# WEEK 5 – Metastable states

In some cases, we have systems that are in one (seemingly) stable state and then decay to a lower energy state by releasing energy.

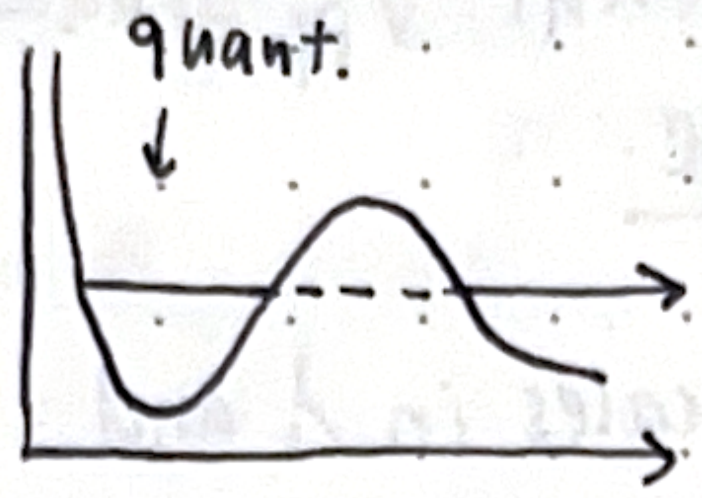
E.g.:

$$A^* \longrightarrow A + \gamma \qquad \text{(excited state} \rightarrow \text{lower state + photon)}$$

$$H_{(2p)} \longrightarrow H_{(2s)} + \gamma_{\hbar\omega} \qquad (n=2,\ \ell=1 \rightarrow \ell=0\text{, photon with energy } \hbar\omega)$$

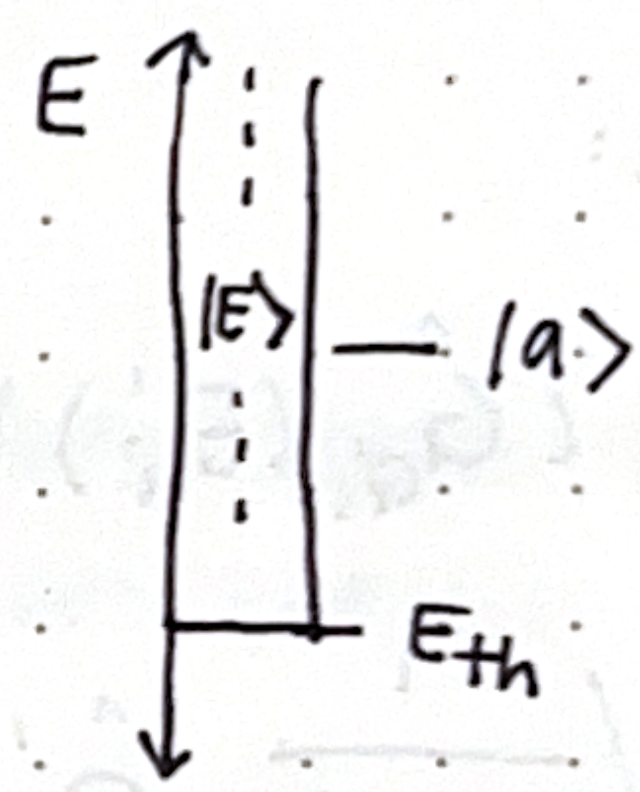
$$|e\rangle \otimes |0\rangle \rightarrow |g\rangle \otimes |1\rangle_\omega \qquad (|1\rangle_\omega = \text{photon with frequency } \omega.)$$

Visually:




a state that is bound slowly tunnels into the continuum until none is left in the bound state.

For some threshold energy $E_{th}$, we can say all possible energies must be greater. This could be the bound ground state energy, some horizontal asymptote for the continuum tail, etc.




Say we have bound state $|a\rangle$ with energy $E_a$. This $E_a$ must be greater than $E_{th}$.

Say we also have the following:

$$\hat{H}_0|E\rangle = E|E\rangle,\quad \hat{H}_0|a\rangle = E_a|a\rangle,\quad E_a > E_{th} \text{ and } E > E_{th}$$

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\langle E|E'\rangle = \delta(E-E') \text{ (continuum)} \quad \langle a|a\rangle = 1,\quad \langle a|E\rangle = 0$$

Evidently, there is some continuum state that also has energy $E_a$, thus $|a\rangle$ is degenerate with the continuum.

For this to be true, $\langle a|\hat{V}|a\rangle$ must clearly be $0$ – if it is not, you can redefine $\hat{H}_0$ so that it is.

We also assume $\langle E|\hat{V}|E'\rangle = 0$ but $V_{aE} : \langle a|\hat{V}|E\rangle \neq 0$, that is, the perturbation does not affect the continuum on its own.

Now, we know $|a\rangle$ escapes and can eventually be described purely as a superposition of continuum states. Thus, in the continuum, we can solve:

$\hat{H}|\psi_E\rangle = E|\psi_E\rangle$ where E is known, as it's in the continuum.

$|\psi_E\rangle$ can be written as linear combination $|a\rangle b_E + \int_{E_{th}}^{\infty} d\xi\, |\xi\rangle C_{\xi,E}$

as is always the case with the continuum, $\langle\psi_E|\psi_{E'}\rangle = N_E\, \delta(E-E')$ which is not normalizable. Thus we expect $C_{\xi,E}$ to <u>not</u> be square integrable. We instead solve for the eigen-functions using a system of equations:

$(E-\hat{H})|\psi_E\rangle = 0$ which means we have infinite system:

$$\begin{cases} \langle a|E-\hat{H}|\psi_E\rangle = 0 \\ \langle E'|E-\hat{H}|\psi_E\rangle = 0, \ \forall E' \end{cases}$$

and $|a\rangle$ ($|E'\rangle$ is an <u>un</u>perturbed eigenfunction)

Plugging in $\hat{H} = \hat{H}_0 + \hat{V}$:

$$\begin{cases} \langle a|(E-\hat{H}_0-\hat{V})\left\{|a\rangle b_E + \int d\xi\, |\xi\rangle C_{\xi E}\right\} = 0 \\ \langle E'|(E-\hat{H}_0-\hat{V})\left\{|a\rangle b_E + \int d\xi\, |\xi\rangle C_{\xi E}\right\} = 0 \end{cases}$$

We know only $\langle a|\hat{V}|E'\rangle$ or $\langle E'|\hat{V}|a\rangle$ are non-zero, $\langle a|\hat{v}|a\rangle$ and $\langle E'|\hat{V}|\xi\rangle$ are both 0. Any $\langle a|E'\rangle = 0$ also, so:

$$\begin{cases} \langle a|E-H_0|a\rangle b_E - 0 + 0 - \int d\xi\, \langle a|V|\xi\rangle C_{\xi E} = 0 \\ 0 - \langle E'|\hat{V}|a\rangle b_E + \int d\xi\, \langle E'|E-\hat{H}_0|\xi\rangle C_{\xi E} + 0 = 0 \end{cases}$$

which simplifies to:

$$\begin{cases} (E-E_a) b_E - \int d\xi\, V_{a\xi}\, C_{\xi E} = 0 \\ -V_{E'a}\, b_E + (E-E')\int d\xi\, \delta(E'-\xi)\, C_{\xi E} = 0 \end{cases}$$

because of the delta function, $\int d\xi\, \delta(E'-\xi) C_{\xi E} = C_{E'E}$ and our "second" equation becomes:

$$\underset{\substack{\uparrow \\ \text{given}}}{V_{E'a}}\, b_E = \underset{\substack{\uparrow \\ \text{param.}}}{(E}-\underset{\substack{\uparrow \\ \text{variable}}}{E'})\, C_{E'E}$$

and we want to know $C_{E'E}$.

Say for a moment we call $V_{E'a} b_E$ some function $g(x)$ and we call $(E-E')C_{E'E}$ some function $x f(x)$, where $C_{E'E} = f(x)$. (Note $f(x)$ does not have to be strictly a function, it could also be a distribution).

For $x \neq 0$, $f(x) = g(x)/x$

For all! $\hat{V} = 0$, $|\Psi_E\rangle = \int d\xi |\xi\rangle C_{\xi E} = \int d\xi |\xi\rangle \delta(\xi - E) = |E\rangle$ so free states must be solutions. There is no perturbation.

Thus $(E-E')C_{E'E} = 0$ must be one possible solution, meaning $C_{E'E} = \delta(E-E')$ is a solution.

In general, for homogenous equations, solution $f(x) = f_p(x) + N\delta(x)$ where $f_p(x)$ is a <u>particular solution</u>:

$$\begin{cases} 1/x & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$$

We want this ? to still leave $f_p(x)$ well defined under integration. It turns out that to find $f_p(x)$ we can do:

$$\lim_{\lambda \to 0^+} \int f_\lambda(x) dx = \lim_{\lambda \to 0^+} \int \frac{g(x)}{x + i\lambda} dx$$ which has general solution

$$\lim_{\lambda \to 0^+} \frac{g(x)}{x + i\lambda}$$ where we often write $\lim_{\lambda \to 0^+} \lambda$ simply as $0^+$, so

$$= \frac{g(x)}{x + i0^+}$$. Also note $\lim_{\lambda \to 0} \frac{1}{x + i\lambda} = \frac{P}{x} - i\pi\,\delta(x)$

↖ Principle part of $x$

Apply this to our original equation:
$(E-E')C_{E'E} = x f(x)$, so $x = E-E'$ and $f(x) = C_{E'E}$ and $V_{E'a} b_E = g(x)$

Thus $f(x) = f_p(x) + N\delta(x) = \frac{g(x)}{x + i0^+} + N\delta(x)$ becomes

$$C_{E'E} = \frac{V_{E'a} b_E}{(E-E') + i0^+} + N\delta(E-E')$$

Note that the delta function prevents us from getting the zero vector instead of an eigen function if $E = E'$ (??) and that if $N = 1$, then $\langle \Psi_E | \Psi_{E'} \rangle = \delta(E-E')$

Thus we have the solution to the second part of our system of equations. We can plug this in to the first part of the system:

$$(E-E_a)b_E - \int d\xi\, V_{a\xi}\, C_{\xi E} = 0$$

$$(E-E_a)\, b_E - \int d\xi\, V_{a\xi}\left[\frac{V_{\xi a} b_E}{(E-\xi)+i0^+} + \delta(E-\xi)\right] = 0$$

$$(E-E_a)b_E - b_E \int d\xi \frac{|V_{a\xi}|^2}{E-\xi+i0^+} - V_{aE} = 0$$

$$b_E\left(E-E_a - \int d\xi \frac{|V_{a\xi}|^2}{E-\xi+i0^+}\right) = V_{aE}$$

Now plug in $\frac{1}{x+i0^+} = \frac{P}{x} - i\pi\,\delta(x)$ to get

$$\Big(E-E_a + \underbrace{\int d\xi \frac{|V_{a\xi}|^2 P}{E-\xi}}_{\text{called } \Delta_a(E)\ \approx \Delta_a(E_a)} \underbrace{- i\pi\,|V_{aE}|^2}_{=\frac{i}{2}2\pi|V_{aE}|^2}\Big) b_E = V_{aE}$$

where $2\pi|V_{aE}|^2 = \Gamma_a(E)$

$\Gamma_a(E)$ is the so-called width of energy resonance.

We also say $\tilde{E}_a(E) = E_a + \Delta_a(E) - \frac{i}{2}\Gamma_a(E)$

$$= \bar{E}_a(E) - i\Gamma_a(E)/2$$

So $\tilde{E}_a$ is a <u>complex</u> energy.

We can also now say $b_E = \frac{V_{aE}}{E-\tilde{E}_a(E)}$ and

$$C_{E'E} = \frac{V_{E'a}}{E-E'+i0^+}\,\frac{V_{aE}}{E-\tilde{E}_a(E)} + \delta(E'-E)$$ from which we get the

final, exact solution:

$$|\Psi_E\rangle = |E\rangle + \left\{|a\rangle + \int d\xi\,|\xi\rangle \frac{V_{\xi a}}{E-\xi+i0^+}\right\}\frac{V_{aE}}{E-\tilde{E}_a(E)}$$

<u>Energy distribution of $|a\rangle$</u>:

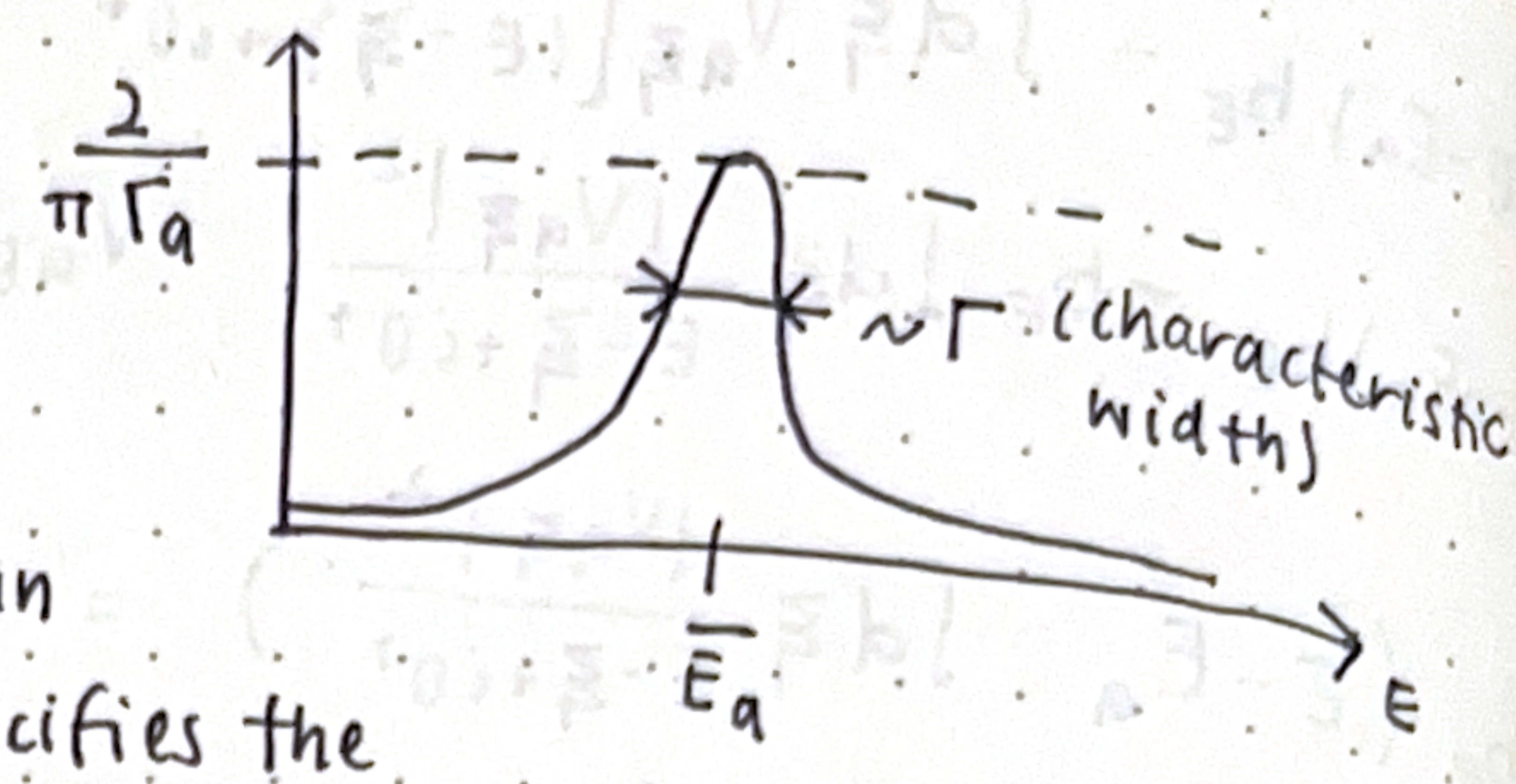
$|a\rangle = \int dE\, |\Psi_E\rangle\langle\Psi_E|a\rangle$ (or a superposition of continuum states.

$\langle a|\Psi_E\rangle$, or $b_E$ as we've been calling it, is $\frac{V_{aE}}{E-\tilde{E}_a(E)}$. The square mod

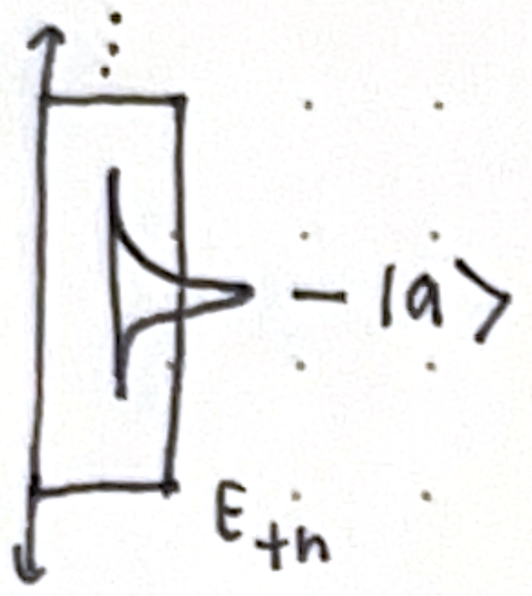
$$|\langle a|\Psi_E\rangle|^2 \text{ is : } \frac{|V_{aE}|^2}{(E-\tilde{E}_a)(E-\tilde{E}_a^*)} = \frac{|V_{aE}|^2}{(E-\bar{E}_a)^2+\Gamma_a^2/4}$$

$$= \frac{1}{\pi}\frac{\pi|V_{aE}|^2}{(E-\bar{E}_a)^2+\Gamma_a^2/4} = \frac{4}{\Gamma_a^2\pi}\frac{\Gamma_a/2}{\left(\frac{E-\bar{E}_a}{\Gamma_a/2}\right)+1}$$

$$= \frac{2}{\pi\Gamma_a}\frac{1}{\left(\frac{E-\bar{E}_a}{\Gamma_a/2}\right)^2+1}$$




which fits the form of a Lorentzian function (see graph), where $\Gamma$ specifies the width. We can also sort of say it looks like this :




where the initial state $|a\rangle$ is "diluted in the continuum", accross an energy range of the order $\Gamma_a$ (the resonance width) around central energy $\bar{E}_a = E_a + \Delta_a$

$\underset{\text{SHIFTED}}{\vee}$

Essentially, a metastable state looks bound but eventually falls apart/decays on its own. (He says to believe him when he says it's exponential decay).

He also does some off the cuff stuff about $\frac{1}{x+i0^+}$ but I won't do that here.