Application: Potential scattering of a spinless particle

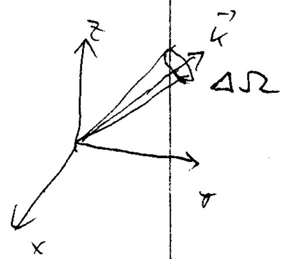
$$H_0 = \frac{|P|^2}{2m}, \qquad V = U(r) \text{ : some localized potential}$$

* Unperturbed eigenstates: free particle, plane wave
* To have proper normalization, place the system in a big box L^3 with periodic B.C. $\quad L >> \text{size of } U(r)$

  At the end of calculation, $L \to \infty$

* $$\langle r | \vec{k} \rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \qquad \langle \vec{k} | \vec{k}' \rangle = \delta_{k,k'}, \qquad E^{(0)} = \frac{\hbar^2 k^2}{2m}$$

  $$\vec{k} = \frac{2\pi}{L}\vec{n}, \qquad \vec{n} = (n_x, n_y, n_z) \qquad n_i : \text{integer}$$



denote $|\vec{k}_i\rangle$: incident plane wave, initial state

$|\vec{k}\rangle$: some final state

* The transition amplitude is:

$$\langle \vec{k} | U_I(t) | \vec{k}_i \rangle \simeq \delta_{k,k_i} - \frac{i}{\hbar}\int_0^t dt' \langle \vec{k} | e^{\frac{+iH_0t'}{\hbar}} U(r) e^{\frac{-iH_0t'}{\hbar}} | \vec{k}_i \rangle$$

$$= \delta_{k,k_i} - \frac{2i}{\hbar} e^{\frac{i\omega t}{2}} \left(\frac{\sin\frac{\omega t}{2}}{\omega} \right) \langle \vec{k} | U(r) | \vec{k}_i \rangle, \qquad \omega = \frac{E_k - E_i}{\hbar} = \frac{\hbar(\vec{k}^2 - \vec{k}_i^2)}{2m}$$

when $t >> 1$, the transition rate is...

$$W = \frac{2\pi}{\hbar} \sum_k \delta(E_k - E_i) \left| \langle \vec{k} | U(r) | \vec{k}_i \rangle \right|^2$$

$$\underbrace{\frac{dW}{d\Omega}}_{} \Delta\Omega = \sum_{k \in \Delta\Omega} \frac{2\pi}{\hbar} \delta(E_k - E_i) \left| \langle \vec{k} | U(r) | \vec{k}_i \rangle \right|^2$$

transition rate per unit solid angle

(in general a function of direction $\hat{n}_f$)

changing variable

$$\delta(E_k - E_i) = \frac{\delta(|\vec{k}| - |\vec{k}_i|)}{\left| \frac{\partial(E_k - E_i)}{\partial|\vec{k}|} \right|} = \frac{m}{\hbar^2 |\vec{k}|} \delta(|\vec{k}| - |\vec{k}_i|)$$

* physical ~~mean~~ limit : $V \to \infty$

but $\psi_{k_i}(r)$ loses meaning, $\rho \simeq \frac{1}{V} \to 0$, as does the $\frac{dW}{d\Omega}$

* However, the differential cross section is well defined.

$$\frac{d\sigma}{d\Omega} = \frac{\text{the differential transition rate } \frac{dW}{d\Omega} \sim \frac{1}{T}}{\text{incident flux } \sim \left(\frac{1}{L^3}\right)\cdot\left(\frac{L}{T}\right)} \sim L^2$$ is same as an area

$$J_{inc} = n_i v_i = \frac{1}{V}\left(\frac{\hbar|k_i|}{m}\right)$$

$$\Rightarrow \frac{d\sigma}{d\Omega}\Delta\Omega = \frac{Vm}{\hbar|k_i|}\sum_{k\in\Delta\Omega}\frac{2\pi}{\hbar}\frac{m}{\hbar^2|\vec{k}|}\,\delta(|\vec{k}|-|\vec{k}_i|)\,|\langle\vec{k}|U(r)|\vec{k}_i\rangle|^2$$

$\because$ $\vec{k} = \frac{2\pi}{L}\vec{n}$, $\quad d^3\vec{n} = \frac{V}{(2\pi)^3}d^3\vec{k}$

$$= \frac{Vm}{\hbar|\vec{k}_i|}\frac{V}{(2\pi)^3}\Delta\Omega\int k^2dk\,\frac{2\pi m}{\hbar^3|\vec{k}|}\,\delta(|\vec{k}|-|\vec{k}_i|)\,|\langle\vec{k}|U(r)|\vec{k}_i\rangle|^2$$

$$= \frac{V^2m^2\Delta\Omega}{(2\pi)^2\hbar^4|\vec{k}_i|}\int_0^\infty\frac{|\vec{k}|^2d|\vec{k}|}{|\vec{k}|}\,\delta(|\vec{k}|-|\vec{k}_i|)\,|\langle\vec{k}|U(r)|\vec{k}_i\rangle|^2$$

$$= \frac{V^2m^2}{(2\pi)^2\hbar^4}\Delta\Omega\,|\langle\vec{k}|U(r)|\vec{k}_i\rangle|^2 \quad \text{where } |\vec{k}| = |\vec{k}_i|$$

Also, $\langle\vec{k}|U(r)|\vec{k}_i\rangle = \int d^3r\,\psi^*_{k}(r)\,U(r)\,\psi_{k_i}(r) = \frac{1}{V}\int d^3r\,e^{-i(\vec{k}-\vec{k}_i)\cdot\vec{r}}\,U(r)$

$$= \frac{(2\pi)^{\frac{3}{2}}}{V}\hat{U}(\vec{k}-\vec{k}_i)$$

the Fourier transform $\hat{U}(q) \equiv \int\frac{d^3r}{(2\pi)^{\frac{3}{2}}}\,e^{-i\vec{q}\cdot\vec{r}}\,U(r)$

The factors of V and $\Delta\Omega$ have cancelled, and the δ-function picks $|\vec{k}| = |\vec{k}_i|$ (but may pointing to diff directions)

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{2\pi m^2}{\hbar^4}|\hat{U}(\vec{q})|^2,$$ q : the momentum transfer $\vec{q} = (\vec{k}-\vec{k}_i)$

This is the so called Born approximation.

eg $U(r) = A\frac{e^{-\lambda r}}{r}$, $\hat{U}(\vec{q}) = \frac{2A}{\sqrt{2\pi}}\frac{1}{\lambda^2+q^2}$, $q^2 = 4k_i^2\sin^2\frac{\theta}{2}$, $\frac{d\sigma}{d\Omega} = \frac{4A^2m^2}{\hbar^4}\frac{1}{(4k_i^2\sin^2\frac{\theta}{2}+\lambda^2)^2}$

two-state system

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}, \quad V(t) = \gamma \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}$$

assume $E_2 > E_1$ (to make H Hermitian)

$$\psi(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-\frac{iE_1 t}{\hbar}} c_1(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-\frac{iE_2 t}{\hbar}} c_2(t) = \begin{pmatrix} c_1 e^{-\frac{iE_1 t}{\hbar}} \\ c_2 e^{-\frac{iE_2 t}{\hbar}} \end{pmatrix}$$

Schrödinger eq

$$i\hbar \frac{\partial}{\partial t} \psi = H \psi$$

$$\Rightarrow \begin{pmatrix} i\hbar \dot{c}_1 e^{-\frac{iE_1 t}{\hbar}} \\ i\hbar \dot{c}_2 e^{-\frac{iE_2 t}{\hbar}} \end{pmatrix} = \begin{pmatrix} \gamma c_2 \, e^{\frac{-i}{\hbar}(E_2 - \hbar\omega)t} \\ \gamma c_1 \, e^{\frac{-i}{\hbar}(E_1 + \hbar\omega)t} \end{pmatrix}$$

differentiate both sides again

$$\Rightarrow \begin{pmatrix} i\hbar \ddot{c}_1 e^{\frac{-iE_1 t}{\hbar}} + E_1 \dot{c}_1 e^{\frac{-iE_1 t}{\hbar}} \\ i\hbar \ddot{c}_2 e^{\frac{-iE_2 t}{\hbar}} + E_2 \dot{c}_2 e^{\frac{-iE_2 t}{\hbar}} \end{pmatrix} = \begin{pmatrix} \gamma \dot{c}_2 e^{\frac{-i}{\hbar}(E_2 - \hbar\omega)t} + c_2 \gamma \left(\frac{-i}{\hbar}\right)(E_2 - \hbar\omega) e^{\frac{-i}{\hbar}(E_2 - \hbar\omega)t} \\ \gamma \dot{c}_1 e^{\frac{-i}{\hbar}(E_1 + \hbar\omega)t} + c_1 \gamma \left(\frac{-i}{\hbar}\right)(E_1 + \hbar\omega) e^{\frac{-i}{\hbar}(E_1 + \hbar\omega)t} \end{pmatrix}$$

$$= \begin{pmatrix} \left[\frac{\gamma^2}{i\hbar} c_1 + (E_2 - \hbar\omega)\dot{c}_1\right] e^{-\frac{iE_1 t}{\hbar}} \\ \left[\frac{\gamma^2}{i\hbar} c_2 + (E_1 + \hbar\omega)\dot{c}_2\right] e^{-\frac{iE_2 t}{\hbar}} \end{pmatrix}$$

or

$$(i\hbar)^2 \ddot{c}_1 + i\hbar(E_1 - E_2 + \hbar\omega)\dot{c}_1 - \gamma^2 c_1 = 0$$

$$(i\hbar)^2 \ddot{c}_2 + i\hbar(E_2 - E_1 - \hbar\omega)\dot{c}_2 - \gamma^2 c_2 = 0$$

denote $\hbar\omega_{21} \equiv E_2 - E_1$,

Assume the general solution $c_1 \sim e^{i\alpha t}$, $c_2 \sim e^{i\beta t}$

$$\Rightarrow \begin{cases} \alpha^2 + (\omega_{21} - \omega)\alpha - \frac{\gamma^2}{\hbar^2} = 0 \\ \beta^2 - (\omega_{21} - \omega)\beta - \frac{\gamma^2}{\hbar^2} = 0 \end{cases}$$

$$\alpha_\pm = \frac{1}{2}\left[\omega - \omega_{21} \pm \sqrt{(\omega_{21} - \omega)^2 + \frac{4\gamma^2}{\hbar^2}}\right], \quad c_1 = A_+ e^{i\alpha_+ t} + A_- e^{i\alpha_- t}$$

$$\beta_\pm = \frac{1}{2}\left[\omega_{21} - \omega \pm \sqrt{(\omega_{21} - \omega)^2 + \frac{4\gamma^2}{\hbar^2}}\right] \quad c_2 = B_+ e^{i\beta_+ t} + B_- e^{i\beta_- t}$$

Impose the B.C. that $C_1(0)=1, \quad C_2(0)=0$

$$\Rightarrow \quad A_+ + A_- = 1 \quad , \quad B_+ + B_- = 0$$

$$\begin{cases} C_1(t) = A e^{i\alpha_+ t} + (1-A) e^{i\alpha_- t} \\ C_2(t) = B e^{i\beta_+ t} + (-B) e^{i\beta_- t} \end{cases}$$

Using the 1st order D.E to determine A & B

$$(i\hbar)\left[i\alpha_+ A e^{i\alpha_+ t} + (i\alpha_-)(1-A) e^{i\alpha_- t} \right] = \gamma B \left[e^{i\alpha_+ t} - e^{i\alpha_- t} \right]$$

$$\Rightarrow \quad B = -\frac{\hbar}{\gamma} \alpha_+ A$$

$$-\hbar \alpha_- (1-A) = \hbar \alpha_+ A$$

We have $$A = \frac{\alpha_-}{\alpha_- - \alpha_+} = \frac{\omega - \omega_{21} - \sqrt{\quad ''}}{2\sqrt{(\omega_{21}-\omega)^2 + \frac{4\gamma^2}{\hbar^2}}}$$

$$(1-A) = \frac{-\alpha_+}{\alpha_- - \alpha_+} = \frac{-\omega + \omega_{21} - \sqrt{\quad ''}}{2\sqrt{\quad ''}}$$

$$B = \frac{\gamma}{\hbar \sqrt{\quad ''}}$$

Therefore

$$C_1(t) = e^{\frac{i(\omega-\omega_{21})}{2} t} \left[\frac{i(\omega-\omega_{21})}{\sqrt{\quad}} \sin \frac{\sqrt{\quad}}{2} t - \cos \frac{\sqrt{\quad}}{2} t \right]$$

$$C_2(t) = e^{\frac{i(\omega-\omega_{21})}{2} t} \left[\frac{2i\gamma}{\hbar} \right) \frac{\sin \frac{\sqrt{\quad}}{2} t}{\sqrt{\quad}}$$

The probability for the state 1 to evolve to state 2 is

$$P(1\to 2, t) = |C_2(t)|^2 = \frac{\frac{4\gamma^2}{\hbar^2}}{(\omega_{21}-\omega)^2 + \frac{4\gamma^2}{\hbar^2}} \sin^2\left(\frac{t}{2} \sqrt{(\omega_{21}-\omega)^2 + \frac{4\gamma^2}{\hbar^2}} \right) \quad , \quad |C_1(t)|^2 = 1 - |C_2|^2$$

This is the important eq (5.5.21a) in Sakurai, Rabi's formula

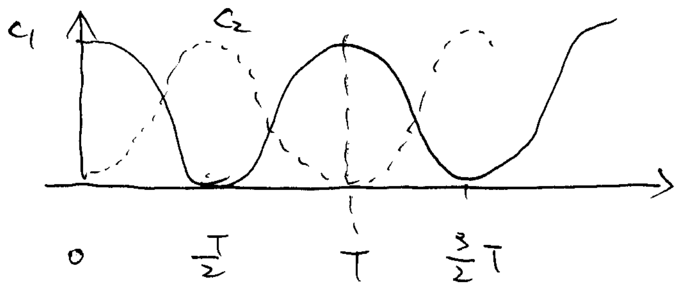
In many cases, the coupling γ is very small, therefore

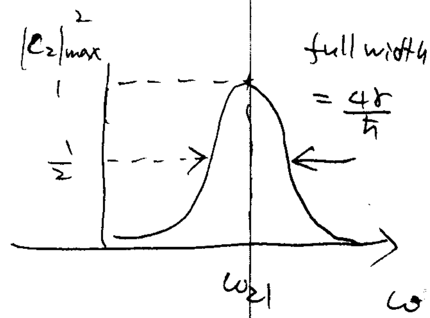
$$|C_2|^2 \leq \left(\frac{2\gamma}{(\omega_{21}-\omega)\hbar} \right)^2 << 1 ,$$ and the transition is negligible.

However, when $|\omega_{21} - \omega| \simeq \frac{\gamma}{\hbar}$, the prob is non-negligible.
In particular, it has a maximum when on resonance $\omega = \omega_{21}$, as $\hbar\omega = E_2 - E_1$

On the resonance, $\sqrt{\quad \text{"}} = \frac{2\gamma}{\hbar}$

$$\begin{cases} c_1(t) = -\cos\left(\frac{\gamma t}{\hbar}\right) \\ c_2(t) = i\sin\left(\frac{\gamma t}{\hbar}\right) \end{cases} \Rightarrow \begin{cases} |c_1(t)|^2 = \cos^2\left(\frac{\gamma}{\hbar}t\right) \\ |c_2(t)|^2 = \sin^2\left(\frac{\gamma}{\hbar}t\right) \end{cases} \qquad T = \frac{\pi\hbar}{\gamma}$$





Away from the resonance $\quad |c_2|^2_{max} < 1$

Note, smaller $\gamma \to$ narrower the resonance peak.

$\Rightarrow$ NMR, Maser, --

Say proton in strong B field, $\vec{B} = B_0\hat{z}$

$$H_0 = -g_p \frac{e}{2m_p c} \vec{S}_p \cdot \vec{B}, \quad \text{in the basis of } |S_z \pm\rangle$$

$$H_0 = 8.79\times10^{-8}\,\text{eV} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \left(\frac{B_0}{\text{Tesla}}\right)$$

The resonance frequency is

$$\nu = \frac{\omega_{21}}{2\pi} = \frac{E_2 - E_1}{2\pi\hbar} = 42.5\ \text{MHz} \left(\frac{B_0}{\text{Tesla}}\right)$$

in the radio range for $B_0 \sim O(T)$)

$\Rightarrow$ Apply a time varying $\vec{B}_x$, then

$$V = -g_p \frac{e}{2m_p c} (\vec{S}_p)_x B_x \cos\omega t$$

Typically $B_x \ll B_0 \to$ resonance is narrow

$$|S_z \pm\rangle = \frac{1}{\sqrt{2}}\left(|S_x+\rangle \pm |S_x-\rangle\right)$$

$$\langle S_z+|V|S_z-\rangle \propto \frac{1}{2}\left(\langle S_x+| + \langle S_x-|\right)\cdot\left(|S_x+\rangle - |S_x-\rangle\right) = 0$$

$$\langle S_z+|V|S_z-\rangle \propto \frac{1}{2}\left(\langle S_x+| + \langle S_x-|\right)\cdot\left(|S_x+\rangle + |S_x-\rangle\right) = 1$$