2.4: Fermi's Golden Rule

We have seen that the width of a resonance is determined by the imaginary part of the self-energy, $\mathrm{Im}[\Sigma]$. In this section, we will show that $\mathrm{Im}[\Sigma]$ has a physical meaning: it represents the **decay rate** of a quasi-bound state. Moreover, it can be approximated using a simple but important formula known as **Fermi's Golden Rule**.

Suppose we set the quantum state of a particle to a quasi-bound state $|\varphi\rangle$ at some initial time $t=0$. Since $|\varphi\rangle$ is not an exact eigenstate of the Hamiltonian, the particle will not remain in that state under time evolution. For $t>0$, its wavefunction should become less and less localized, which can be interpreted as the escape of the particle to infinity or the "decay" of the quasi-bound state into the free state continuum.

The decay process can be described by

$$P(t)=\left|\langle\varphi|\exp\left(-i\hat{H}t/\hbar\right)|\varphi\rangle\right|^2, \tag{2.4.1}$$

which is the probability for the system to continue occupying state $|\varphi\rangle$ after time t. In order to calculate $P(t)$, let us define the function

$$f(t)=\begin{cases}\langle\varphi|\exp\left(-i\hat{H}t/\hbar\right)|\varphi\rangle\, e^{-\varepsilon t}, & t\geq 0\\ 0, & t<0,\end{cases} \tag{2.4.2}$$

where $\varepsilon\in\mathbb{R}^+$. For $t\geq 0$ and $\varepsilon\to 0^+$, we see that $|f(t)|^2\to P(t)$. The reason we deal with $f(t)$ is that it is more well-behaved than the actual amplitude $\langle\varphi|\exp(-i\hat{H}t/\hbar)|\varphi\rangle$. The function is designed so that firstly, it vanishes at negative times prior to start of our thought experiment; and secondly, it vanishes as $t\to\infty$ due to the "regulator" ε. The latter enforces the idea that the bound state decays permanently into the continuum of free states, and is never re-populated by waves "bouncing back" from infinity.

We can determine $f(t)$ by first studying its Fourier transform,

$$F(\omega)\;=\;\int_{-\infty}^{\infty} dt\; e^{i\omega t}\, f(t)\;=\;\int_0^{\infty} dt\; e^{i(\omega+i\varepsilon)t}\;\langle\varphi|e^{-i\hat{H}t/\hbar}|\varphi\rangle. \tag{2.4.3}$$

Now insert a resolution of the identity, $\hat{I}=\sum_n|n\rangle\langle n|$, where $\{|n\rangle\}$ denotes the exact eigenstates of $\hat{H}$ (for free states, the sum goes to an integral in the usual way):

$$\begin{aligned}F(\omega)&=\int_0^{\infty} dt\; e^{i(\omega+i\varepsilon)t}\;\sum_n\langle\varphi|e^{-i\hat{H}t/\hbar}|n\rangle\langle n|\varphi\rangle\\ &=\sum_n\langle\varphi|n\rangle\left(\int_0^{\infty}dt\;\exp\left[i\left(\omega-\frac{E_n}{\hbar}+i\varepsilon\right)t\right]\right)\langle n|\varphi\rangle\\ &=\sum_n\langle\varphi|n\rangle\frac{i}{\omega-\frac{E_n}{\hbar}+i\varepsilon}\langle n|\varphi\rangle\\ &=i\hbar\,\langle\varphi|\left(\hbar\omega-\hat{H}+i\hbar\varepsilon\right)^{-1}|\varphi\rangle.\end{aligned} \tag{2.4.4}$$

In the third line, the regulator ε removes any contribution from the $t\to\infty$ limit of the integral, in accordance with our requirement that the decay of the bound state is permanent. Hence, we obtain

$$\lim_{\varepsilon\to 0^+}F(\omega)=i\hbar\,\langle\varphi|\hat{G}(\hbar\omega)|\varphi\rangle, \tag{2.4.5}$$

where $\hat{G}$ is our old friend the causal Green's function. The fact that the *causal* Green's function shows up is due to our definition of $f(t)$, which vanishes for $t<0$.

As discussed in the previous section, when the resonance condition is satisfied,

$$\langle\varphi|\,\hat{G}(E)\,|\varphi\rangle\approx\frac{1}{E-E_{\text{res}}-i\mathrm{Im}[\Sigma]}, \tag{2.4.6}$$

where E_{res} is the resonance energy and Σ is the self-energy of the quasi-bound state. We can now perform the inverse Fourier transform

$$\begin{aligned}\lim_{\varepsilon\rightarrow 0^+} f(t) &= \lim_{\varepsilon\rightarrow 0^+} \int_{-\infty}^\infty \frac{d\omega}{2\pi}\, e^{-i\omega t}\, F(\omega) \\ &= \frac{i}{2\pi}\int_{-\infty}^\infty d\omega\, \frac{e^{-i\omega t}}{\omega - (E_{\mathrm{res}} + i\mathrm{Im}[\Sigma])/\hbar} \\ &= \exp\left(-\frac{iE_{\mathrm{res}}t}{\hbar}\right)\, \exp\left(-\frac{|\mathrm{Im}[\Sigma]|}{\hbar}\,t\right).\end{aligned} \tag{2.4.7}$$

In deriving the last line, we performed a contour integration assuming that $\mathrm{Im}[\Sigma] < 0$; this assumption will be proven shortly. The final result is

$$P(t) = e^{-\kappa t}, \quad \text{where}\;\; \kappa = \frac{2|\mathrm{Im}[\Sigma]|}{\hbar}. \tag{2.4.8}$$

Let us now take a closer look at the self-energy. From our earlier definition,

$$\Sigma(E) \equiv \lim_{\varepsilon\rightarrow 0^+} \int d^dk\, \frac{|\langle\psi_k|\hat{V}_1|\varphi\rangle|^2}{E - E_k + i\varepsilon}, \tag{2.4.9}$$

where $|\varphi\rangle$ and $\{|\psi_k\rangle\}$ are the bound and free states of the model in the absence of $\hat{V}_1$, and E_k is the energy of the k-th free state. The imaginary part is

$$\begin{aligned}\mathrm{Im}\big[\Sigma(E)\big] &= \lim_{\varepsilon\rightarrow 0^+} \int d^dk\, \Big|\langle\psi_k|\hat{V}_1|\varphi\rangle\Big|^2\, \mathrm{Im}\left(\frac{1}{E-E_k+i\varepsilon}\right) \\ &= -\int d^dk\, \Big|\langle\psi_k|\hat{V}_1|\varphi\rangle\Big|^2\, \left[\lim_{\varepsilon\rightarrow 0^+}\; \frac{\varepsilon}{(E-E_k)^2+\varepsilon^2}\right].\end{aligned} \tag{2.4.10}$$

The quantity inside the square brackets is a Lorentzian function, which is always positive; hence, $\mathrm{Im}(\Sigma) < 0$, as previously asserted. The Lorentzian function has the limiting form

$$\lim_{\varepsilon\rightarrow 0^+} \frac{\varepsilon}{x^2+\varepsilon^2} = \pi\delta(x). \tag{2.4.11}$$

This comes from the fact that as $\varepsilon \rightarrow 0^+$, the Lorentzian curve describes a sharper and sharper peak, but the area under the curve is fixed as π. Hence,

$$\mathrm{Im}\big[\Sigma(E)\big] = -\pi \int d^dk\, \Big|\langle\psi_k|\hat{V}_1|\varphi\rangle\Big|^2\, \delta(E-E_k). \tag{2.4.12}$$

Because of the delta function, we see that the only non-vanishing contributions to the integral come from the parts of k-space where $E = E_k$.

We can further simplify the result by defining the **density of states**,

$$\mathcal{D}(E) = \int d^dk\; \delta(E-E_k). \tag{2.4.13}$$

Roughly speaking, this measures the number of free states that exist at energy E. The k-space volume d^dk is proportional to the number of free states at each k, while the delta function restricts the contributions to only those free states with energy E. (In the next section, we'll see an explicit example of how to calculate $\mathcal{D}(E)$.) Now, for any function $f(k)$,

$$\int d^dk\; f(k)\,\delta(E-E_k) = \overline{f(k(E))}\;\mathcal{D}(E), \tag{2.4.14}$$

where $\overline{f(k(E))}$ denotes the mean value of $f(k)$ for the free states satisfying $E_k = E$. Applying this to the imaginary part of the self-energy gives

$$\mathrm{Im}\big[\Sigma(E)\big] = -\pi\; \overline{\Big|\langle\psi_{k(E)}|\hat{V}_1|\varphi\rangle\Big|^2}\; \mathcal{D}(E). \tag{2.4.15}$$

Hence, the quasi-bound state's decay rate is

Definition: Fermi's Golden Rule

$$\kappa = -\frac{2}{\hbar}\mathrm{Im}\left[\Sigma(E_{\mathrm{res}})\right] = \frac{2\pi}{\hbar}\,\overline{\left|\langle\psi_{k(E_{\mathrm{res}})}|\hat{V}_1|\varphi\rangle\right|^2}\,\mathcal{D}(E_{\mathrm{res}}). \tag{2.4.16}$$

This extremely important result is called **Fermi's golden rule**. It says that the decay rate of a quasi-bound mode is directly proportional to two factors. The first factor describes how strongly $\hat{V}_1$ couples the quasi-bound state and the free states, as determined by the quantity $\langle\psi_k|\hat{V}_1|\varphi\rangle$, called the **transition amplitude**. It goes to zero when $\hat{V}_1 = 0$, which is the case where $|\varphi\rangle$ is a true bound state that does not decay. The second factor is the density of free states, and describes how many free states are available for $|\varphi\rangle$ to decay into. Both factors depend on energy, and must be evaluated at the resonance energy E_{res}.