6. Unstable States

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Let's go back to Harmonic potential $V = M e^{\pm i\omega t}$

Assuming @ $t=0$ $|\psi\rangle = |i\rangle$, we derived

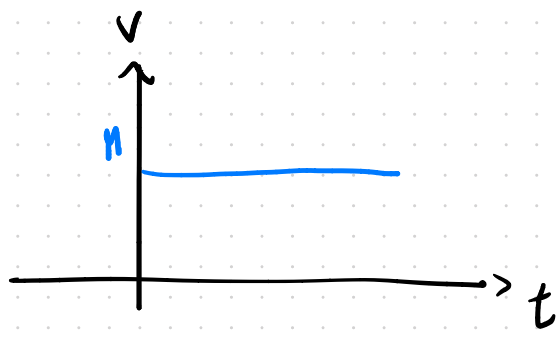
$$\Gamma_{i\to f} = \frac{|C_f^{(1)}(t)|^2}{t} = \frac{|\langle f|M|i\rangle|^2}{\hbar^2}\frac{1}{t}\left[\frac{\sin\left(\frac{\omega_{fi}\pm\omega}{2}t\right)}{\frac{\omega_{fi}\pm\omega}{2}}\right]^2$$

which in the $t\to\infty$ becomes F.G.R.

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}|\langle f|M|i\rangle|^2\,\delta(E_f - E_i \pm \hbar\omega)$$

Very same steps can be repeated for a CONSTANT POTENTIAL

$$V = \begin{cases} M & t \geq 0 \\ 0 & t < 0 \end{cases}$$



$\Rightarrow$ same result with

$\omega = 0$!

$$\frac{|c_f(t)|^2}{t} = \frac{4}{t} \underbrace{\frac{|\langle f|H|i\rangle|^2}{\hbar^2 \omega_{fi}^2}}_{\Downarrow} \left[\sin\left(\frac{\omega_{fi}}{2} t\right)\right]^2$$

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

$(E_f - E_i)^2$ simply

so before, when $t \to \infty$ F.G.R.

$$\Gamma_{i\to f} \sim \frac{2\pi}{\hbar} |\langle f|H|i\rangle|^2 \delta(E_f - E_i)$$

energy conservation

δ function might appear problematic

physically, we are usually interested in transitions to a "group" of final states with energy

$$E_f \simeq E_i \Rightarrow \sum_{f;\, E_f \sim E_i} |c_f(t)|^2 = ?$$

indeed, the Energy alone usually DOES NOT SPECIFY UNIQUELY THE STATE

For example:

$|i\rangle$ = some Atom in some excited state

$$|i\rangle \to |f\rangle + \gamma$$

lower state

photon

γ- momentum not fixed & we want to sum over all possibilities!

In general, we define a DENSITY OF STATES $\rho(E)$ such that $\rho(E)\,dE$ = # states with $(E, E+dE)$

So we write

$$\sum_f |C_f(t)|^2 \Longrightarrow \int_{E_f \sim E_i} dE_f\, \rho(E_f)\, |C_f^{(1)}(t)|^2$$

using our formula (stay with $V = M$ constant)

$$\Rightarrow 4 \int \sin^2\left(\frac{E_f - E_i}{2\hbar} t\right) \frac{|\langle f|M|i\rangle|^2}{|E_f - E_i|^2} \rho(E_f)\, dE_f$$

$$\xrightarrow{t \to \infty} \frac{2\pi}{\hbar} \int |\langle f|M|i\rangle|^2 \rho(E_f) \cdot t\, \delta(E_f - E_i)\, dE_f$$

such that we sometimes write for $\Gamma_{f \to i} = \frac{|c_f(t)|^2}{t}$

$$\Gamma_{f \to i} = \frac{2\pi}{\hbar} \overline{|\langle f|M|i\rangle|^2} \rho(E_i)$$

Also called FERMI GOLDEN RULE

see exercises!

pay attention here, in general for states with similar energy, if they are "close" in continuum, these $|\langle\ \rangle|^2$ are also similar $\Rightarrow$ CASE BY CASE

Before looking at explicit applications of the F.G.R, we will get back to the question

WHAT HAPPENS TO THE INITIAL STATE $|i\rangle$?

Clearly if $|c_f(t)|^2 \sim \Gamma \cdot t + \dots$

then by conservation of probability

$$|c_i(t)|^2 \sim 1 - \Gamma t + \dots$$

When $t \to \infty$ $\begin{cases} |c_f(t)|^2 > 1 \\ |c_i(t)|^2 < 0 \end{cases}$ $\Rightarrow$ <u>NON-SENSE</u> ?

Indeed it turns out that these first order results can be "resummed" and the right behaviour is

$$|c_i(t)|^2 \sim e^{-\Gamma t} \qquad |c_f(t)|^2 = 1 - e^{-\Gamma t}$$

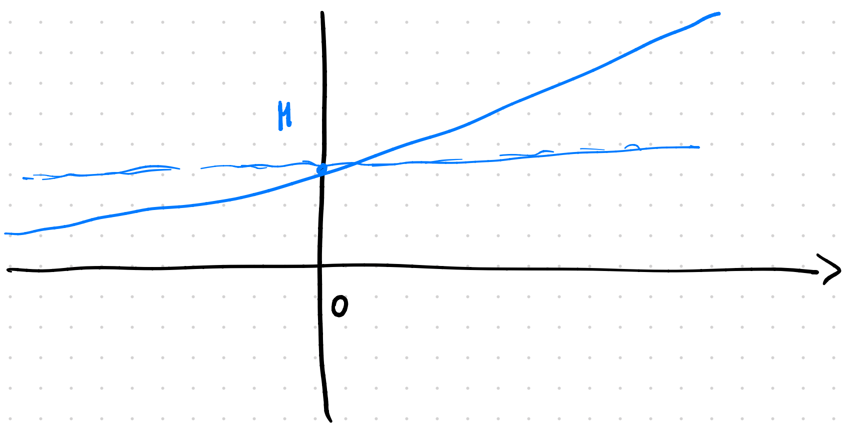
Exponential Decay

Let's see how this works in explicit case of constant potential.

By switching on potential at once, we have a DISCONTINUITY $\Rightarrow$ we try to work around this as follows: modify potential as

$$V_\eta = \begin{cases} 0 & @ \; t = -\infty \\ e^{\eta t} H & \forall t, \text{ with } \eta > 0, \; |\eta| \ll 1 \end{cases}$$

we use η as a "regulator" to turn potential on slowly at $t = -\infty$.



IMPORTANT: we start now @ $t = -\infty$, so we won't need to send $t \to \infty$ anymore!

at $t = -\infty$ assume system in $|i\rangle$

let us evaluate $c_f(t)$ & $c_i(t)$ in this framework

Same formulas give

$$c_f^{(0)}(t) = 0$$

$$c_f^{(1)}(t) = -\frac{i}{\hbar} \langle f|M|i\rangle \int_{-\infty}^{t} e^{\eta t'} e^{i\omega_{fi} t'} dt'$$

$t_0 = -\infty$ when $V \neq 0$

$$= -\frac{i}{\hbar} \langle f|M|i\rangle \frac{e^{\eta t + i\omega_{fi} t}}{\eta + i\omega_{fi}}$$

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

and therefore

$$|c_f^{(1)}(t)|^2 = \frac{1}{\hbar^2} |\langle f|M|i\rangle|^2 \frac{e^{2\eta t}}{\eta^2 + \omega_{fi}^2}$$

$\hookrightarrow$ again, any t is very FAR from $t = -\infty$

no $t \to \infty$ limit needed !

this is not $\propto t$, how do we compute $\Gamma_{i\to f}$?

$$\Gamma_{i\to f} = \frac{d}{dt}|c_f(t)|^2 = \frac{2\,|\langle f|H|i\rangle|^2}{\hbar^2}\;\frac{\eta e^{2\eta t}}{\eta^2+\omega_{fi}^2}$$

now notice $\lim\limits_{\eta\to 0} \dfrac{\eta}{\eta^2+\omega^2} = \pi\,\delta(\omega)$ another rep. of Dirac δ

so using $\omega_{fi} = \dfrac{E_f - E_i}{\hbar}$ we get :

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}|\langle f|H|i\rangle|^2\,\delta(E_f - E_i)$$

we recovered F.G.R.

so far so good ; now what about $c_i(t)$?

we will compute it up to SECOND ORDER

in perturbation theory !

• $c_i^{(0)}(t) = 1$ nothing happens

• $c_i^{(1)}(t) = -\frac{i}{\hbar}\langle i|M|i\rangle \int_{-\infty}^{t} e^{\eta t'} dt'$

$\omega_{ii} = \frac{E_i - E_i}{\hbar} = 0$!

$= -\frac{i}{\hbar\eta} e^{\eta t} \underbrace{\langle i|M|i\rangle}$

"energy shift" time indep

behaves badly when $\underline{\eta \to 0}$

up to this order

$$\frac{dc_i(t)}{dt} = -\frac{i}{\hbar}\frac{1}{\cancel{\eta}}\cancel{\eta} e^{\eta t}\langle i|M|i\rangle$$

$$\xrightarrow{\eta \to 0} -\frac{i}{\hbar}\langle i|M|i\rangle = -\frac{i}{\hbar} M_{ii}$$

to go one order higher, remember the general formula for $U_I(t,t_0)$ derived in previous lecture

$$U_I^{(2)}(t,t_0) = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, V_I(t') V_I(t'')$$

interaction picture!

and

@ $t = t_0$

$$C_f(t) = \langle f | U_I(t,t_0) | \psi_i \, t_0 \rangle_I$$

$= |i\rangle$

so in our case [$f = i$!]

$$c_i^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \, \langle i | V_I(t') V_I(t'') | i \rangle$$

insert $\sum_n |n\rangle\langle n| = \mathbb{1}$

$$= \left(-\frac{i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \sum_n \langle i | V(t') | n \rangle \langle n | V(t'') | i \rangle \cdot e^{i\omega_{in} t'} e^{i\omega_{ni} t''}$$

$$V(t) = M e^{\eta t} \quad \text{gives}$$

$$c_i^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \sum_n |M_{ni}|^2$$

$$\times \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \, e^{i\omega_{in}t' + \eta t'} \, e^{i\omega_{ni}t'' + \eta t''}$$

$$= \left(-\frac{i}{\hbar}\right)^2 \sum_n |M_{ni}|^2 \int_{-\infty}^{t} dt' \, e^{i\omega_{in}t' + \eta t'} \, \frac{e^{i\omega_{ni}t' + \eta t'}}{\eta + i\omega_{ni}}$$

$\omega_{ni} = -\omega_{in}$ so

$$= \left(-\frac{i}{\hbar}\right)^2 \sum_n |M_{ni}|^2 \int_{-\infty}^{t} dt' \, \frac{e^{2\eta t'}}{\eta + i\omega_{ni}}$$

$$= \left(-\frac{i}{\hbar}\right)^2 \sum_n |M_{ni}|^2 \, \frac{e^{2\eta t}}{2\eta(\eta + i\omega_{ni})}$$

now separate $n = i$ from the rest

$$= \left(-\frac{i}{\hbar}\right)^2 |M_{ii}|^2 \frac{e^{2\eta t}}{2\eta^2} +$$

$$+ \left(-\frac{i}{\hbar}\right)^2 \sum_{n\neq i} |M_{ni}|^2 \frac{e^{2\eta t}}{i 2\eta \left(\frac{E_n - E_i}{\hbar} - i\eta\right)}$$

$$= \left(-\frac{i}{\hbar}\right)^2 |M_{ii}|^2 \frac{e^{2\eta t}}{2\eta^2} +$$

$$+ \cancel{\left(-\frac{i}{\hbar}\right)^2 \left[\frac{1}{-\frac{i}{\hbar}}\right]} \sum_{n\neq i} |M_{ni}|^2 \frac{e^{2\eta t}}{2\eta \left(E_i - E_n + i\eta\hbar\right)}$$

$$= c_i^{(2)}(t)$$

Once more, compute $\Gamma_{i\to i} \sim \frac{dc_i(t)}{dt}$

$$\frac{dc_i(t)}{dt} = \frac{d}{dt}\left[1 - \frac{i}{\hbar\eta} M_{ii} e^{\eta t} + \left(-\frac{i}{\hbar}\right)^2 |M_{ii}|^2 \frac{e^{2\eta t}}{2\eta^2}\right.$$

$$\left. + \left(-\frac{i}{\hbar}\right) \sum_{n \neq i} |M_{ni}|^2 \frac{e^{2\eta t}}{2\eta (E_i - E_n + i\eta\hbar)}\right]$$

$$= -\frac{i}{\hbar} M_{ii} e^{\eta t} + \left(-\frac{i}{\hbar}\right)^2 |M_{ii}|^2 \frac{e^{2\eta t}}{\eta}$$

$$\underbrace{+ \left(-\frac{i}{\hbar}\right) \sum_{n \neq i} |M_{ni}|^2 \frac{e^{2\eta t}}{(E_i - E_n + i\eta\hbar)}}$$

now compute

$$\frac{1}{c_i(t)} \frac{dc_i(t)}{dt} = \frac{[\;\dots\;]}{1 - \frac{i}{\hbar} \frac{M_{ii}}{\eta} e^{\eta t}}$$

don't need II order here because numerator starts @ first order already !

Cross term cancels term with $\frac{1}{\eta}$ pole !

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$$\frac{1}{c_i(t)}\frac{dc_i(t)}{dt} \simeq -\frac{i}{\hbar} M_{ii}\, e^{\eta t} + \left(-\frac{i}{\hbar}\right)\sum_{n\neq i} |M_{ni}|^2 \frac{e^{2\eta t}}{(E_i - E_n + i\hbar\eta)}$$

take now limit $\eta \to 0$

keep η here since $E_i \sim E_n$ dangerous

$$\frac{1}{c_i(t)}\frac{dc_i(t)}{dt} = \underbrace{-\frac{i}{\hbar} M_{ii}}_{\text{imaginary}} + \left(-\frac{i}{\hbar}\right)\sum_{n\neq i} \underbrace{\frac{|M_{ni}|^2}{E_i - E_n + i\hbar\eta}}_{?}$$

$$\lim_{\varepsilon\to 0} \frac{1}{x \pm i\varepsilon} = PV\left(\frac{1}{x}\right) \mp i\pi\,\delta(x)$$

Principal Value

so we can write

$$\frac{1}{c_i(t)}\frac{d c_i(t)}{dt} = -\underbrace{\frac{i}{\hbar}}_{\text{extra } i}\Bigg[\overbrace{M_{ii} + PV\left(\sum_{n\neq i}\frac{|M_{ni}|^2}{E_i-E_n}\right)}^{\text{Real}} \underbrace{- i\pi\sum_{n\neq i}|M_{ni}|^2\,\delta(E_i-E_n)}_{\text{Imaginary}}\Bigg]$$

$$= -\frac{\Gamma_i}{2} - \frac{i}{\hbar}\Delta_i \quad \text{by defining:}$$

$$\Gamma_i = \frac{2\pi}{\hbar}\sum_{n\neq i}|M_{ni}|^2\,\delta(E_i-E_n)$$

$$\Delta_i = M_{ii} + PV\left(\sum_{n\neq i}\frac{|M_{ni}|^2}{E_i-E_n}\right)$$

notice $\Gamma_i = \sum_{n\neq i}\Gamma_{i\to n}$ sum of transition RATES from

FERMI GOLDEN RULE

notice that r.h.s of differential equation is time independent up to second order in pert. theory!

$$\dot{c}_i(t) = \left[-\frac{\Gamma_i}{2} - \frac{i}{\hbar} \Delta_i \right] c_i(t)$$

$$\Rightarrow \quad c_i(t) = c_{i0} \cdot e^{-\frac{\Gamma_i t}{2} - \frac{i}{\hbar}\Delta_i t}$$

Let's interpret Δ_i & Γ_i :

1] remember

$$|\psi_i, t\rangle_S = \sum_n c_n(t) e^{-i E_n t/\hbar} |n\rangle$$

$$|\psi_i, t\rangle_I = \sum_n c_n(t) |n\rangle$$

so if we start from state $|i\rangle$ and look at its evolution we have in Schrödinger Picture

$$|i\rangle \longrightarrow c_i(t)\, e^{-iE_i t/\hbar} \; |i\rangle$$

$$\sim e^{-\frac{\Gamma_i t}{2} - i[E_i + \Delta_i] t/\hbar} \; |i\rangle$$

Δ_i gives the ENERGY SHIFT of the level $|i\rangle$

2] If we look at probability $|c_i(t)|^2$

$$|c_i(t)|^2 = |c_{i0}|^2 \, e^{-\Gamma_i t}$$

consistent with FERMI GOLDEN RULE !

Γ_i gives the DECAY RATE of state $|i\rangle \rightarrow \sum_{n \neq i} |n\rangle$

one often introduces also the mean lifetime

$$\tau_i = \frac{1}{\Gamma_i}$$

so we write also $|c_i|^2 \sim e^{-t/\tau_i}$

Let's go back to Γ_i $\Rightarrow$ called <u>DECAY WIDTH</u>

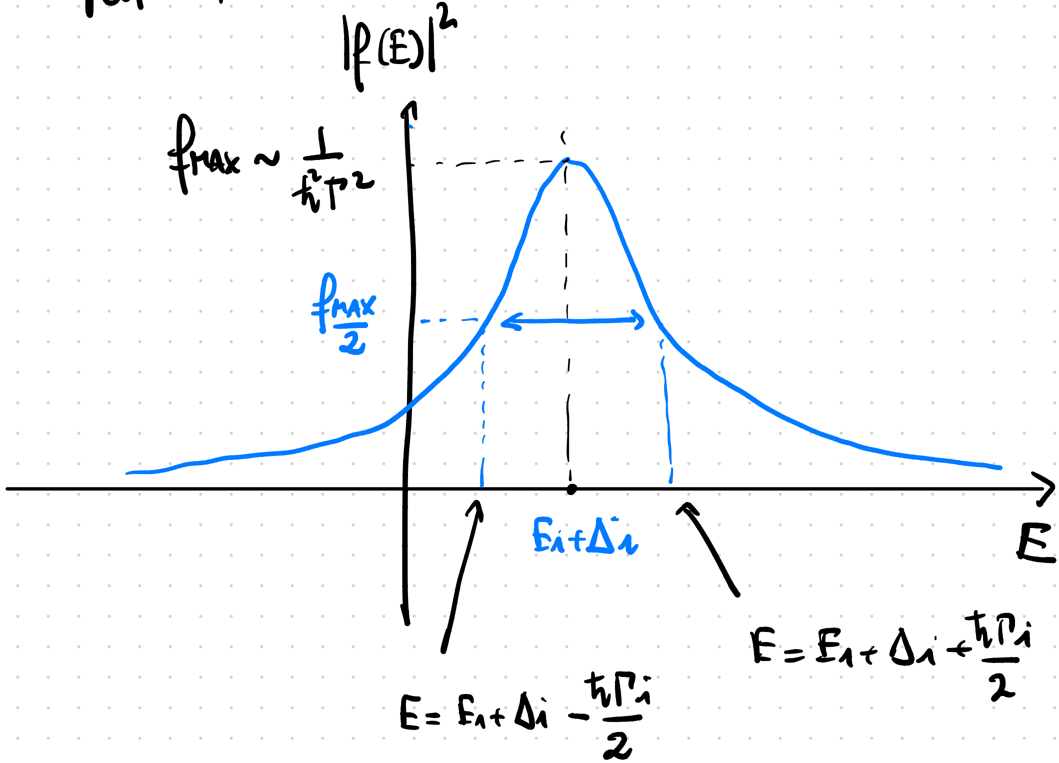
to see why, go from t to E (Fourier transf.)

$$f(E) \propto \int_0^{+\infty} dt' \, e^{-i(E_i+\Delta_i)t'/\hbar - \frac{\Gamma_i t'}{2}} \, e^{iEt'/\hbar}$$

$$= \frac{i\hbar}{E-(E_i+\Delta_i)+i\hbar\Gamma_i/2}$$

$$\Rightarrow |f(E)|^2 \propto \frac{1}{[E-(E_i+\Delta_i)]^2+\hbar^2\Gamma_i^2/4}$$

let's plot it



Γ_i gives the width of the probability distribution at half-maximum!