

Derivation of Fermi's Golden Rule #2

Fermi's Golden Rule #2 is one of the central equations in radiation physics, as it is employed to obtain decay rates and cross sections. Thus, a clear derivation is called for.

Consider the Schrödinger equation for a single particle in a static binding potential:

$$\mathcal{H}_0 \Psi(\vec{x}, t) = \frac{i}{\hbar} \Psi(\vec{x}, t) \quad (1)$$

where

$$\begin{aligned} \mathcal{H}_0 &= \mathcal{T} + V(\vec{x}) \\ \mathcal{T} &= -\frac{\hbar^2}{2m} \nabla^2 \end{aligned} \quad (2)$$

We know that such a potential has a set of orthonormal eigenstates:

$$|j\rangle = \Psi_j(\vec{x}, t) = \Psi_j(\vec{x}) e^{-E_j t / \hbar} , \quad (3)$$

with eigenenergies, E_j . These eigenstates are orthonormal, that is,

$$\langle i | j \rangle = \delta_{ij} . \quad (4)$$

We know that the E_j 's are constants, and fixed. By Heisenberg's Uncertainty Principle, we also know that all eigenstates are stable, as there is no mechanism for decay. In Nature, we know that excited states eventually decay to the ground state, and the purpose of this derivation is to obtain an expression for that decay rate.

We start by assuming that there is a perturbation potential that is time dependent, $V_p(\vec{x}, t)$.

Now we solve:

$$(\mathcal{H}_0 + V_p) \Psi = \frac{i}{\hbar} \frac{\partial \Psi}{\partial t} , \quad (5)$$

where Ψ is the general solution to the entire problem, with both static and perturbation potentials included.

To start, we write $\Psi(\vec{x}, t)$ as a superposition of the eigenstates of the $\mathcal{H}_0$ operator, that is:

$$\Psi(\vec{x}, t) = \sum_j a_j(t) \Psi_j(\vec{x}, t) \quad (6)$$

Taking the partial derivative (6) with respect to t gives: (Henceforth, for brevity, obvious functional dependences on space and time will usually be suppressed.)

$$\frac{\partial \Psi}{\partial t} = \sum_j \left(\dot{a}_j - i \frac{E_j}{\hbar} \right) \Psi_j . \quad (7)$$

$$(7) + (6) \longrightarrow (5) \Rightarrow$$

$$\sum_j a_j (\mathcal{H}_0 - E_j) \Psi_j + \sum_j (a_j V_p - i \hbar \dot{a}_j) \Psi_j = 0 . \quad (8)$$

The first summation is zero, because each Ψ_j is a eigenfunction of the unperturbed $\mathcal{H}_0$ with eigenenergy E_j . Thus,

$$\sum_j (a_j V_p - i \hbar \dot{a}_j) \Psi_j = 0 , \quad (9)$$

or,

$$\sum_j (a_j V_p - i \hbar \dot{a}_j) |j\rangle = 0 . \quad (10)$$

Let $|f\rangle$ be the state that the excited states $|j\rangle$ transitions to. You can think of $|f\rangle$ as the ground state, or at least a lower excited state.

$$\langle f | \otimes (10) \Rightarrow$$

$$\sum_j (a_j \langle f | V_p | j \rangle e^{i(E_j - E_f)/\hbar} - i \hbar \dot{a}_j) \delta_{jf} = 0 . \quad (11)$$

Using the shorthand notation $V_{jf} \equiv \langle f | V_p | j \rangle$ and $\omega_{jf} \equiv (E_j - E_f)/\hbar$, we have:

$$i \hbar \dot{a}_f = \sum_j a_j V_{jf} e^{i(E_j - E_f)/\hbar} . \quad (12)$$

(12) represents, at least in principle, an exact solution the problem. All one needs to do is to set an initial condition, say, $a_n(0) = 1$ (the excited state) and then al the other a 's, potentially an infinite number (!) to zero, and then let the solution evolve. Note that every single eigenstate can be involved in the eventual de-excitation of $|n\rangle$. This approach is more amenable to numerical solution. So, to proceed with the analysis, we make the

Small perturbation approximation

In this approximation, we only have two states, the initial excited and final states, $|i\rangle$ and $|f\rangle$. None of the other states are assumed to be involved. In the spirit of this approximation, we treat the a 's on the right hand side of (12) as constants. (This is how the system would evolve for small t for any perturbation, large or small.)

Hence we set $a_i(t) = 1 \forall t$, $a_f(0) = 0$, we allow these to change with time, and all the other a 's are set to zero for all time. This allows us to integrate the equation, resulting in:

$$a_f = V_{if} \frac{1 - e^{i\omega_{if}t}}{\hbar\omega_{if}} . \quad (13)$$

Now, we evaluate the occupation probability of the state to which the transition is made,

$$P = |a_f|^2 = |V_{if}|^2 \frac{(1 - e^{i\omega_{if}t})(1 - e^{-i\omega_{if}t})}{(\hbar\omega_{if})^2} . \quad (14)$$

Using some trigonometric identities, this can be recast into the following form:

$$P = |a_f|^2 = \frac{|V_{if}|^2}{\hbar^2} \frac{\sin^2(\omega_{if}t/2)}{(\omega_{if}/2)^2} . \quad (15)$$

The derivation of (15) assumed that the energy of the initial state $|i\rangle$ is precisely known. However, we know from the Heisenberg's Uncertainty Principle, $\Delta E \Delta t \geq \hbar/2$, that the energy of an excited state can not be known precisely, but distributed in some way. So, assume that the energy of the excited state is distributed according to some distribution $\rho(\omega)$. We must integrate over all of these to obtain the occupation probability:

$$P = \int_{-\infty}^{\infty} d\omega \frac{|V_{if}|^2}{\hbar^2} \rho(\omega) \frac{\sin^2((\omega_{if} - \omega)t/2)}{((\omega_{if} - \omega)/2)^2} . \quad (16)$$

The

$$\frac{\sin^2((\omega_{if} - \omega)t/2)}{((\omega_{if} - \omega)/2)^2}$$

term in the above equation acts as a delta function for large t , narrowing as t increases. We eventually want to consider the decay of the excited state to the final state, so we take the large t limit to obtain, after a change of variables:

$$P = \frac{|V_{if}|^2}{\hbar^2} \rho(\omega_{if}) 2t \int_{-\infty}^{\infty} dx \frac{\sin^2 x}{x^2} . \quad (17)$$

The integral evaluates numerically to π , thus

$$P = \frac{2\pi}{\hbar^2} |V_{if}|^2 \rho(\omega_{if}) t \quad (18)$$

We can also rewrite $\rho(\omega_{if})$ in terms of E_{if} . Since $E_{if} = \hbar\omega_{if}$,

$$P = \frac{2\pi}{\hbar} |V_{if}|^2 \rho(E_{if}) t . \quad (19)$$

Finally, the rate of decay, $\lambda = dP/dt$. Hence,

$$\lambda = \frac{2\pi}{\hbar} |V_{if}|^2 \rho(E_{if}) , \quad (20)$$

and we have derived Fermi's Golden Rule #2.

A few comments are in order.

The “blurring” function $\rho(E_{if})$ is sometimes referred to as the “density of final states”. We had to introduce it, in a somewhat *ad hoc* fashion to recognize that excited states are, indeed, “blurred”. However, it is fascinating to note, that this blurring is directly connected to the existence of final states for the system to accept the decay. For example, a typical nuclear decay involves the release of a γ . Unless this γ has a quantum state to occupy it, there can be no quantum mechanical transition. Hence, our interpretation of the “blurring” of excited states depends on our ability to measure its decay. If there is no decay mode, then this density of states function drops to zero, the decay does not occur, and hence, the energy of the excited state is precise! (But not measurable!)

What is the nature of this “blurring”?

The Lorentz distribution

If an excited state can decay, we may write its wavefunction in the following form:

$$\Psi(\vec{x}, t) = \Psi(\vec{x}) e^{iE_i t/\hbar} \frac{e^{-t/(2\tau)}}{\sqrt{\tau}} , \quad (21)$$

where τ is its mean life. This interpretation follows directly from the probability density of the excited state:

$$|\Psi(\vec{x}, t)|^2 = |\Psi(\vec{x})|^2 \frac{e^{-t/\tau}}{\tau} , \quad (22)$$

giving the well-known exponential decay law, properly normalized over the domain $0 \leq t < \infty$. Here we are adopting the normalization convention that

$$\int_0^\infty dt |\Psi(\vec{x}, t)|^2 = |\Psi(\vec{x})|^2 .$$

Just as the dynamic variables k and x are related by Fourier transforms in the operational sense, this is true as well for ω and t . Hence the above distribution in time, namely $e^{-t/\tau}$, is converted to a distribution in frequency by its Fourier transform, namely,

$$\Psi_i(\vec{x}, \omega) = \Psi_i(\vec{x}) \frac{1}{\sqrt{2\pi\tau}} \int_0^\infty dt e^{i(\omega_i - \omega)t} e^{-t/(2\tau)} , \quad (23)$$

where $\omega_i = E_i$ and $\omega = E$.

After performing the integral

$$\Psi_i(\vec{x}, \omega) = \Psi_i(\vec{x}) \frac{1}{\sqrt{2\pi\tau}} \frac{1}{i(\omega_i - \omega) + 1/(2\tau)} , \quad (24)$$

Therefore,

$$|\Psi_i(\vec{x}, \omega)|^2 = |\Psi_i(\vec{x})|^2 \frac{1}{2\pi\tau} \left(\frac{1}{(\omega_i - \omega)^2 + (1/(2\tau))^2} \right) . \quad (25)$$

In terms of E rather than ω ,

$$|\Psi_i(\vec{x}, E)|^2 = |\Psi_i(\vec{x})|^2 \frac{\Gamma}{2\pi} \left(\frac{1}{(E_i - E)^2 + (\Gamma/2)^2} \right) , \quad (26)$$

where $\Gamma \equiv \hbar/\tau$.

Thus we have found the form of the Lorentz distribution:

$$|\Psi_i(\vec{x}, E)|^2 = |\Psi_i(\vec{x})|^2 \frac{\Gamma}{2\pi} \left(\frac{1}{(E_i - E)^2 + (\Gamma/2)^2} \right) . \quad (27)$$

One may easily verify that:

$$\int_{-\infty}^{\infty} dE |\Psi_i(\vec{x}, E)|^2 = |\Psi(\vec{x})|^2 . \quad (28)$$