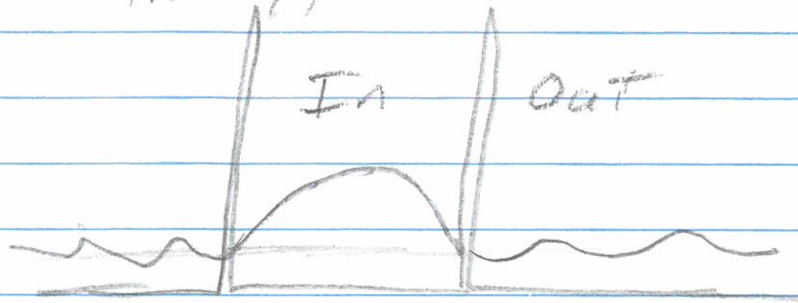
Resonances, Time Dependent Perturbation Theory, and Fermi's Golden Rule

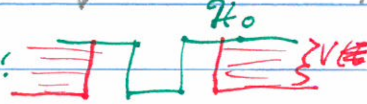


Double-δ model

α-decay

Lowers δ-function from ∞.

$\mathcal{H} = \mathcal{H}_{square\ well} + V$ $\quad |n\rangle$ unperturbed basis

(Sensible example: 

$\mathcal{H}_{square\ well}|n\rangle = E_n|n\rangle$

$|0\rangle = \sqrt{\frac{2}{L}}\sin \pi x/L \qquad E_0 = \frac{\hbar^2\pi^2}{2mL^2}$

Adding V (lowering barrier) turns bound states like $|0\rangle$ into <u>resonances</u>,

energy $E_0' + i\Gamma$ $\Big\}$ You calculated actual eigenstates, ~~e~~

Actual eigenstates: ~~mix pts~~ plane waves mix with $|0\rangle$ only in range Γ of energies

How to get $E_0' + i\Gamma$ more formally?

(Not today, but can compute decay rate Γ!)

Strategy:

(1) Turn on V slowly, and multiply by ε (later $\varepsilon = 1$)

$$\mathcal{H} = \mathcal{H}_0 + \varepsilon \overbrace{e^{\eta t} V}^{\text{generally } V(t)}$$

$V(t)$ couples $|0_{in}\rangle$ to plane waves $|k_{out}\rangle$
energy $E_k = \frac{\hbar^2 k^2}{2m}$

(2) Time evolve initial state $|0\rangle$

$$|\alpha(t)\rangle = \mathcal{U}(t)|0\rangle = c_0(t)\, \overbrace{e^{-iE_0 t/\hbar}}^{\text{boring } \mathcal{H}_0 \text{ dependence}} |0_{in}\rangle + \sum_k c_k(t) \underbrace{e^{-iE_k t/\hbar}}_{\text{Interaction } \cancel{\text{Representation}} \text{ Picture}} |k_{out}\rangle$$

(like Heisenberg picture, but $\mathcal{H}_0$ only)

(3) Expand $c_0(t)$, $c_k(t)$ in formal power series in ε

$$c_0(t) = 1 + \varepsilon c_0^{(1)}(t) + \varepsilon^2 c_0^{(2)}(t) + \dots$$

$$c_k(t) = \varepsilon c_k^{(1)}(t) + \dots$$

- $\varepsilon = 0 \Rightarrow \frac{dc_0}{dt} = \frac{dc_k}{dt} = 0$. interaction picture.
-

Equate $\frac{d}{dt}$(series) to Schrödinger

$$\frac{d|\alpha\rangle}{dt} = \frac{1}{i\hbar}(\mathcal{H}_0+V)|\alpha\rangle$$

$$\frac{d|\alpha\rangle}{dt} = \left(\varepsilon\frac{dc_0^{(1)}}{dt} + \varepsilon^2\frac{dc_0^{(2)}}{dt}\right)e^{-iE_0t/\hbar}|0\rangle$$

$$+\underbrace{\cancel{c_0(t)\left(\frac{-iE_0}{\hbar}\right)e^{-iE_0t/\hbar}|0\rangle}}_{\frac{1}{i\hbar}\mathcal{H}_0|\alpha\rangle}$$

$$+\varepsilon\sum_k\frac{dc_k^{(1)}}{dt}e^{-iE_kt/\hbar}|k\rangle$$

$$\underbrace{\cancel{\sum_k c_k(t)\,e^{-iE_kt/\hbar}|0\rangle}}_{\frac{1}{i\hbar}\mathcal{H}_0|\alpha\rangle}$$

$$= \frac{1}{i\hbar}(\underbrace{\mathcal{H}_0}_{\text{interaction}}+\varepsilon V)\underbrace{|\alpha\rangle}_{\text{expand}}$$

$$= \cancel{\frac{1}{i\hbar}\mathcal{H}_0|\alpha\rangle} + \frac{\varepsilon V}{i\hbar}\Big[\big(1+\varepsilon c_0^{(1)}(t)+\cancel{\varepsilon^2 c_0(t)}\big)e^{-iE_0t/\hbar}|0\rangle$$

$$+\sum_k \varepsilon c_0^{(1)}(t)\,e^{-iE_kt/\hbar}|k\rangle\Big]$$

$\cancel{\sum c_0 e^{-iE_0t/\hbar}}$ $O(\varepsilon^3)$

Multiply by $\langle k| e^{iE_k t/\hbar}$, find decay rate into state $|k\rangle$

$$\varepsilon \frac{dc_k^{(1)}}{dt} = \langle k| e^{iE_k t/\hbar}\left(\frac{\varepsilon V}{i\hbar} + O(\varepsilon^2)\right) e^{-iE_0 t/\hbar}|0\rangle$$

$$= \frac{\varepsilon}{i\hbar}\, e^{\overbrace{i(E_k - E_0)t/\hbar}^{\omega_{k0} t}} \underbrace{\langle k|V|0\rangle}_{V_{k0}}$$

$$\frac{dc_k^{(1)}}{dt} = \frac{1}{i\hbar} e^{i\omega_{k0} t} \underbrace{V_{k0}(t)}_{V(t)e^{\eta t}}$$

turn on potential

$$= \frac{1}{i\hbar} e^{(\eta + i\omega_{k0})t} V_{k0}$$

$$c_k(t) = \frac{1}{i\hbar} V_{k0} \frac{e^{(\eta + i\omega_{k0})t}}{\eta + i\omega_{k0}}$$

$$|c_k(t)|^2 = \frac{|V_{k0}|^2}{\hbar^2} \frac{e^{2\eta t}}{\eta^2 + \omega_{k0}^2}$$

$$\frac{d|c_k(t)|^2}{dt} = \frac{2|V_{k0}|^2}{\hbar^2} \frac{\eta}{\eta^2 + \omega_{ki}^2} e^{2\eta t}$$

Total decay rate at $t=0$ $(e^{2\eta t}=1)$

$$\frac{d}{dt}|c_0|^2 = -\int \frac{d}{dt}|c_k|^2 dk$$

$$= -\int \frac{2|V_{k0}|^2}{\hbar^2} \underbrace{\frac{\eta}{\eta^2+\omega_{ki}^2}} dk$$

Take $\eta \to 0$ (turn on slowly)

$$\lim_{\eta \to 0} \frac{\eta}{\eta^2+\omega_{ki}^2} = \pi\,\delta(\omega_{ki}) = \hbar\,\delta(E_k - E_i)$$

$$\frac{d|c_0|^2}{dt} = \frac{2\pi}{\hbar}|V_{k0}|^2\,\delta(E_k - E_0)$$

Fermi's Golden Rule

Time Dependent Perturbations and Fermi's Golden Rule

Time-dependent perturbation on time-independent Hamiltonian

$\mathcal{H}(t) = \mathcal{H}_0 + V(t)$

* AC (classical) electromagnetic fields: absorption and stimulated emission
* Slowly varying fields: the adiabatic theorem and Berry's phase
* Rapidly varying fields: the sudden approximation

* Turning on interactions and watching the decay of excited states
  - Excited atom + coupling to electromagnetic waves = decay rate via photon emission
  - Uranium nucleus + transmission through Coulomb barrier = alpha-decay rate
  - Electron on quantum dot + hopping to lead = metastable state
  - Electron-hole excitation of noninteracting electron gas + e-e interactions = Quasiparticle lifetimes

[No actual time dependence! Need to start without interactions: will use formal trick

V(t) = lim_eta->0 V exp(eta t)]

Imaginary Energies

$|E(t)\rangle = e^{-\frac{i}{\hbar}Et}$

Decay $P(t) \sim e^{-\Gamma t}$

Q: Guess what to add to E to make decay?

Q2: If $E = E_0 \mp i\Delta$, what is Γ in terms of Δ?

$$\mathcal{H} = \mathcal{H}_0 + \underset{\sim}{\overset{\text{Perturb in } V}{\varepsilon}} V(t)$$

$V(t)$ general fct x, p, t

$\mathcal{H}_0 |n\rangle = E_n |n\rangle$ Work in unperturbed basis of $\mathcal{H}_0$

General initial state

$$|\alpha\rangle = \sum c_n(0)\,|n\rangle$$

$$\mathcal{U}(t)|\alpha\rangle = \sum \underbrace{c_n(t)}_{\text{New Occupation Amplitudes}} \overbrace{e^{-iE_n t/\hbar}}^{\text{Boring } \mathcal{H}_0 \text{ dependence}} |n\rangle$$

<u>Transitions.</u>

Expand $c_n(t)$ in formal power series in ε

Q: What is $c_n^{(0)}(t)$, $c_n(t)$ for $\varepsilon = 0$?

A: Since $\mathcal{U}_0(t)|n\rangle = e^{-i\mathcal{H}t/\hbar}|n\rangle$, $c_n^{(0)}$ is constant

$$c_n(t) = c_n^{(0)} + \varepsilon c_n^{(1)}(t) + \varepsilon^2 c_n^{(2)}(t)$$

Schrödinger's Eqn $i\hbar \frac{d|\alpha\rangle}{dt} = (\mathcal{H}_0 + V(t))\,|\alpha\rangle$

$\rightarrow$ Equations for $c_n^{(1)}, c_n^{(2)}, \dots$

$$\frac{d|\alpha\rangle}{dt} = \sum_n \left(\frac{dc_n^{(0)}}{dt} + \varepsilon \frac{dc_n^{(1)}}{dt} + \varepsilon^2 \frac{dc_n^{(2)}}{dt} \right) e^{-iE_n t/\hbar} \overbrace{|n\rangle}^{\text{Fixed in time}}$$

$$\cancel{+ \left(c_n^{(0)} + \varepsilon c_n^{(1)} + \varepsilon^2 c_n^{(2)}\right) \left(\frac{-iE_n}{\hbar}\right) e^{-iE_n t/\hbar} |n\rangle}$$

$$= \frac{1}{i\hbar} (\mathcal{H}_0 + \varepsilon V)\,|\alpha(t)\rangle \quad e^{iE_n t/\hbar}$$

$$= \sum_i \left(c_i^{(0)} + \varepsilon c_i^{(1)} + \varepsilon^2 c_i^{(2)}\right) \left(-\frac{i}{\hbar}\right)\left(\overset{E_n}{\cancel{\mathcal{H}_0}} + \varepsilon V\right) e^{-iE_i t/\hbar} |i\rangle$$

Q: What equation does $\varepsilon = 0$ give?

A: $\frac{dc_n^{(0)}}{dt} e^{-iE_n t/\hbar} |n\rangle = 0 \quad \Rightarrow \frac{dc_n^{(0)}}{dt} = 0$

Take both sides times $\langle n| e^{iE_n t/\hbar}$:

$$\varepsilon \frac{dc_n^{(1)}}{dt} + \varepsilon^2 \frac{dc_n^{(2)}}{dt} = -\frac{i}{\hbar} \sum_i \left[\varepsilon c_i^{(0)} + \varepsilon^2 c_i^{(1)}(t)\right] \underbrace{\langle n| e^{+iE_n t/\hbar} V e^{-iE_i t/\hbar} |i\rangle}_{V_{ni}\, e^{i(E_n - E_i)t/\hbar}}$$

$\omega_{ni} = (E_n - E_i)/\hbar$ = Frequency difference $\quad = V_{ni}\, e^{i\omega_{ni} t}$

$$e^{i\mathcal{H}_0 t/\hbar}\, V\, e^{-i\mathcal{H}_0 t/\hbar} = V_I$$: Interaction Picture

(Like Heisenburg representation
Useful in field theory)

Q: What is $\frac{dc^{(1)}}{dt}$?

A: $\frac{dc^{(1)}}{dt} = \left(-\frac{i}{\hbar}\right) \sum_n V_{ni}\, e^{i\omega_{ni} t}\, c_i^{(0)}$

Q: If at $t=0$, $|\alpha\rangle = |i\rangle$ (so $c_n^{(0)} = \delta_{ni}$), what is $c_1(t)$?

A: $c^{(1)}(t) = -\frac{i}{\hbar} \int^t e^{i\omega_{ni} t'}\, V_{ni}(t')\, dt'$

Now consider $V(t) = e^{\eta t} V$, gradually turning on potentual, as $\eta \to 0$. For $n \neq i$,

$$c_n^{(1)}(t) = -\frac{i}{\hbar} V_{ni} \int^t e^{\eta t'} e^{i\omega_{ni} t'} dt' = -\frac{i}{\hbar} V_{ni} \frac{e^{\eta t + i\omega_{ni} t}}{\eta + i\omega_{ni}}$$

$c_n^{(1)}(t)$ is amplitude for decay into state n after time t

Q: What is the decay rate, $\frac{d|c_n^{(1)}(t)|^2}{dt}$?

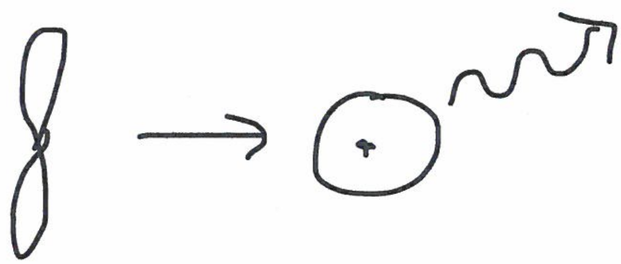
A: $|c_n(t)|^2 = \frac{|V_{ni}|^2}{\hbar^2} \frac{e^{2\eta t}}{\eta^2 + \omega_{ni}^2} \Rightarrow \frac{d|c_n(t)|^2}{dt} = \frac{2|V_{ni}|^2}{\hbar^2} \frac{\eta}{\eta^2 + \omega_{ni}^2} e^{2\eta t}$

But as $\eta \to 0$, this vanishes unless $\omega_{ni} = 0$?

(Energy conservation. Adiabatic theorem.)

If $\omega_{ni} = 0$, degenerate perturbation...

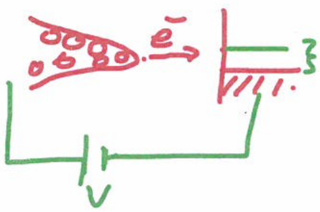
But, what if there are a continuum of final states?



Continuum of final photon energies

H 2p state $\to$ 1s + photon

STM e^- tunnel into metal



$$\frac{d|c_n(t)|^2}{dt} = \lim_{\eta \to 0} \frac{|V_{ni}|^2}{\hbar^2} \frac{2\eta}{\eta^2 + \omega_{ni}^2} e^{2\eta t}$$

Q: What is $\lim_{\eta \to 0} \frac{\eta}{\eta^2+\omega^2}$? Where have you seen this?

A: Exercise 2.2; sharply peaked, integral = $\arctan \Big|_{-\infty}^{\infty} = \pi$,

$$\lim_{\eta \to 0} \frac{\eta}{\eta^2+\omega^2} = \pi\delta(\omega)$$

$\delta(\omega_{ni}) = \hbar\,\delta(E_n - E_i)$, so

$$\frac{d|c_n(t)|^2}{dt} \simeq \frac{2\pi}{\hbar} |V_{ni}|^2 \delta(E_n - E_i) \qquad \text{Fermi's Golden Rule}$$

Total decay rate, sum (integrate) over final states.

If V_{ni} varies smoothly over energy $V_{ni} = V_i(E_n)$

$$\frac{dP}{dt} = \frac{2\pi}{\hbar} |V_i(E_i)|^2 \underbrace{\int dn\, \delta(E_n - E_i)}_{\substack{\text{Density of} \\ \text{Final States} \\ \text{at } E_i}}$$

Resonances

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

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

$$= \sum_{n \neq i} \frac{d|c_n(t)|^2}{dt} =$$

What happens to c_i(t)? Is probability conserved? Today we'll see that the state |i > 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

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

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

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

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

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

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

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

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

$$dc_i^{(2)}/dt = -\frac{i}{\hbar}\sum_m c_m^{(1)}(t)\, V_{im} e^{\eta t} e^{i\omega_{im}t} \qquad V_{im} = V_{mi}^*,\ \omega_{im} = -\omega_{mi}$$
$$= -\frac{i}{\hbar}\sum_m \left(-\frac{i}{\hbar} V_{mi}\frac{e^{\eta t + i\omega_{mi}t}}{\eta + i\omega_{mi}}\right) V_{im} e^{\eta t + \omega_{im} t}$$
$$= \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{mi}|^2 \frac{e^{2\eta t}}{\eta + i\omega_{mi}}$$

Hence, we integrate to find

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

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 $\eta\to 0$):

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

$\ast\ast$ $$c_i = 1 - \frac{iV_{ii}}{\hbar\eta} \qquad \frac{1}{c_i} \cong 1 + \frac{iV_{ii}}{\hbar\eta}$$

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

$$\Delta_i = V_{ii} + \sum \frac{|V_{mi}|^2}{E_m - E_i + i\hbar\eta}$$

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

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

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

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

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

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

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

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

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

Γ_i is called decay <u>width</u>, 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

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

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

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

prepared atom at $t=0$

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, ...