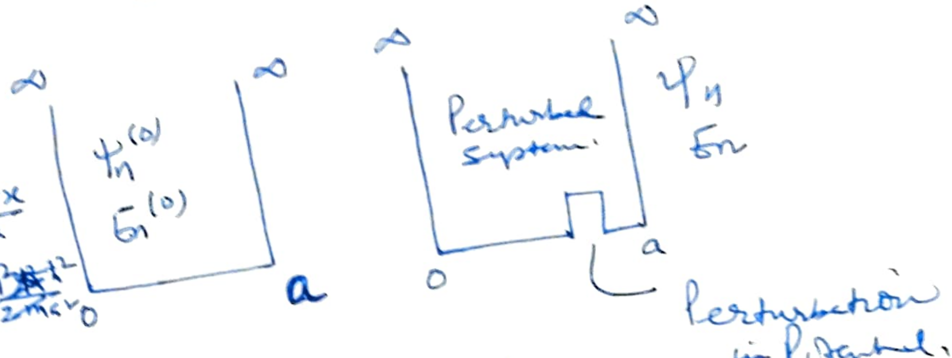
Perturbation Theory

Small change/disturbance in Hamiltonian of the system.

$$H = T + V$$

Slight change in potential

Example



$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$E_n = \frac{n^2 \cancel{a^2} \hbar^2}{2m \cancel{a^2}} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

How to find out the solution of Approximate ~~~~ Schrödinger Equation i.e. How to find out Eigen wave function and Eigen Energy of the perturbed system, using solutions of unperturbed system.

$$H = H_0 + H'$$

- Time Independent Perturbation Theory
- Time Dependent Perturbation Theory

→ Hamiltonian is constant in time
$\Rightarrow$ H' is not changing with time

- Non-degenerate Perturbation Theory (T.I)
- Degenerate Perturbation Theory (T.I)

$$H_0\psi_1 = E_1\psi_1$$
$$H_0\psi_2 = E_2\psi_2$$

$$H_0\psi_1 = E_1\psi_1$$
$$H_0\psi_2 = E_1\psi_2$$

Same Energy Eigen value

$$E = \frac{n^2 h^2}{8mL^2} \text{ or } \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$n \longrightarrow n_x \; n_y \; n_z$$

(1)

Perturbation Theory

$$H = H_0 + H'$$

*should be small

Example [

* Approximate solutions
Wavefunction
Energy Eigen value

Perturbed unperturbed Correction

$$E_n = E_n^{(0)} + E_n^{(1)} + \dots$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + |\psi_n^{(1)}\rangle + |\psi_n^{(2)}\rangle + \dots$$ Ist order Correction

Perturbed

unperturbed wave function

$$H = H_0 + H' \quad \text{--- (1)}$$

Eigen function & Eigen values of H_0 are known and the effect of H' is assumed to be small.

For unperturbed system:

$$H_0 u_n = \underline{E_n} u_n \quad \text{--- (2)}$$

For perturbed system

$$H \psi_n = \underline{W_n} \psi_n \quad \text{--- (3)}$$

Introducing another parameter 'g' (0-1)

$$H = H_0 + g H' \quad \text{--- (4)}$$

Expressing ψ_0 and W_n in power series

$$\psi_n = \psi_n^{(0)} + g\,\psi_n^{(1)} + g^2 \psi_n^{(2)} + \dots \quad (5)$$

$$W_n = W_n^{(0)} + g\,W_n^{(1)} + g^2 W_n^{(2)} \dots \quad (6)$$

(5) & (6) in (3)

$$(H_0 + g H')(\psi_n^{(0)} + g\,\psi_n^{(1)} + g^2 \psi_n^{(2)} + \dots)$$

$$= (W_n^{(0)} + g W_n^{(1)} + g^2 W_n^{(2)} + \dots)(\psi_n^{(0)} + g\,\psi_n^{(1)} + g^2 \psi_n^{(2)} + \dots)$$

$$(H_0 + gH')(\psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \cdots) = (W_n^{(0)} + gW_n^{(1)} + g^2W_n^{(2)} + \cdots)(\psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \cdots) \quad (7)$$

This is valid for all values of g lying between 0 and 1, The coefficients of equal powers of g on either side of the equation must be the same. (8)

$$H_0\psi_n^{(0)} = W_n^{(0)}\psi_n^{(0)} \quad (9)$$

$$H_0\psi_n^{(1)} + H'\psi_n^{(0)} = W_n^{(0)}\psi_n^{(1)} + W_n^{(1)}\psi_n^{(0)}$$

$$H_0\psi_n^{(2)} + H'\psi_n^{(1)} = W_n^{(0)}\psi_n^{(2)} + W_n^{(1)}\psi_n^{(1)} + W_n^{(2)}\psi_n^{(0)} \quad (10)$$

$\psi_n^{(0)}$ and $W_n^{(0)}$ are the Eigen functions and Eigen values of unperturbed Hamiltonian. (11)

$$\psi_n^{(0)} = u_n \quad (12)$$
$$\& \quad W_n^{(0)} = E_n$$

First order Perturbation correction.

We assume that the Eigen functions of the unperturbed Hamiltonian H_0 form a complete set, thus we may write $\psi_n^{(1)}$ as a linear combination of the functions u_n

$$\psi_n^{(1)} = \sum_m a_m^{(1)} u_m \quad (13)$$

Substituting (13) in equation (9)

$$H_0 \sum_m a_m^{(1)} u_m + H'\psi_n^{(0)} = W_n^{(0)} \sum_m a_m^{(1)} u_m + W_n^{(1)} u_n$$

$$H_0 \sum a_m^{(1)} u_m + H' \psi_n^{(0)} = W_n^{(0)} \psi_n^{(1)} + W_n^{(1)} \psi_n^{(0)} \quad \text{— (14)}$$

$$\Rightarrow \quad \sum_m a_m^{(1)} E_m u_m + H' u_n = E_n \sum a_m^{(1)} u_m + W_n^{(1)} u_n \quad \text{— (15)}$$

Here we have used Equation (2) & (11)

Multiplying Equation 15 by. u_k^* and integrate

$$\left(\int u_k^* u_m = \delta_{km}\right)$$

$$\sum_m a_m^{(1)} E_m \delta_{km} + \int u_k H' u_n \, d\tau = E_n \sum a_m^{(1)} \delta_{km} + W_n^{(1)} \delta_{kn}$$

when $m = k$

$$a_k^{(1)} E_k + H'_{kn} = E_n \cancel{\#} a_k^{(1)} + W_n^{(1)} \delta_{kn}$$

$$\Rightarrow \quad a_k^{(1)} (E_n - E_k) + W_n^{(1)} \delta_{kn} = H'_{kn} \quad \text{— (16)}$$

where $H'_{kn} = \int u_k^* H' u_n \delta\tau$ — (17)

For $k = n$, Equation (16) gives

$$\boxed{W_n^{(1)} = H'_{nn} = \int u_n^* H' u_n \, d\tau} \quad \text{— (18)}$$

First-order Correction in Energy Eigen value.

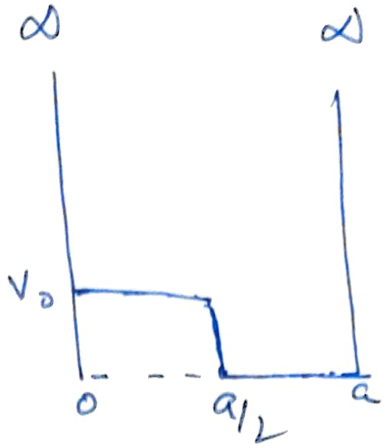
$\int \psi_n^* H' \psi$ = First order correction.

For $k \neq n$

from Eq^n. (16)

$$\boxed{a_k^{(1)} = \frac{H'_{kn}}{E_n - E_k}}.$$

Example



A particle of mass is confined in an asymmetric potential well as shown

Find $E_n^{(1)}$, first order correction

$$E_n^{(1)} = \langle \psi_n | H' | \psi_n \rangle$$

Here $|\psi_n\rangle = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

Here $H' = V_0 \qquad 0 < x < \frac{a}{2}$

$$E_n^{(1)} = \int_0^{a/2} \frac{2}{a} \sin^2 \frac{n\pi x}{a} V_0 \, dx$$

$$= \frac{V_0}{2}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} + \frac{V_0}{2} + \cdots$$

$$E_n^{(1)} = \int_0^{a/2} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot V_0 \cdot \sqrt{\frac{2}{a}} \cdot \sin \frac{n\pi x}{a} \cdot dx$$

$$= \frac{V_0}{2}$$