Fermi Golden Rule

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Fermi Golden Rule is an equation that describes the transition rate between 2 states. Before we derive the equation, we can obtain the form of the equation by using some physical arguments.

Physical Intuition

Consider a Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + V,$$

where V is a small perturbation to the unperturbed system $\mathcal{H}_0$. Suppose the unperturbed system has eigenstates

$$\mathcal{H}_0 |n\rangle = |n\rangle E_n .$$

We are interested in the transition probability between different states under the perturbation V. Naturally, we are looking at final states that are different from the initial state. Then, the transition probability amplitude should be proportional to

$$\langle m| \underbrace{e^{-\frac{it}{\hbar}\mathcal{H}}}_{\text{time-evolution operator}} |n\rangle = \langle m| e^{-\frac{it}{\hbar}(\mathcal{H}_0 + V)} |n\rangle$$

$$\sim \langle m| e^{-\frac{it}{\hbar}\mathcal{H}_0} e^{-\frac{it}{\hbar}V} |n\rangle$$

P/S: Remember that this is not a rigorous derivation, put a rough physical argument

Since V is a small perturbation,

$$e^{-\frac{it}{\hbar}V} \sim \left(1 - \frac{it}{\hbar}V\right)$$

$$\sim \underbrace{\langle m| e^{-\frac{it}{\hbar}\mathcal{H}_0} |n\rangle}_{=0 \text{ for } m \neq n} - \frac{it}{\hbar} \langle m| e^{-\frac{it}{\hbar}\mathcal{H}_0} V |n\rangle$$

$$\sim -\frac{it}{\hbar} e^{-\frac{it}{\hbar}E_m} \langle m|V|n\rangle$$

Hence, the transition rate is proportional to:

$$\gamma_{n\to m} \propto |\langle m|V|n\rangle|^2 .$$

Also, if there are more number of final states, there is a higher chance for the system to transit into the final state. Therefore,

$$\gamma_{n\to m} \propto |\langle m|V|n\rangle|^2 \rho(E_m),$$

where $\rho(E_m)$ is the density of states.

Since transition rate is probability per unit time, it has a dimension of

$$\gamma_{n\to m} \sim \frac{1}{[\text{time}]} .$$

By dimensional analysis,

$$|\langle m|V|n\rangle|^2 \sim [\text{energy}]^2 ,$$

$$\rho(E_n) \sim \frac{1}{[\text{energy}]} ,$$

We must have

$$\gamma_{n\to m} \propto \frac{1}{\hbar} |\langle m|V|n\rangle|^2 \rho(E_m)$$

dimension [energy][time]

This is exactly the form of the Fermi Golden Rule, which states that

$$\boxed{\gamma_{n\to m} = \frac{2\pi}{\hbar} |\langle m|V|n\rangle|^2 \rho(E_m).}$$

P/S: This transition rate was actually mainly due to Dirac,

$$\boxed{\gamma_{n\to m} = \frac{2\pi}{\hbar} |\langle m|V|n\rangle|^2 \rho(E_m).}$$

P/s: This transition rate was actually mainly due to Dirac, despite the name

Derivation from Perturbation Theory

To derive the factor of 2π, we need to use perturbation theory. Consider the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \lambda V,$$

where we include the small parameter λ more explicitly to use perturbation theory. The dynamics of the system is governed by the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle.$$

Since λV is a small perturbation, as before, we expand $|\Psi\rangle$ in the unperturbed eigenbasis:

$$\mathcal{H}_0 |n\rangle = |n\rangle E_n,$$

so that

$$|\Psi\rangle = \sum_n a_n e^{-\frac{it}{\hbar}E_n} |n\rangle.$$

By applying it into the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = i\hbar \frac{\partial}{\partial t}\sum_n a_n e^{-\frac{it}{\hbar}E_n}|n\rangle$$

$$= i\hbar \sum_n \left(\frac{\partial a_n}{\partial t} - a_n \frac{iE_n}{\hbar}\right) e^{-\frac{it}{\hbar}E_n}|n\rangle$$

$$= \sum_n \left(i\hbar\frac{\partial a_n}{\partial t} + \underline{a_n E_n}\right) e^{-\frac{it}{\hbar}E_n}|n\rangle$$

$$\mathcal{H}|\Psi\rangle = (\mathcal{H}_0 + \lambda V)\sum_n a_n e^{-\frac{it}{\hbar}E_n}|n\rangle$$

$$= \sum_n (\underline{a_n E_n} + \lambda a_n V) e^{-\frac{it}{\hbar}E_n}|n\rangle$$

still an operator

Hence:

$$\sum_n i\hbar \frac{\partial a_n}{\partial t} e^{-\frac{it}{\hbar}E_n}|n\rangle = \sum_n \lambda a_n e^{-\frac{it}{\hbar}E_n} V|n\rangle$$

By applying a bra $\langle m|$ in both sides:

$$i\hbar \frac{\partial a_m}{\partial t} e^{-\frac{it}{\hbar}E_m} = \lambda \sum_n a_n e^{-\frac{it}{\hbar}E_n}\langle m|V|n\rangle$$

$$i\hbar \frac{\partial a_m}{\partial t} = \lambda\sum_n a_n e^{-\frac{it}{\hbar}(E_n - E_m)}\langle m|V|n\rangle$$

Although a_n are present on both sides of the equation, there is a small parameter λ at the right hand side. We can use the self-consistent solution method, which effectively expands a_n in powers of λ.

Firstly, when $\lambda = 0$ at the zeroth order,

$$i\hbar \frac{\partial a_m^{(0)}}{\partial t} = 0 \Rightarrow a_m^{(0)} = \text{constant}.$$

Substituting this into the right hand side,

$$i\hbar\frac{\partial a_m^{(1)}}{\partial t} = \lambda \sum_n a_n^{(0)} e^{-\frac{it}{\hbar}(E_n - E_m)}\langle m|V|n\rangle,$$

where $a_m^{(1)}$ is the first order approximation. For convenience, we define $\omega_{nm} \equiv \frac{E_n - E_m}{\hbar}$

and solve the differential equation:

$$i\hbar \frac{\partial a_m^{(1)}}{\partial t} = \lambda\sum_n a_n^{(0)} e^{-it\omega_{nm}}\langle m|V|n\rangle$$

$$\frac{\partial a_m^{(1)}}{\partial t} = -\frac{i}{\hbar}\lambda\sum_n a_n^{(0)} e^{-it\omega_{nm}}\langle m|V|n\rangle$$

$$a_m^{(1)}(T) - \underbrace{a_m^{(1)}(0)} = -\frac{i}{\hbar}\lambda\sum_n a_n^{(0)}\int_0^T dt\, e^{-it\omega_{nm}}\langle m|V|n\rangle,$$

$$a_m^{(1)}(T) - \underbrace{a_m^{(1)}(0)}_{} = -\frac{i}{\hbar}\lambda \sum_n a_n^{(0)} \int_0^T dt\, e^{-it\omega_{nm}} \langle m|V|n\rangle,$$

↳ at $t=0$, this is the zeroth order solution

$$\Rightarrow a_m^{(1)}(T) = a_m^{(0)} - \frac{i}{\hbar}\lambda \sum_n a_n^{(0)} \int_0^T dt\, e^{-it\omega_{nm}} \langle m|V|n\rangle,$$

where we observe that $a_m^{(1)}(T)$ is first order in λ. We can continue to substitute into the differential equation to obtain higher order $a_m^{(n)}(T)$ with higher order λ expansion.

For the purpose of the Fermi Golden Rule, we stop at the first order approximation. We are interested in the transition rate from initial state $|i\rangle$ to final state $|f\rangle$ when $i \neq f$. Therefore, we start with $|i\rangle$,

$$a_n^{(0)} = 0 \quad \forall\, n \neq i \quad \text{and} \quad a_i^{(0)} = 1.$$

For the final state f, we have:

$$a_f(T) \sim \underbrace{a_f^{(0)}}_{=0} - \frac{i}{\hbar}\lambda \sum_n \underbrace{a_n^{(0)}}_{=0 \text{ except } a_i^{(0)}=1} \int_0^T dt\, e^{-it\omega_{nf}} \langle f|V|n\rangle$$

$$= -\frac{i}{\hbar}\lambda \int_0^T dt\, e^{-it\omega_{if}} \langle f|V|i\rangle.$$

Since by Ansatz:

$$|\Psi\rangle = \sum_n a_n(t)\, e^{-\frac{it}{\hbar}E_n} |n\rangle,$$

the probability of being in $|n\rangle$ is $|a_n(t)|^2$. Then, the probability of being in $|f\rangle$ after time T from $|i\rangle$ is

$$|\langle f|U(T)|i\rangle|^2 = |a_f(T)|^2$$

$$= \frac{\lambda^2}{\hbar^2} |\langle f|V|i\rangle|^2 \left| \int_0^T dt\, e^{-it\omega_{if}} \right|^2$$

$$\int_0^T dt\, e^{-it\omega} = \left[-\frac{1}{i\omega} e^{-it\omega} \right]_{t=0}^T$$

$$= \frac{1 - e^{-iT\omega}}{i\omega}$$

$$= \frac{1}{i\omega} e^{-\frac{iT\omega}{2}} \underbrace{\left(e^{\frac{iT\omega}{2}} - e^{-\frac{iT\omega}{2}} \right)}_{= 2i \sin\frac{\omega T}{2}}$$

$$= \frac{2}{\omega} e^{-\frac{iT\omega}{2}} \sin\frac{\omega T}{2}$$

$$= \frac{\lambda^2}{\hbar^2} |\langle f|V|i\rangle|^2 \left(\frac{2}{\omega_{if}} \sin\frac{\omega_{if} T}{2} \right)^2.$$

To proceed, recall that we are interested in obtaining the transition rate, which is the transition probability per unit time.

$$|\langle f|U(T)|i\rangle|^2 \sim \gamma_{i\to f}\, T.$$

If time T is too small, then there is not enough time for transition, since

$$|\langle i|U(T)|i\rangle|^2 = |\langle i| e^{-\frac{iT}{\hbar}\mathcal{H}} |i\rangle|^2$$

$$\sim \left|\langle i| \left[1 - \frac{iT}{\hbar}\mathcal{H} + \frac{1}{2}\left(-\frac{iT}{\hbar}\mathcal{H}\right)^2\right] |i\rangle\right|^2, \quad T \ll 1$$

$$= \left| \left(1 - \frac{iT}{\hbar}\langle\mathcal{H}\rangle - \frac{T^2}{2\hbar^2}\langle\mathcal{H}^2\rangle\right) \right|^2$$

$$= \left(1 - \frac{T^2}{2\hbar^2}\langle\mathcal{H}^2\rangle\right)^2 + \frac{T^2}{\hbar^2}\langle\mathcal{H}\rangle^2$$

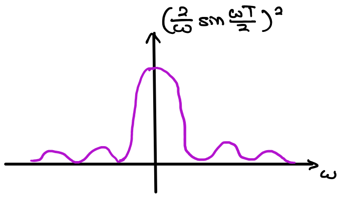
$$\sim 1 - \frac{T^2}{\hbar^2}\left(\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2\right)$$

$$= 1 - \frac{T^2}{\hbar^2}\delta\mathcal{H}^2,$$ variance

and the probability differs in the order of $\mathcal{O}(T^2)$. Therefore,

$$= 1 - \frac{T^2}{\hbar^2} \delta H^2 \quad \swarrow \text{variance}$$

and the probability differs in the order of $O(T^2)$. Therefore, for the system to transit, T must be long enough, but long with respect to what? With respect to the time scale set by the transition frequency. Therefore, we are looking at a regime where $\omega_{if} T \to \infty$.



Consider

$$\lim_{\omega T \to \infty} \left(\frac{2}{\omega} \sin \frac{\omega T}{2}\right)^2 .$$

From the graph, we see that as $\omega T \to \infty$, it looks like a Dirac delta function.

To show that it is a Dirac delta function, we use its definition $\int_{-\infty}^{\infty} dx\, f(x)\, \delta(x) = f(0)$

and consider

$$\int_{-\infty}^{\infty} d\omega\, f(\omega) \left(\frac{2}{\omega} \sin \frac{\omega T}{2}\right)^2 , \quad T >> 1$$

$$= \Big[\underbrace{\int_{-\infty}^{-\epsilon}}_{③} + \underbrace{\int_{-\epsilon}^{\epsilon}}_{②} + \underbrace{\int_{\epsilon}^{\infty}}_{①} \Big] d\omega\, f(\omega) \left(\frac{2}{\omega} \sin \frac{\omega T}{2}\right)^2$$

Consider ①:

$$\int_{\epsilon}^{\infty} d\omega\, f(\omega) \left(\frac{2}{\omega} \sin \frac{\omega T}{2}\right)^2$$

$$= \int_{\epsilon}^{\infty} d\left(\frac{\omega T}{2}\right) f(\omega) \left(\frac{2}{\omega T} \sin \frac{\omega T}{2}\right)^2 2T$$

Let $y = \frac{\omega T}{2}$

$$= \int_{\epsilon T/2}^{\infty} dy\, f\left(\frac{2y}{T}\right) \left(\frac{\sin y}{y}\right)^2 2T$$

$$\xrightarrow{T \to \infty} \int_{\infty}^{\infty} \cdots \to 0$$

The same applies to ③

$$= \int_{-\epsilon}^{\epsilon} d\omega\, f(\omega) \left(\frac{2}{\omega} \sin \frac{\omega T}{2}\right)^2$$

The integral is evaluated around $-\epsilon \leq \omega \leq \epsilon$ for $\epsilon \ll 1$. Therefore, at this region, $f(\omega) \sim f(0)$

$$\sim f(0) \int_{-\epsilon}^{\epsilon} d\omega \left(\frac{2}{\omega} \sin \frac{\omega T}{2}\right)^2$$

Repeat the substitution

$$y = \frac{\omega T}{2}$$

$$= f(0) \int_{-\epsilon T/2}^{\epsilon T/2} dy \left(\frac{\sin y}{y}\right)^2 2T$$

$$\sim 2 f(0) T \int_{-\infty}^{\infty} dy \left(\frac{\sin y}{y}\right)^2$$

$$\int_{-\infty}^{\infty} dy \left(\frac{\sin y}{y}\right)^2 = - \int_{-\infty}^{\infty} d\left(\frac{1}{y}\right) (\sin y)^2$$

$$= \underbrace{- \frac{(\sin y)^2}{y} \Big|_{y=-\infty}^{\infty}}_{=0} + \int_{-\infty}^{\infty} dy\, \frac{2 \sin y \cos y}{y}$$

$$= \int_{-\infty}^{\infty} d(2y)\, \frac{\sin 2y}{2y}$$

$$= \int_{-\infty}^{\infty} dy\, \frac{\sin y}{y}$$

To get the integration of a sinc function, consider

$$\int_{-\infty}^{\infty} dx\, \frac{\sin x}{x} = 2 \int_{0}^{\infty} \frac{\sin x}{x}$$

Define $I(t) = \int_{0}^{\infty} dx\, \frac{\sin x}{x} e^{-xt}$ — ④

Then

Define $I(t) = \int_0^\infty dx \, \frac{\sin x}{x} e^{-xt}$ —— ④

Then,

$$\frac{dI(t)}{dt} = \int_0^\infty dx \, \frac{\sin x}{x} e^{-xt}(-x)$$

$$= -\int_0^\infty dx \, \sin x \, e^{-xt}$$

$$= \int_0^\infty d(-xt) \, \frac{\sin x}{t} e^{-xt}$$

$$= \int_0^\infty d(e^{-xt}) \, \frac{\sin x}{t}$$

$$= \underbrace{\frac{\sin x}{t} e^{-xt}\Big|_{x=0}^{\infty}}_{=0} - \int_0^\infty dx \, \frac{\cos x}{t} e^{-xt}$$

$$= \int_0^\infty d(-xt) \, \frac{\cos x}{t^2} e^{-xt}$$

$$= \underbrace{\frac{\cos x}{t^2} e^{-xt}\Big|_{x=0}^{\infty}}_{= -\frac{1}{t^2}} + \int_0^\infty dx \, \frac{\sin x}{t^2} e^{-xt}$$

$$= \frac{1}{t^2}\left(-1 + \int_0^\infty dx \, \sin x \, e^{-xt}\right)$$

$$\Rightarrow \int_0^\infty dx \, e^{-xt} \sin x = \frac{1}{t^2} \frac{1}{\frac{1}{t^2}+1}$$

$$\frac{dI(t)}{dt} = \frac{-1}{1+t^2}$$

$$I(t) = C_0 - \arctan(t)$$

From ④:

$$I(t\to\infty) = 0 = C_0 - \frac{\pi}{2} \Rightarrow C_0 = \frac{\pi}{2}$$

Hence $I(t) = \frac{\pi}{2} - \arctan(t)$

$$I(0) = \frac{\pi}{2} = \int_0^\infty dx \, \frac{\sin x}{x}$$

$$\therefore \int_{-\infty}^\infty dx \, \frac{\sin x}{x} = \pi$$

$$= \pi$$

$$= 2\pi T f(0)$$

Hence,

$$\lim_{\omega T\to\infty} \left(\frac{2}{\omega} \sin\frac{\omega T}{2}\right)^2 = 2\pi T \, \delta(\omega).$$

Then,

$$|\langle f|U(T)|i\rangle|^2 \longrightarrow \frac{\lambda^2}{\hbar^2} |\langle f|V|i\rangle|^2 \, 2\pi T \, \delta(\omega_{if})$$

and

$$\gamma_{i\to f} = \frac{\lambda^2}{\hbar^2} |\langle f|V|i\rangle|^2 \, 2\pi \, \delta\left(\frac{E_f - E_i}{\hbar}\right)$$

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

Finally, if we integrate over all degenerate final states by using the density of states, the total transition rate is

$$\gamma = \int dE_f \, \rho(E_f) \, \frac{2\pi}{\hbar} |\langle f|\lambda V|i\rangle|^2 \, \delta(E_f - E_i)$$

$$\boxed{\gamma = \frac{2\pi}{\hbar} |\langle f|\lambda V|i\rangle|^2 \, \rho(E_i)}$$

$= \rho(E_f)$ because of Dirac delta function

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This is the Fermi Golden Rule.

P/S: We could obtain the limit through Fourier transform:

$$\mathcal{F}\left[\left(\frac{2}{\omega}\sin\frac{\omega T}{2}\right)^2\right]$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, \frac{4}{\omega^2} \sin^2\frac{\omega T}{2} \, e^{-i\omega t}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, \frac{4}{\omega^2} \left(\frac{1}{2i}\right)^2 \left(e^{i\omega T/2} - e^{-i\omega T/2}\right)^2 e^{-i\omega t}$$

$$= -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, \frac{1}{\omega^2} \left(e^{i\omega T} + e^{-i\omega T} - 2\right) e^{-i\omega t}$$

$$= -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \, \frac{1}{\omega^2} \left(e^{i\omega(T-t)} + e^{-i\omega(T+t)} - 2e^{-i\omega t}\right)$$

We can use Residue theorem to evaluate

$$\int_{-\infty}^{\infty} d\omega \, \frac{e^{-i\omega t}}{\omega^2}.$$

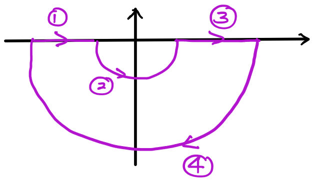
There is only a pole at $\omega = 0$. To find its residue, we expand it into Laurent series

$$\frac{1}{\omega^2} e^{-i\omega t} = \frac{1}{\omega^2} \sum_n \frac{(-i\omega t)^n}{n!}$$

$$= \frac{1}{\omega^2} - \frac{i\omega t}{\omega^2} - \frac{\omega^2 t^2}{2\omega^2} + O(\omega)$$

The residue is $-it$.

We then consider the contour: for $t > 0$



By residue theorem:

① + ② + ③ + ④ = 0

① + ③ = integral we want

② = $2\pi i \times \text{Residue} \times \frac{1}{2}$

$= \pi t$

$$\Rightarrow \int_{-\infty}^{\infty} d\omega \, \frac{e^{-i\omega t}}{\omega^2} = -\pi t$$

Similarly, if $t < 0$, $\int_{-\infty}^{\infty} d\omega \, \frac{e^{-i\omega t}}{\omega^2} = \pi t$

$$= \frac{1}{\sqrt{2\pi}} \left[\pi(t-T)\,\mathrm{sgn}(t-T) + \pi(T+t)\,\mathrm{sgn}(T+t) - 2\pi t\,\mathrm{sgn}\, t \right]$$

We take limit $t < T \to \infty$

$$= \frac{1}{\sqrt{2\pi}} \left[\pi(T-t) + \pi(T+t) - 2\pi|t|\right]$$

$$= \sqrt{\frac{\pi}{2}} \, 2\,(T - |t|)$$

$\to \sqrt{2\pi}\, T$, which is a constant

The inverse Fourier transform is:

$$\lim_{T\to\infty} \mathcal{F}^{-1}\left[\mathcal{F}\left[\left(\frac{2}{\omega}\sin\frac{\omega T}{2}\right)^2\right]\right]$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt \, \sqrt{2\pi}\, T \, e^{i\omega t}$$

$$= 2\pi T \, \delta(\omega)$$

as expected