen state = old + λ correction