Phys 487 Discussion 11 – Fermi's Golden Rule

Given • $H(t) = H^{(0)} + H'(t)$, • $\left\{ E_n^{(0)}, |n^{(0)}\rangle \right\}$ = the eigen-* of $H^{(0)}$ • initial state $|\psi(t=0)\rangle = |i^{(0)}\rangle$

then $\boxed{|\psi(t)\rangle = \sum_n c_n(t)\, e^{-i\omega_n t} |n^{(0)}\rangle}$ with $\boxed{i\hbar \dot{c}_f(t) = \sum_n H'_{fn}\, e^{i\omega_{fn}t} c_n(t)}$ • $\omega_{fn} \equiv \left(E_f^{(0)} - E_n^{(0)}\right)/\hbar$ • $H'_{fn} \equiv \langle f^{(0)}|H'|n^{(0)}\rangle$

& to <u>1st order</u> in $H' \ll H^{(0)}$, $\boxed{c_f(t) \approx \delta_{fi} + \frac{1}{i\hbar}\int_0^t H'_{fi}(t') e^{i\omega_{fi}t'} dt'}$ $\rightarrow$ $\boxed{P_{i\to f} = \left| c_f(t) \right|^2}$

Problem 1 : Fermi's Golden Rule for a constant perturbation

In class, we derived Fermi's Golden Rule for a perturbation that **oscillates sinusoidally with time** (typically in the form of EM radiation) and that is ON for a very long time. As it happens, Fermi's Golden Rule *also* applies for another extremely common type of perturbation: a potential that is **constant with time**, it merely turns on and off. An example: a simple Stark and/or Zeeman effect experiment when a field $\vec{E}(\vec{r})$ and/or $\vec{B}(\vec{r})$ is turned on at some time $t = 0$ and turned off later. So off we go!

The simplest time-dependent perturbation is a constant potential V that just "turns on" at some time $t = 0$:

$V(t) = 0$ for $t < 0$ & $V(t) = V =$ constant for $t \geq 0$.

Important: we are NOT saying that V is constant versus POSITION, only with respect to time. In all of our time-dependent PT work, it is implied that the perturbation labelled "V" or "H'" DOES in general have some $\vec{r}$-dependence, it will just end up in a transition matrix element $V_{fi} = \langle \psi_f | V | \psi_i \rangle$ that we will have to calculate (as an integral over position) if we want a specific answer for a specific V. If we ever need to specify a potential that is independent of position, we will call it something like "V_0" to denote one single scalar value.

Now suppose we have a system with a solvable unperturbed Hamiltonian H_0 plus the on/off perturbation $V(t)$ given above. What is the transition probability $P_{i\to f} = | c_f(t) |^2$ to first order?

(a) Derive the following result : $P_{i\to f} = \frac{|V_{fi}|^2}{\hbar^2}\left[\frac{\sin(\omega_{fi}t/2)}{\omega_{fi}t/2}\right]^2 t^2$ for $i \neq f$.

You will need the "half-angle formula" $1 - \cos\theta = 2\sin^2(\theta/2)$.

▶ Is your first thought that the result is a typo? It is always my first thought when seeing that expression for a simple *time-independent* perturbation that just turns ON once and OFF once! "We saw that $\sin^2(\omega t/2)$ stuff when we worked with sinusoidal perturbations in class, surely it is just a copy/paste error?" Indeed one would think that such a term only appears for sinusoidal perturbations, but no! Start your calculation from time-dependent PT basics (back to the formula sheet!), and observe how that same time-dependent term arises even for our much simpler ON/OFF perturbation. (Actually, look closely: is $P_{i\to f}$ the same or just similar to the sinusoidal case?)

(b) Prove the following weird but important Dirac delta-function relation : $\delta(ax) = \frac{\delta(x)}{a}$.

▶ Remember that the <u>defining properties</u> of the Dirac delta are on your 486 formula sheet, consult those to derive/prove the above relation, and the one in the next part.

(c) Prove that the following is a delta function : $\lim_{a\to\infty} \frac{1}{\pi}\frac{\sin^2(ax)}{ax^2} = \delta(x)$. (You will need $\int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx = \pi$.)

(d) Combining the above, show that the **transition rate** $\boxed{R_{i\to f} \equiv \frac{P_{i\to f}}{t} = \frac{2\pi}{\hbar}\left|V_{fi}\right|^2 \delta\left(E_f - E_i\right)}$ in the limit where energy is conserved, i.e. where $\left(E_f - E_i\right) \to 0$.

This relation is one form of **Fermi's Golden Rule** for energy-conserving transitions.

(e) Is it reasonable to insist that energy is conserved despite the change in potential energy? Return to expression (a) and consider its dependence on $\omega_{fi} = \hbar(E_f - E_i)$. As you can quickly check with some sort of machine, the function $\sin^2 x / x^2$ is peaked at x=0 and has a width of about π. (It reaches 0.4 ≈ ½ at $x = \pm\pi/2$). Given this info, what range of ω_{fi} values keeps the transition probability $P_{i\to f}$ within a factor of about 2 of its maximum value? Your answer will involve time, t. Does the range of probable transition frequencies increase or decrease with t?

(f) Hopefully what you found was that, as $t \to \infty$, the width in reasonably-probable transition frequencies goes to zero. This is a very important result! What does t represent, exactly? Once you know, you can say something like this

> "In the limit that the perturbation $V(t)$ ____(words)____, the only transition frequency with any finite probability is ωfi = ____, which means that energy is _____ in this limit."

We have thus clarified the conditions under which part (d) is a valid result.

(g) You just found that **energy is conserved more exactly** in the transition from state i to state f **as the time t that the perturbation has been ON increases**. What relation involving a German name is this related to?

(h) The perturbation can never be on *forever*, i.e. we can never reach the limit $t \to \infty$, so there is always some non-zero *range* of final-state energies $E_f \approx E_i$ that can be reached from an initial-state energy E_i … but a transition $E_i \to E_f$ can only occur if there a state with energy E_f actually *exists*. It is customary to inject information about the availability of final states into Fermi's Golden Rule using the quantity $\rho(E_f)$ = the density of final states = #states per unit energy. This quantity has units of 1/energy. The energy-conserving delta function $\delta(E_f - E_i)$ in our earlier version of Fermi's Golden Rule *also* has units of 1/energy. To get the most familiar form of F.G.R., we simply replace the one-final-state-only δ-function with the density of states:

$$\boxed{R_{i\to f} \equiv \frac{P_{i\to f}}{t} = \frac{2\pi}{\hbar}\left|V_{fi}\right|^2 \rho\left(E_f\right)\Big|_{E_f \approx E_i}} \quad \textbf{Fermi's Golden Rule}$$