Resonances

We used the growth of c_n^1(t) to derive Fermi's Golden Rule, telling us how the state $|i\rangle$ decays with time; it decayed with a rate

$$\Gamma = \frac{2\pi}{\hbar} \sum_{m \neq i} |V_{mi}|^2 \, \delta(E_m - E_i)$$

What happens to c_i(t)? Is probability conserved? Today we'll see that the state $|i\rangle$ can be described as an eigenstate with a complex energy...

By equating $d|\alpha\rangle/dt = (1/i\hbar)[\mathcal{H}_0 + V(t)]\,|\alpha\rangle$, we saw

$$\varepsilon \frac{dc_n^{(1)}}{dt} + \varepsilon^2 \frac{dc_n^{(2)}}{dt} = -\frac{i}{\hbar} \sum_m \left[\varepsilon c_m^{(0)} + \varepsilon^2 c_m^{(1)}(t)\right] V_{nm} e^{i\omega_{nm} t}$$

where $\omega_{nm} = (E_n - E_m)/\hbar$.

Q: If $|\alpha\rangle = |i\rangle$ at $t=0$, what is $\frac{dc_i^{(1)}}{dt}$?

A: $dc_i^{(1)}/dt = -i/\hbar \; V_{ii}(t)$

To get the Golden Rule, we took $V(t) = Ve^{\eta t}$, then $\eta \to 0$.
So $dc_i^{(1)}/dt = -i/\hbar \; V_{ii}$.

Q: What does this mean physically about $|i\rangle$?

A: $c_i(t) \sim e^{i/\hbar V_{ii} t}$ corresponds to an energy shift for $|i\rangle$: $E_i \to E_i - V_{ii}$ (as expected from 1st order perturbation theory)

We need to look at $c_i^{(2)}$ to see decays...

Q: What is $dc_i^{(2)}/dt$, in terms of $c_m^{(1)}(t)$?

A: $dc_i^{(2)}/dt = -i/\hbar \sum_m c_m^{(1)}(t) \, V_{nm}(t) \, e^{i\omega_{nm} t}$, by equating ε^2 terms

We solved for $c_m^{(1)}(t)$ before: $c_m^{(1)}(t) = -\frac{i}{\hbar}\int^t e^{i\omega_{mi}t'} V_{mi}(t')\,dt'$

Q: If $V(t) = V e^{\eta t}$, what is $dc_i^{(2)}/dt$?

A: $c_m^{(1)}(t) = -i/\hbar \int^t e^{i\omega_{mi}t'} e^{\eta t'} V_{mi}\,dt'$

$$= -i/\hbar\, V_{mi} \frac{e^{\eta t + i\omega_{mi}t}}{\eta + i\omega_{mi}}$$

$$dc_i^{(2)}/dt = -i/\hbar \sum_m c_m^{(1)}(t)\, V_{im} e^{\eta t} e^{i\omega_{im}t}$$

$V_{im} = V_{mi}^*$, $\omega_{im} = -\omega_{mi}$

$$= -i/\hbar \sum_m \left(-i/\hbar\, V_{mi} \frac{e^{\eta t + i\omega_{mi}t}}{\eta + i\omega_{mi}}\right) V_{im} e^{\eta t + \omega_{im}t}$$

$$= (-i/\hbar)^2 \sum_m |V_{mi}|^2 \frac{e^{2\eta t}}{\eta + i\omega_{mi}}$$

Hence, we integrate to find

$$c_i^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{mi}|^2 \frac{1}{2\eta} \frac{e^{2\eta t}}{\eta + i\omega_{mi}}$$

(Separate $m = i$)

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

$\left(\eta + i\omega_{mi} = \frac{-i}{\hbar}(E_m - E_i + i\hbar\eta)\right)$

$$+ \left(\frac{-i}{\hbar}\right) \sum_{m \neq i} \frac{|V_{mi}|^2 e^{2\eta t}}{2\eta(E_i - E_m + i\hbar\eta)}$$

So, to second order, we have

$$c_i(t) = 1 - \frac{i}{\hbar\eta} V_{ii} e^{\eta t} + \left(\frac{-i}{\hbar}\right)^2 |V_{ii}| \frac{e^{2\eta t}}{2\eta^2} + \left(\frac{-i}{\hbar}\right) \sum_{m \neq i} \frac{|V_{mi}|^2 e^{2\eta t}}{2\eta(E_i - E_m + i\hbar\eta)}$$

- The first three terms look like $e^{-\frac{i}{\hbar\eta} V_{ii} e^{\eta t}}$, to second order
- We want decay rate, $\dot{c}_i$, compared to (decaying) c.

Try $\dot{c}_i/c$, now taking $e^{\eta t} \to 1$ (since $\eta \to 0^+$):

$$\dot{c}_i = -\frac{i}{\hbar} V_{ii} + \left(\frac{-i}{\hbar}\right)^2 \frac{|V_{ii}|^2}{\eta} + \left(-\frac{i}{\hbar}\right) \sum_{m \neq i}^{\infty} \frac{|V_{mi}|^2}{E_i - E_m + i\hbar\eta}$$

$$c = 1 - \frac{i V_{ii}}{\hbar\eta} \qquad \frac{1}{c} \cong 1 + \frac{i V_{ii}}{\hbar\eta}$$

$$\dot{c}_i / c_i = -\frac{i}{\hbar} V_{ii} + \left(\frac{-i}{\hbar}\right) \sum_{m \neq i} \frac{|V_{mi}|^2}{(E_i - E_m + i\hbar\eta)} = \frac{-i}{\hbar} \Delta_i \quad \text{as } \eta \to 0^+$$

* Independent of time
* Ignores 'backscattering' into c_i from other states
* Effective change in energy eigenvalue $E_i \to E_i + \Delta_i$

$$\mathcal{U}(t)|i\rangle = c_i(t)\, e^{-\frac{i}{\hbar} E_i(t)} |i\rangle = e^{-\frac{i}{\hbar}(E_i + \Delta_i)t} |i\rangle$$

So, Δ_i = energy shift = $\Delta^{(1)} + \Delta^{(2)} + \ldots$

$\Delta^{(1)} = V_{ii}$ first order perturbation theory

$$\Delta^{(2)} = \sum_{m \neq i} \frac{|V_{mi}|^2}{E_i - E_m + i\hbar\eta}$$ <u>Complex</u>.

Q: What does this have to do with the decay rate

(Fermi's Golden Rule:

$$\Gamma = \frac{2\pi}{\hbar} \sum_{m \neq i} |V_{mi}|^2 \, \delta(E_m - E_i) \;)$$

A: $$\lim_{\varepsilon \to 0} \frac{1}{x + i\varepsilon} = \mathrm{Pr.} \frac{1}{x} - i\pi\delta(x)$$

$$\mathrm{Im}\, \Delta^{(2)} = -\pi \sum_{m \neq i} |V_{mi}|^2 \, \delta(E_m - E_i) = -\frac{\hbar}{2} \Gamma$$

Check: $$e^{-\frac{i}{\hbar}(E_i + \Delta_i)t} = \underbrace{e^{-\frac{i}{\hbar}(i\,\mathrm{Im}\,\Delta)t}}_{e^{+\Delta/\hbar\, t} = e^{-\Gamma/2\, t}} e^{-\frac{i}{\hbar}(E_i + \mathrm{Re}\,\Delta)t}$$ ✓

Remember!
Probability ~ $\langle\alpha|\alpha\rangle$
~ $e^{2\Delta/\hbar\, t}$, hence 2

Γ_i is called decay width, because light absorbed or emitted from the state $|i\rangle$ will be spread in frequency over a width $\Gamma_i/\hbar$.

Without derivation, motivate by Fourier transform

$$\left|\int_0^\infty e^{-\frac{i}{\hbar}(E_i+\mathrm{Re}(\Delta_i))t}\, e^{-\Gamma_i t/2\hbar}\, e^{i\omega t}\, dt\right|^2$$

$$=\left|\frac{1}{i(\omega-(E_i+\mathrm{Re}\,\Delta)/\hbar)+\Gamma_i/2\hbar}\right|^2$$

$$=\frac{1}{|\omega-E/\hbar|^2+\Gamma^2/4\hbar}$$

Q: What is the full width at half maximum of this curve?

A: When $|\omega-E/\hbar|=\Gamma/2\hbar$, the height is half max, so

$\Gamma/\hbar =$ FWHM.

* Decaying states are not energy eigenstates!
* They are resonances -- with complex energies including the decay rate as the imaginary part
* Above is 'physicist's derivation'
* More mathematical approach: analytic continuation, ...