Phys 487 Discussion 11 – Fermi's Golden Rule

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

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

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

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

Right at the end of last class, we derived a relation called 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 common type of perturbation: a potential that is **constant with time**, it merely TURNS ON at some moment. An example: a simple Stark or Zeeman effect experiment where a field $\vec{E}(\vec{r})$ and/or $\vec{B}(\vec{r})$ is turned on at some time $t = 0$. 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 versus 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. The position dependence will end up in a transition matrix element $V_{fi} = \langle\, \psi_f \,|\, V \,|\, \psi_i \,\rangle$ = an integral over position that we will have to calculate. 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 that we have a system with a solvable unperturbed Hamiltonian H_0 plus the off/on 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 : for $i \neq f$, $P_{i\to f} = \frac{\left|V_{fi}\right|^2}{\hbar^2}\left[\frac{\sin(\omega_{fi}\, t/2)}{\omega_{fi}\, t/2}\right]^2 t^2$.

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! "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 OFF/ON perturbation. (Actually, look closely: is $P_{i\to f}$ exactly 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 the time t that the perturbation is ON goes to ∞.
This is one form of **Fermi's Golden Rule**.

(e) That delta function insists that the energy of the system is conserved in the transition. Is that reasonable when we have a changing potential energy $V(t)$ around that turned on at some moment and caused the transition? Return to expression (a) and consider its dependence on the transition frequency $\omega_{fi}=\hbar\,(E_f-E_i)$. The transition frequency is a measure of the energy mismatch between the initial and final states, and so of the energy that the system gained or lost as a result of the perturbation. 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 FWHM (full width at half maximum) of about 3. 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) 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 that can be reached from an initial-state energy E_i. And now for a new consideration: a transition $E_i\to E_f$ can only occur if 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

$n(E_f)$ = the **density of final states**.

This quantity has units of 1/energy because it stands for the number of states per energy-interval:

$$\boxed{n(E)\,dE\equiv\text{number of states in the interval } E-\tfrac{1}{2}dE\ \to\ E+\tfrac{1}{2}dE}$$

The 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 replace the one-final-state-only δ-function with the density of states:

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