Time Independent Perturbation Theory

Perturbation?

Let's Say we have Solved $\hat{H}\psi = E\psi$

For a complete Set of ψ_n^s and E_n^s

Assume 1: Non-degenerate → unique ψ_n → unique E_n

2: Complete $\langle \psi_n | \psi_m \rangle = \delta_{nm}$

Now - relabel $H^0 \psi_n^0 = E_n^0 \psi_n^0$ 0 means zeroth order Solution To unperturbed Hamiltonian

$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{nm}$

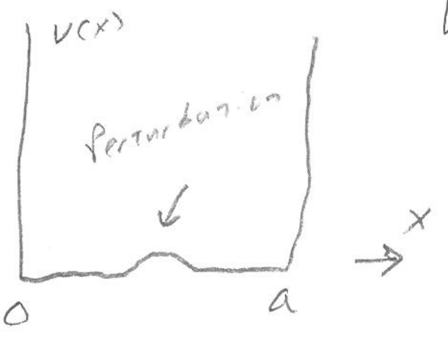
Now Perturb → add Small change to H^0

and try to Solve $\hat{H}\psi_n = E_n \psi_n$

want to find approximate Solutions using Known Solutions

Works for Small changes

Ex. ISW



H is now $H^0 + \lambda H'$

$$\psi_n = \psi_n^0 + \lambda \psi_n' + \overset{\text{Power}}{\lambda^{2<}}\,\overset{2\text{nd order}}{\psi_n} + \ldots$$

$$E_n = E_n^0 + \lambda E_n' + \underset{\text{power}}{\lambda^2}\,\underset{\text{order}}{E_n^2} + \ldots$$

λ is simply a record keeping tool!

The # corresponds to the ORDER of the correction

Now $(H^0 + \lambda H')\psi_n = E_n \psi_n$

$$(H^0 + \lambda H')[\psi_n^0 + \lambda\psi_n' + \lambda^2\psi_n^2 + \ldots] = (E_n^0 + \lambda E_n' + \lambda^2 E_n^2 + \ldots)(\psi_n^0 + \lambda\psi_n' + \lambda^2\psi_n^2$$

1st order perturbation theory keep just λ' terms

$$H_0\psi_n^0 + \lambda[H'\psi_n^0 + H^0\psi_n'] + \lambda^2[H_0\psi_n^2 + H'\psi_n^1] + \ldots$$

$$= E^0\psi_n^0 + \lambda[E_n^0\psi_n' + E_n'\psi_n^0] + \lambda^2[E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0]$$

Notice orders add to 0, 1, 2 ....

Equate orders → $H_0\psi_n^0 = E^0\psi_n^0$ <u>Old Form</u> order = 0

$$\boxed{H'\psi_n^0 + H_0\psi_n' = E_n^0\psi_n' + E_n'\psi_n^0}$$ order = 1

$$\boxed{H_0\psi_n^2 + H'\psi_n' = E_n^0\psi_n^2 + E_n'\psi_n' + E_n^2\psi_n^0 \quad \text{order} = 2}$$

1st Order

$$\boxed{H^0\psi_n^1 + H^1\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0}$$

Take inner product with $(\psi_n^0)^*$

$$\overset{1}{\langle \psi_n^0 | H^0 | \psi_n^1 \rangle} \overset{+}{+} \overset{2}{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle} \overset{=}{=} \overset{3}{\langle \psi_n^0 | E_n^0 | \psi_n^1 \rangle} \overset{+}{+} \overset{4}{\langle \psi_n^0 | E_n^1 | \psi_n^0 \rangle}$$

H^0 is hermetian $\langle f | \hat{Q} | g \rangle = \langle \hat{Q} f | g \rangle$

$$\langle \psi_n^0 | H^0 | \psi_n^1 \rangle = \langle H^0 \psi_n^0 | \psi_n^1 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle$$

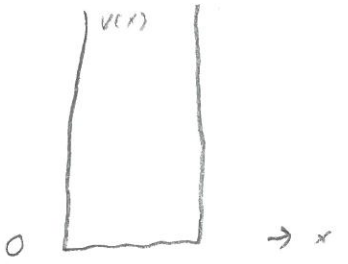
So 1 = 3

Or $\langle \psi_n^0 | H^1 | \psi_n^0 \rangle = E_n^1 \underset{\downarrow 1}{\langle \psi_n^0 | \psi_n^0 \rangle}$

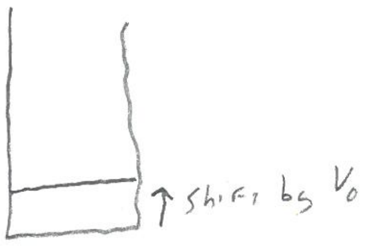
So $E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle$ → 1st order Energy correction is simply the expectation value of the perturbed Hamiltonian

Ex. Let $\psi_n^0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

go from



To



$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \langle \psi_n^0 | V_0 | \psi_n^0 \rangle = V_0 \langle \psi_n^0 | \psi_n^0 \rangle = V_0$

$E \sim E_n^0 + E_n^1 = E_n^0 + V_0$ Exact because H' is constant

what about $H' = V_0 \quad x \in [0, \frac{a}{2}]$

0 else

Then $E_n^1 = \underbrace{\int_0^{a/2} \frac{2}{a} V_0 \sin^2\left(\frac{n\pi x}{a}\right) dx}_{\frac{V_0}{2}} + \underbrace{\int_{a/2}^{a} 0 \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right) dx}_{0}$

$E \sim E_n^0 + \frac{V_0}{2} \rightarrow$ approximate

ψ_n^1? Let's rewrite $H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$

known

$(H^0 - E_n^0)\psi_n^1 = -[H' - E_n^1]\psi_n^0$

known

not known

Differential Equation For ψ_n^1

Now ψ_n^0 Form a complete Set

So $\psi_n^1 = \sum_{m \neq n} C_m^{(n)} \psi_m^0$ essentiall Each ψ_n^1 get's it's own

infinite Series

So $(H_0 - E_n^0) \sum_{m \neq n} C_m^{(n)} \psi_m^0 = -(H' - E_n') \psi_n^0$

n= fixed
m= free

but $H_0 \psi_m^0 = E_m^0$

$$\sum_{m \neq n} (E_m^0 - E_n^0) C_m^{(n)} \psi_m^0 = -(H' - E_n') \psi_n^0$$

Take inner product with $\psi_\ell^0 \rightarrow \langle \psi_\ell^0 |$

$$\sum_{m \neq n} (E_m^0 - E_n^0) C_m^{(n)} \langle \psi_\ell^0 | \psi_m^0 \rangle = -\langle \psi_\ell^0 | H' | \psi_n^0 \rangle + E_n' \langle \psi_\ell | \psi_n \rangle$$

Now $\langle \psi_\ell^0 | \psi_m^0 \rangle = \delta_{m\ell}^0$ and if $\ell = n \rightarrow = \delta_{nm}^0$

but $m \neq n$ so LHS=0

or $\langle \psi_n^0 | H' | \psi_n^0 \rangle = E_n' \underset{\downarrow 1}{\langle \psi_n | \psi_n \rangle}$. Same as we found

If $\ell \neq n$ all $\langle \psi_\ell^0 | \psi_m^0 \rangle$ vanish Except where $m = \ell$

Or $(E_\ell^0 - E_n^0) C_\ell^{(n)} = -\langle \psi_\ell^0 | H' | \psi_n^0 \rangle$ $\quad \ell \rightarrow m$

$$(E_m^0 - E_n^0) C_m^{(n)} = -\langle \psi_m^0 | H' | \psi_n^0 \rangle$$

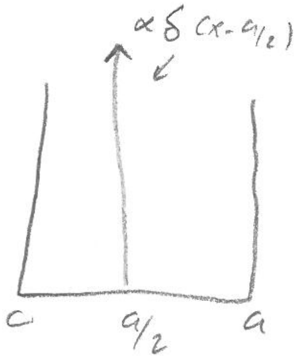
↑ not zero $\langle \psi_m^0 | H^0 | \psi_n^0 \rangle = 0$
but H' Not H^0

$$\boxed{C_m^{(n)} = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}}$$

So $$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \psi_n^0$$

Safe if $E_n^0 \neq E_m^0$ → Non-degenerate Spectrum

Problem 6.1



$H' = \alpha\delta(x - a/2)$ in ISW

$$\psi_n^0 = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$\langle \psi_n^0 | \alpha\delta(x - a/2) | \psi_n^0 \rangle = \frac{2}{a} \int_0^a \alpha\delta\left(x - \frac{a}{2}\right) \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$E_n^1 = \frac{2}{a} \alpha \sin^2\left(\frac{n\pi}{2}\right) \rightarrow \begin{matrix} 0 \text{ n even} \\ \frac{2\alpha}{a} \text{ n odd} \end{matrix}$$

$$\langle \psi_m^0 | \alpha\delta\left(x - \frac{a}{2}\right) | \psi_1^0 \rangle = \frac{2\alpha}{a} \int_0^a \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) \delta\left(x - \frac{a}{2}\right) dx$$

$$= \frac{2\alpha}{a} \sin\left(\frac{m\pi}{2}\right) \sin\left(\frac{\pi}{2}\right) = \frac{2\alpha}{a} \sin\left(\frac{m\pi}{2}\right)$$ Now the sum runs from $m \neq 1$

or $$\psi_1^1 = \sum_{m=2} \frac{\frac{2\alpha}{a} \sin\left(\frac{m\pi}{2}\right)}{E_n^0 - E_m^0}$$

even m are zero

So $$\sum_{m=3,5,7,\ldots} \frac{2\alpha/a \ \text{SIN}(m\pi/2)}{E_1' - E_m^0} \psi_m^0 \qquad E_1^0 - E_m^0 = \frac{\pi^2\hbar^2}{2ma^2}(1-m^2)$$

$$\frac{2\alpha}{a} \cdot \frac{2ma^2}{\pi^2\hbar^2} \left[\frac{-1}{1-9}\psi_3^0 + \frac{1}{1-25}\psi_5^0 - \frac{1}{1-49}\psi_7^0 + \cdots \right]$$

$$\frac{4ma\alpha}{\pi^2\hbar^2} \cdot \sqrt{\frac{2}{a}} \left[\frac{1}{8}\text{SIN}\left(\frac{3\pi x}{a}\right) - \frac{1}{24}\text{SIN}\left(\frac{5\pi x}{a}\right) + \frac{1}{48}\text{SIN}\left(\frac{7\pi x}{a}\right) + \cdots \right.$$