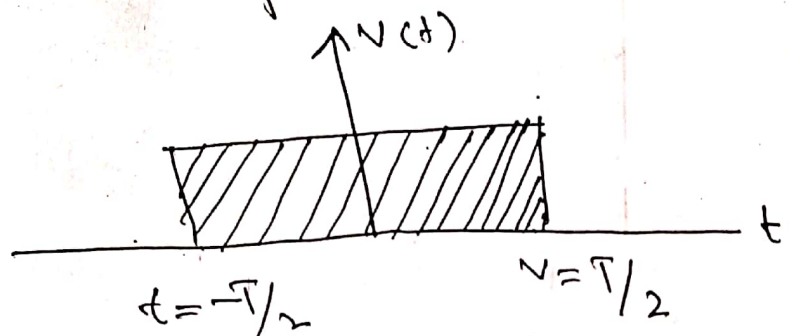


Transition Probability for a Constant Perturbation: (1)

We consider the case when the perturbation $V(t) = 0$ for $t < -T/2$ and $t > T/2$, and constant over the period $-T/2 \leq t \leq T/2$, i.e. V does not depend on time.



For a given interval of perturbation and V being sufficiently weak, then equ (3) becomes

$$T_{fi} = -\frac{2i}{\hbar} V_{fi} \int_{-T/2}^{T/2} dt e^{i\omega_{fi}t}$$

where

$$\hbar \omega_{fi} = E_f - E_i$$

↳ first order perturbation

Now

$$T_{fi} = \frac{-V_{fi}}{\hbar \omega_{fi}} \Big|_{-T/2}^{T/2} e^{i\omega_{fi}t}$$

$$T_{fi} = -\frac{V_{fi}}{\hbar \omega_{fi}} \left(e^{i\omega_{fi}T/2} - e^{-i\omega_{fi}T/2} \right)$$

$$= -\frac{V_{fi}}{\hbar \omega_{fi}} \left(2i \sin(\omega_{fi}T/2) \right)$$

because

$$e^{ix} = \cos x + i \sin x$$

$$e^{-ix} = \cos x - i \sin x$$

$$|T_{fi}|^2 = \frac{4}{\hbar^2} |V_{fi}|^2 \frac{\sin^2(\omega_{fi}T/2)}{\omega_{fi}^2}$$

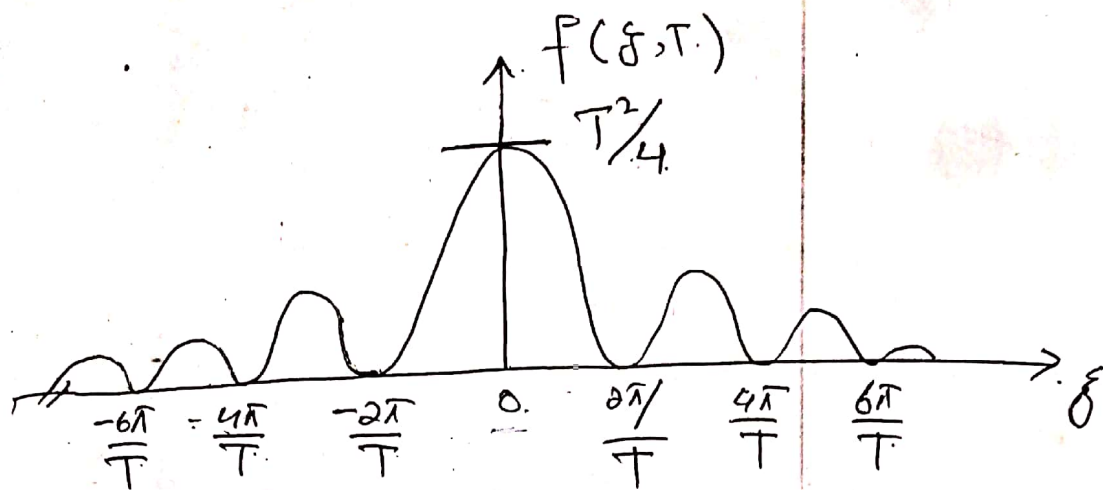
$$= \frac{4}{\hbar^2} |V_{fi}|^2 f(\xi, T)$$

$$f(\xi, T) = \frac{\sin^2(\xi T/2)}{\xi^2}, \quad \xi = \omega_{fi}$$

$$= \frac{1}{\xi^2} \left[\left(\frac{\xi T}{2} \right)^2 - \left(\frac{\xi T}{2} \right)^4 \frac{1}{3!} + \dots \right]^2$$

$f(\xi, T)$ is maximum when $\xi \rightarrow 0$

As a function of time, this transition probability is an oscillating sinusoidal with function with a period $2\pi/\omega_{fi}$



(5)

As shown in fig above, the transition probability is maximum only when $\delta = \omega_{fi} = 0$ and decay rapidly as δ move away from zero. This means that the

transition probability of finding the system in a state $|\Phi_f\rangle$ of energy E_f is maximum only when $E_i \cong E_f$ or when $\omega_{fi} = 0$.

The height and width of the main peak, centered around $\delta = 0$, are proportional to T^2 and $1/T$, respectively. Hence, the

transition probability is proportional to T and grows linearly with time. The central peak becomes narrower and higher as time increases, this is exactly the property of a delta function.

$$\int_{-\infty}^{\infty} dg \frac{\sin^2(\delta T/2)}{g^2} = \frac{\pi T}{2}$$

since $\int \frac{\sin^2 x}{x^2} dx = \pi$

The function $f(g, T)$ goes to $\frac{\pi T}{2} \delta(g)$ for $T \rightarrow \infty$ i.e. the maximum of $f(g, T)$ at $g=0$ becomes very sharp

$$\lim_{T \rightarrow \infty} f(g, T) = \frac{\pi T}{2} \delta(g)$$

Transition Into a Continuum of final states

Now we calculate the total transition rate associated with a transition from an initial state $|\Phi_i\rangle$ into a continuum of final states $|\Phi_f\rangle$. For energy to be conserved during the transition, i.e.

$$\Delta E = |E_f - E_i| = 0,$$

The uncertainty principle $\Delta E \Delta t \geq \hbar/2$ ⁽¹⁾ implies that an infinite time separates the initial and the final states. So the physically important quantity is not $|T_{fi}|^2$ but the transition probability per unit time.

$$W_{fi} = \frac{|T_{fi}|^2}{T} = \frac{4}{\hbar^2} |V_{fi}|^2 f(\delta, T)$$

$$= \frac{4}{\hbar^2} |V_{fi}|^2 \frac{\pi T}{2} \delta(\delta)$$

$$= \frac{2\pi}{\hbar} |V_{fi}|^2 \delta\left(\frac{E_f - E_i}{\hbar}\right)$$

$$\hbar \delta = \hbar \omega_{fi} = E_f - E_i$$

$$W_{fi} = \frac{2\pi}{\hbar} |\langle f | V | i \rangle|^2 \delta(E_f - E_i)$$

Fermi's Golden Rule I

Now consider the density of final states $\rho(E_f)$, where the number N_f of final states lying in the energy range E_f to $E_f + dE_f$ is

$$N_f = \rho(E_f) dE_f$$

The transition probability per unit time is then

$$W_{f_i} = \int dE_f \rho(E_f) \frac{2\pi}{\hbar} |V_{f_i}|^2 \delta(E_f - E_i)$$

$$= \frac{2\pi}{\hbar} |\langle f | V | i \rangle|^2 \rho(E_f = E_i)$$

$$= \frac{2\pi}{\hbar} |\langle f | V | i \rangle|^2 \int \rho(E_f) \delta(E_f - E_i) dE_f$$

$$W_{f_i} = \frac{2\pi}{\hbar} |\langle f | V | i \rangle|^2 \rho(E_i)$$

Fermi's Golden Rule II

It implies that in the case of a constant perturbation, the total transition rate becomes constant (time-independent).

VARIATIONAL METHOD ⁽¹⁾ (12)

The ground state of a quantum mechanical system can be determined without solving the Schrodinger equation explicitly. The method is the variational method in which one requires that the low energy of the ground state be the lowest of all possible energies of all possible states.

Let " E_0 " be the energy of the ground state of a system described by a Hamiltonian H and having a spectrum of energies $\{E_n\}$ such that

$$H|\phi_n\rangle = E_n |\phi_n\rangle$$

$$n = 0, 1, 2, \dots$$

with

$$E_0 \leq E_n = \langle \phi_n | H | \phi_n \rangle \quad (n \neq 0)$$

If $\{|\phi_n\rangle\}$ be the complete set of eigenstates of H , then any arbitrary state ψ can be expanded as

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle,$$

$$\langle\psi|\psi\rangle = \sum_n |a_n|^2 = 1$$

The mean energy of $|\psi\rangle$ is

$$\langle\psi|H|\psi\rangle = \int \psi^* H \psi dx$$

$$\neq \frac{\int \psi^* H \psi dx}{\int \psi^* \psi dx}$$

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle$$

$$\langle\psi| = \sum_m a_m \langle\phi_m|$$

$$\langle\psi|H|\psi\rangle = \sum_n \sum_m a_n^* a_m \langle\phi_n|H|\phi_m\rangle$$

$$= \sum_n \sum_m a_n^* a_m E_m \delta_{nm}$$

$$= \sum_n E_n |a_n|^2$$

$$\geq E_0 \sum_n |a_n|^2 + \sum_n |a_n|^2 (E_n - E_0)$$

$$\geq E_0 \sum_n |a_n|^2$$

$$\langle \psi | H | \psi \rangle \geq E_0, \quad \sum_n |A_n|^2 = 1. \quad (1)$$

This means that $E_0 < E_1 < E_2 < \dots$
 i.e. the energy of the ground state of a quantum system is equivalent to finding the minimum of the integral

$$\langle \psi | H | \psi \rangle = \int \psi^* H \psi dx$$

i.e.

$$E_0 = \min_{\psi \in L^2} \left[\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \right]$$

The necessary condition for the extremum is that

$$\delta (E_\psi) = \delta \left[\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \right] = 0$$

$$\frac{\delta \langle \psi | H | \psi \rangle \langle \psi | \psi \rangle - \langle \psi | H | \psi \rangle (\delta \langle \psi | \psi \rangle)}{\langle \psi | \psi \rangle^2} = 0$$

$$\langle \psi_m | \psi_m \rangle = \int$$

Applications:-

One-dimensional harmonic oscillator:

The Hamiltonian of the system is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$$

Let $\psi_\alpha = A e^{-\alpha x^2}$ be a one-parameter family of wave-functions:

$$\langle \psi_\alpha | H | \psi_\alpha \rangle = E_\psi(\alpha)$$

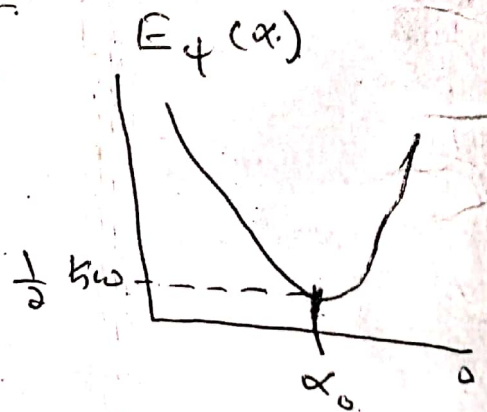
$$\langle \psi_\alpha | \psi_\alpha \rangle$$

$$E_\psi(\alpha) = \frac{\int_{-\infty}^{\infty} \psi_\alpha^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi_\alpha dx}{\int_{-\infty}^{\infty} \psi_\alpha^* \psi_\alpha dx}$$

$$\int_{-\infty}^{\infty} \psi_\alpha^* \psi_\alpha dx$$

$$E_\psi(\alpha) = \frac{\hbar^2}{2m} \alpha + \frac{m\omega^2}{8\alpha}$$

The value of α_0 correspond to the lowest point of the curve and can be obtained



from the minimization of $E_\psi(\alpha)$ with respect to α i.e.

$$\frac{d}{d\alpha} E_{\Psi}(\alpha) \Big|_{\alpha=\alpha_0} = 0 \rightarrow \text{condition for minimum}$$

so

$$\frac{d}{d\alpha} E_{\Psi}(\alpha) = \frac{\hbar^2}{2m} - \frac{1}{8} m \omega^2 \frac{1}{\alpha^2}$$

Hence, the minimum is at $\alpha = \alpha_0$.

$$\frac{\hbar^2}{2m} - \frac{1}{8} m \omega^2 \frac{1}{\alpha_0^2} = 0$$

$$\text{or } \alpha_0 = \frac{m\omega}{2\hbar}$$

Hence the wave function of the ground state is

$$\Psi_{\alpha_0} = \Psi_0 = A e^{-m\omega x^2 / 2\hbar}$$

and the energy of the ground state is (from equ ①)

$$E_0 = \min. \left[\frac{\langle \Psi_{\alpha} | H | \Psi_{\alpha} \rangle}{\langle \Psi_{\alpha} | \Psi_{\alpha} \rangle} \right]$$

$$E_0 = \frac{\hbar^2}{2m} \alpha_0 + \frac{1}{8} m \omega^2 \frac{1}{\alpha_0}$$

$$E_0 = \frac{1}{2} \hbar \omega$$

— ground state
energy of
the Harmonic
oscillator.