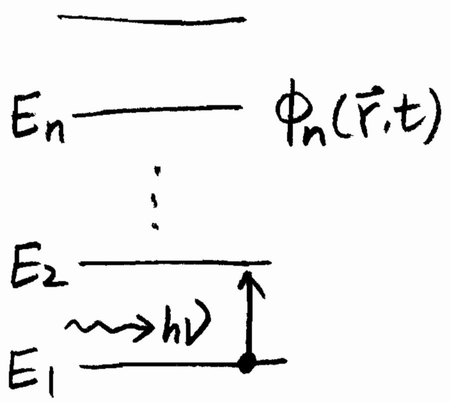
Time-dependent Perturbation

Consider a system



$$H_0 \phi_n(\vec{r},t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\phi_n(r,t)$$

$$\phi_n(\vec{r},t) = \phi_n(r)\, e^{-iE_n t/\hbar}$$

$\phi_n(\vec{r},t)$ are eigenstates

If the system is perturbed by a time-varying stimulus.

$$H = H_0 + H'(r,t)$$

$$H\psi(\vec{r},t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(\vec{r},t)$$

Assume a single frequency perturbation

$$H'(r,t) = \begin{cases} H'(r)\, e^{-i\omega t} + H'^{+} e^{i\omega t} & t \geq 0 \\ 0 & t < 0 \end{cases}$$

and $|H'| \ll |H|$

$\Rightarrow$ Solution of the new Schrodinger's Eq does not deviate too much from the unperturbed system.

$$\psi(\vec{r},t) = \sum_n a_n(t)\, \underbrace{\phi_n(\vec{r})\, e^{-iE_nt/\hbar}}$$

basis of unperturbed system

$\phi_n(\vec{r})$ form orthonormal set,

i.e. $\langle \phi_m(\vec{r}) | \phi_n(\vec{r}) \rangle = \langle m | n \rangle$

$$= \int \phi_m^*(\vec{r})\, \phi_n(\vec{r})\, d\vec{r} = \delta_{mn} = \begin{cases} 1 & m=n \\ 0 & m\neq n \end{cases}$$

$|a_n(t)|^2$ = Probability that the electron is in state n ($\phi_n(\vec{r})$) at time t.

Schrodinger Eq. becomes.

$$(\cancel{H_0} + H') \sum_n a_n(t)\, \phi_n(\vec{r})\, e^{-iE_nt/\hbar}$$

$$= -\frac{\hbar}{i}\left[\sum_n \frac{da_n(t)}{dt}\, \phi_n(\vec{r})\, e^{-iE_nt/\hbar} \right.$$

$$\left. + \cancel{\sum_n a_n(t)\, \phi_n(\vec{r}) \left(-\frac{iE_n}{\hbar}\right) e^{-iE_nt/\hbar}} \right]$$

$$\Rightarrow \sum_n \frac{da_n(t)}{dt}\, \phi_n(\vec{r})\, e^{-iE_nt/\hbar} = -\frac{i}{\hbar} \sum_n H'(\vec{r},t)\, a_n(t)\, \phi_n(\vec{r})\, e^{\frac{-iE_nt}{\hbar}}$$

$$\int \phi_m^*(\vec{r}) \left[\qquad \right] d\vec{r}$$

$$\Rightarrow \frac{da_m(t)}{dt}\, e^{-iE_mt/\hbar} = -\frac{i}{\hbar} \sum_n a_n(t)\, \overbrace{\int \phi_m^*(\vec{r})\, H'(\vec{r},t)\, \phi_n(\vec{r})\, d\vec{r}}^{H'_{mn}}\; e^{-iE_nt/\hbar}$$

$$\frac{d a_m(t)}{dt} = -\frac{i}{\hbar}\sum_n a_n(t)\cdot H'_{mn}(t)\cdot e^{i\omega_{mn}t}$$

$$\omega_{mn} = \frac{E_m - E_n}{t}$$

To track the order of perturbation

$$H = H_0 + \lambda H'(\vec{r},t)$$

$$a_n(t) = a_n^{(0)}(t) + \underbrace{\lambda\, a_n^{(1)}(t)}_{\text{First-order perturbation}} + \underbrace{\lambda^2 a_n^{(2)}(t)}_{\text{second-order 〃}}$$

$$\frac{d a_m^{(0)}(t)}{dt} = 0 \quad \Rightarrow \quad a_m^{(0)}(t) = \text{constant}$$

λ term $$\frac{d a_m^{(1)}(t)}{dt} = -\frac{i}{\hbar}\sum_n a_n^{(0)}(t)\cdot H'_{mn}(t)\cdot e^{i\omega_{mn}t}$$

λ^2 term: $$\frac{d a_m^{(2)}(t)}{dt} = -\frac{i}{\hbar}\sum_n a_n^{(1)}(t)\cdot H'_{mn}(t)\cdot e^{i\omega_{mn}t}$$

Assume the electron is at state i at $t=0$

$$a_i^{(0)}(t=0) = 1$$

$$a_m^{(0)}(t=0) = 0 \quad \text{for } m \neq i$$

Since $\frac{d a_m^{(0)}(t)}{dt} = 0 \Rightarrow$ $a_i^{(0)}(t) = 1$

$a_m^{(0)}(t) = 0 \quad m \neq i$

$$\frac{d}{dt} a_m^{(1)}(t) = \frac{-i}{\hbar} H'_{mi}(t)\, e^{i\omega_{mn} t}$$

Recall $\quad H'(r,t) = H'(r) e^{-i\omega t} + H'^{+} e^{i\omega t}$

$$\frac{d}{dt} a_m^{(1)}(t) = \frac{-i}{\hbar}\left(H'_{mi}\, e^{i(\omega_{mi}-\omega)t} + H'^{+}_{mi}\, e^{i(\omega_{mi}+\omega)t} \right)$$

For final state $f = m$

$$a_f^{(1)}(t) = \frac{-1}{\hbar}\left(H'_{fi}\, \frac{e^{i(\omega_{fi}-\omega)t} - 1}{\omega_{fi}-\omega} + H'^{+}_{fi}\, \frac{e^{i(\omega_{fi}+\omega)t} - 1}{\omega_{fi}+\omega} \right)$$

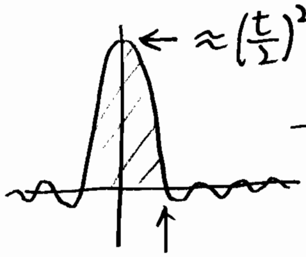
Usually we are interested in near resonance perturbations. i.e.,

$\omega \sim \omega_{fi}$ or $\omega \sim -\omega_{fi}$

$$|a_f^{(1)}(t)|^2 = \frac{4|H'_{fi}|^2}{\hbar^2} \frac{\sin^2\left(\frac{\omega_{fi}-\omega}{2} t\right)}{(\omega_{fi}-\omega)^2} + \frac{4|H'^{+}_{fi}|^2}{\hbar^2} \cdot \frac{\sin^2\left(\frac{\omega_{fi}+\omega}{2} t\right)}{(\omega_{fi}+\omega)^2}$$

t is large, $\quad \dfrac{\sin^2\left(\frac{t x}{2}\right)}{x^2} \longrightarrow \dfrac{\pi t}{2} \delta(x)$

Graphically:



$\longrightarrow \dfrac{\pi t}{2} \delta(x)$

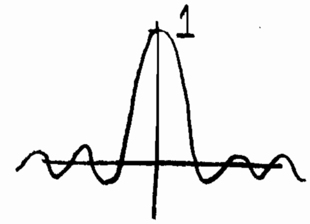
$\frac{t x_0}{2} = \pi \Rightarrow x_0 = \frac{2\pi}{t}$

Shape $\rightarrow$ δ function as $t \to \infty$

Area $\approx \left(\frac{t^2}{4}\right)\left(\frac{2\pi}{t}\right) = \frac{\pi t}{2}$

Mathematically

$$\mathrm{sinc}(x) = \frac{\sin x}{x}$$



$$\int_{-\infty}^{\infty} \mathrm{sinc}(x)\, dx = \pi$$

$$\int_{-\infty}^{\infty} \mathrm{sinc}^2(x)\, dx = \pi$$

$$\frac{\sin^2\left(\frac{t x}{2}\right)}{x^2} = \frac{\sin^2(x')}{x'^2} \cdot \frac{t^2}{4} = \mathrm{sinc}^2(x') \cdot \frac{t^2}{4}$$

$$\int_{-\infty}^{\infty} \frac{\sin^2\left(\frac{t x}{2}\right)}{x^2} dx = \int_{-\infty}^{\infty} \mathrm{sinc}^2(x') \frac{t^2}{4} \cdot \frac{1}{\left(\frac{t}{2}\right)} dx' = \frac{t}{2} \cdot \pi$$

$$|a_f^{(1)}(t)|^2 \simeq \frac{2\pi t}{\hbar^2}|H'_{fi}|^2\cdot\delta(\omega_{fi}-\omega) + \frac{2\pi t}{\hbar^2}|H'^{+}_{fi}|^2\cdot\delta(\omega_{fi}+\omega)$$

Transition rate:

$$W_{i\to f} = \frac{d}{dt}|a_f^{(1)}(t)|^2$$

$$= \frac{2\pi}{\hbar^2}|H'_{fi}|^2\cdot\delta(\omega_{fi}-\omega) + \frac{2\pi}{\hbar^2}|H'^{+}_{fi}|^2\cdot\delta(\omega_{fi}+\omega)$$

$$\delta(\omega_{fi}-\omega) = \delta\left(\frac{\hbar\omega_{fi}-\hbar\omega}{\hbar}\right) = \delta\left(\frac{E_f-E_i-\hbar\omega}{\hbar}\right)$$

$$= \hbar\,\delta(E_f-E_i-\hbar\omega)$$

Math Note:

$$\int \delta(x)\,dx = 1$$

$$\int \delta(ax)\,dx = \int \delta(y)\cdot\frac{1}{a}dy = \frac{1}{a}\int\delta(y)\,dy$$

$$y = ax \qquad\qquad = \frac{1}{a}\int\delta(x)\,dx$$

$$\delta(ax) = \frac{1}{a}\delta(x)$$

Fermi's golden rule:

$$W_{i\to f} = \underbrace{\frac{2\pi}{\hbar}|H'_{fi}|^2\cdot\delta(E_f-E_i-\hbar\omega)}_{} + \underbrace{\frac{2\pi}{\hbar}|H'^{+}_{fi}|^2\cdot\delta(E_f-E_i+\hbar\omega)}_{}$$

$\uparrow$

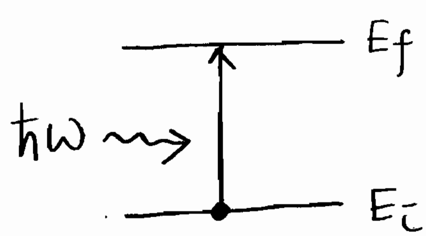
(unit: $\frac{1}{\text{sec}}$)

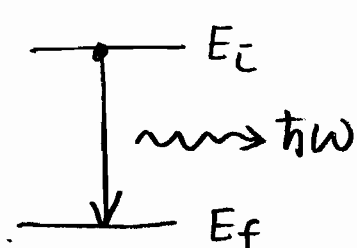
$E_f = E_i + \hbar\omega$

Absorption of a photon

$E_f = E_i - \hbar\omega$

Emission of a photon.





Interpretation:

* Conservation of energy
* Transition rate is determined by how strongly the initial and the final states are coupled.

$$\propto |H'_{fi}|^2 = \left| \int \phi_f^*(\vec{r})\, H'(\vec{r})\, \phi_i(\vec{r})\, d\vec{r} \right|^2$$

In the derivation, we have assumed a simple 2-level system. In case the final state is composed of several states with the same energy, the transition rate is proportional to the density of states of the final state:

$$W_{i\to f} = \frac{2\pi}{\hbar} |H'_{fi}|^2 \cdot \rho_f \cdot \delta(E_f - E_i - \hbar\omega) + \frac{2\pi}{\hbar} |H'^{+}_{fi}|^2 \rho_f\, \delta(E_f - E_i + \hbar\omega)$$