Phys 506 lecture 32: Fermi's golden rule and the sudden approximation

1 Transition probabilities

When we discussed time-dependent perturbation theory, we found the probability for a transition form state m to state n in the first Born approximation was

$$P_{n\leftarrow m}(t) = \frac{1}{\hbar^2}\left|\int_{t_0}^{t} dt_1 e^{i\omega_{nm}(t_1-t_0)}V_{nm}\left(t_1\right)\right|^2$$

If $\hat{V}$ is independent of time and $t_0 = 0$, we have

$$P_{n\leftarrow m}(t) = \frac{4\sin^2\left(\frac{\omega_{nm}t}{2}\right)}{\hbar^2\omega_{nm}^2}\left|V_{nm}\right|^2.$$

This is the result for a discrete spectrum. Consider generalizing to a continuous spectrum and plot the transition probability as a function of the "energy" ω.

$$f(\omega) = \frac{4\sin^2\frac{\omega t}{z}}{\hbar^2\omega^2}$$

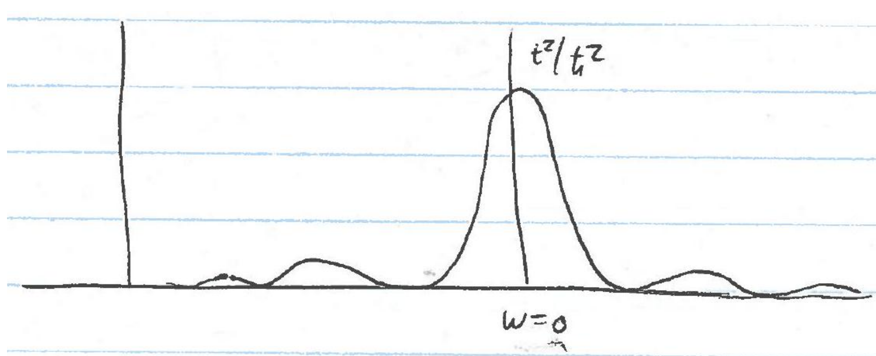

Figure 1: The plot of probability (vertical) versus frequency (horizontal) has a large central peaks with much smaller amplitude oscillating peaks to the left and right, which decrease rapidly in amplitude the further we go from the center.

It is always positive. Furthermore, as $t\to\infty$ we have $f(\omega)\to ct\delta(\omega)$. But $\int_{-\infty}^{+\infty} d\omega f(\omega)d\omega = \frac{2\pi t}{\hbar^2} \Rightarrow c = \frac{2\pi}{\hbar^2}$. So, $\lim_{t\to\infty} P_{n\leftarrow m}(t) \to \frac{|V_{nm}|^2}{\hbar^2}2\pi t\delta\left(\frac{E_n^{(0)}-E_n^{(0)}}{\hbar}\right) = \frac{2\pi}{\hbar}t\delta\left(E_n^{(0)}-E_m^{(0)}\right)\left|V_{nm}\right|^2.$

The rate at which P increases is then

$$\frac{dP_{n\leftarrow m}(t)}{dt} = \dot{P}_{n\leftarrow m}(t) = \frac{2\pi}{\hbar}\delta\left(E_n^0 - E_m^{(0)}\right)|V_{nm}|^2 .$$

In the continuum, all energy levels are allowed, so we drop the superscript (0).

Let $n = f =$ final and $m = i =$ initial, to get

$$\boxed{\dot{P}_{f\leftarrow i}(t) = \frac{2\pi}{\hbar}\delta\left(E_f - E_i\right)|V_{fi}|^2}$$

called Fermi's Golden Rue (actually derived by Dirac).

In order to solve the depletion problem, we sometimes add an extra factor of P on the RHS since the rate should be proportional to the number of states.

$$\dot{P}_{f\leftarrow i}(t) = \frac{2\pi}{\hbar}\delta\left(E_f - E_i\right)|V_{fi}|^2 P(t)$$

In this case, the probability will always be bounded.

2 Example: muonic Helium

Example: Consider a Helium-like atom $(z = 2)$ with a muon and an electron orbiting it.

$$\text{electron} \quad (r, p, m) \quad \text{and} \quad \text{muon} \quad (R, P, M) \quad \text{for} \quad M \gg m :$$

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{ze^2}{\hat{r}} + \frac{\hat{p}^2}{2M} - \frac{ze^2}{\hat{R}} + \frac{e^2}{|\mathbf{R}-\mathbf{r}|}$$

Since $M \gg m$, the muon orbits close to the nucleus, $\Rightarrow$ electron sees effective charge $z_{\text{eff}} = 1$.

Write $\hat{H} = \hat{H}_0 + \hat{V}$

$$= \underbrace{\frac{\hat{p}^2}{2m} - \frac{e^2}{\hat{r}} + \frac{\hat{P}^2}{2M} - \frac{2e^2}{\hat{R}}}_{H_0} + \underbrace{\frac{e^2}{|\hat{\mathbf{R}}-\hat{\mathbf{r}}|} - \frac{e^2}{\hat{r}}}_{V} .$$

Unperturbed wavefunctions are electron in H field and muon in the field.

$$H_0|\psi(r,R)\rangle = E(\Psi(r,R)\rangle$$
$$|\psi(r,R)\rangle_{nlm;n'l'm'} = \underbrace{U_{n'l'm'}(R)}_{\text{Helium field}} \; \underbrace{u_{nlm}(r)}_{\text{Hydrogen field}}$$

$$E_{nn'} = -\frac{me^4}{2\hbar^2 n^2} - \frac{2Me^4}{\hbar^2 a^{12}}$$

$$\text{ground state} \qquad n = n' = 1 \qquad E_{\text{gs}} = -\frac{e^4}{2\hbar^2}[m + 4M]$$

$$\text{excited state} \qquad n = 1, n' = 2 \qquad E_{12} = -\frac{e^4}{2\hbar^2}[m + M]$$

$$E_{12} - E_{\rm gs} = \frac{3Me^4}{2\hbar^2}.$$

Suppose the system starts in the excited state and drops to G.S. if the electron absorbs this energy (instead of a photon taking it away), its energy is

$$\frac{e^4}{2\hbar^2}[-m + 3M] \gg 0$$

$\Rightarrow$ the electron goes to the continuum and is ejected (like a so-called Auger transition).

Suppose at time $t = 0$ we are in the state $n' = 2 \quad n = 1$. What is the electron ejection rate at large t ? You may assume that the emitted electron is a free particle, because it is a high-energy state.

$$\begin{aligned}
&\text{Rate } = \frac{2\pi}{\hbar}\left|V_{fi}\right|^2 \delta\left(E_f - E_i\right) \\
&E_i = -\frac{e^4}{2\hbar^2}[M+m] \qquad E_f = -\frac{e^4}{2\hbar^2}[4M] + \frac{\hbar^2 k^2}{2m^2} \\
&|\psi_i\rangle = U_{2lm_l}(R)U_{100}(r) \\
&|\psi_f\rangle = U_{100}(R)e^{ik\cdot r}.
\end{aligned}$$

Sum over all final momenta to get the total rate

$$\sum_k \to \frac{1}{(2\pi)^3}\int d^3k$$

$$\begin{aligned}
\text{Rate } &= \int \frac{d^3k}{(2\pi)^3}\frac{2\pi}{\hbar}\left|V_{fi}(k)\right|^2 \delta\left(E_f - E_i\right) \\
d^3k &= k^2 dk d\Omega = k\frac{dk^2}{2}d\Omega \quad \text{and} \quad \varepsilon_k = \frac{\hbar^2k^2}{2m} \\
&= \left(\frac{2m\varepsilon_k}{\hbar^2}\right)^{1/2}\frac{m}{\hbar^2}d\varepsilon_k d\Omega \quad \text{and} \quad d\varepsilon_k = d\varepsilon_f
\end{aligned}$$

$$\begin{aligned}
R &= \int \frac{d\varepsilon_f}{(2a)^3}d\Omega\left(\frac{2m\varepsilon_k}{\hbar^2}\right)^{1/2}\frac{m}{\hbar^2}(-\frac{2\pi}{\hbar})|V_{fi}(k)|^2\delta\left(E_f - E_i\right) \\
&= \int \frac{d\Omega}{(2\pi)^3}\left(\frac{2m\frac{e^4}{2\hbar^2}(3M-m)}{\hbar^2}\right)^{1/2}\frac{m}{\hbar^2}\frac{2\pi}{\hbar}\left|V_{fi}(\mathbf{k})\right|^2 \\
&= \frac{1}{(2\pi)^2\hbar^5}e^2 m\sqrt{m(3M-m)}\int d\Omega\left|V_{fi}(\mathbf{k})\right|^2 \\
|V_{fi}(k)|^2 &= \int d^3R \quad U_{2lm_l}(R)U_{100}(R)\int d^3r e^{-ik\cdot r}U_{100}(r)\times\left[\frac{e^2}{|\mathbf{R}-\mathbf{r}|} - \frac{e^2}{r}\right].
\end{aligned}$$

3 The sudden approximation

Now we consider the sudden approximation.

Suppose the system is in a given time independent potential for $t < 0$. At $t = 0$. The potential suddenly changes to a new potential, which remains for all $t > 0$. What happens to the states of the quantum system?

In practice, no potential changes instantly but these changes can be very fast (like in radioactive decay). In these cases the sudden approximation is valid.

Strategy - find the eigenfunctions of $H(t<0) = |\psi_i\rangle$ and of $\bar{H}(t>0) = |\psi_f\rangle$. The probability to find the system in one of the f states given that it started in an i state is just the overlap:

$$P_{f\leftarrow i} = |\langle\psi_f|\psi_i\rangle|^2 \, .$$

It is that simple.

4 Example of the sudden approximation

Example: particle on a box of length L. Assume it starts in the ground state

At $t=0$ the box increases in size to $2L$. What is the probability to be in each of the eigenstates of the wider box?

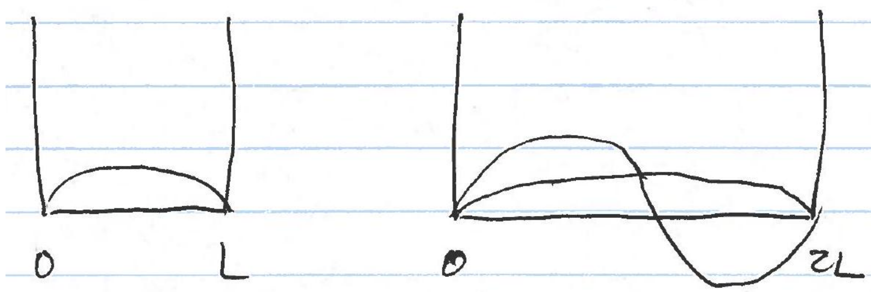

Figure 2: On the left, we see a particle in a box of a box of length L, with the different wavefucntions sketched. On the right, we see the same, but now the box is length $2L$.

The wavefunctions for a particle in a box are

$$\begin{aligned} |\psi_n\rangle &= \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \qquad n = 1, 2, \cdots \\ \text{so } |\psi_i\rangle &= \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \qquad 0 < x < L \\ &= 0 \qquad\qquad\qquad x > L \\ |\,\psi_f(n)\rangle &= \frac{1}{\sqrt{L}} \sin\frac{n\pi x}{2L} \qquad n = 1, 2, \ldots \end{aligned}$$

$$
\begin{aligned}
P_{f\leftarrow i} &= |\langle \psi_f(n) \mid \psi_i\rangle|^2 \\
&= \left| \int_0^L dx \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \sqrt{\frac{1}{L}} \sin\frac{n\pi x}{2L} \right|^2 \\
&= \frac{2}{L^2} \left| \int_0^L dx \frac{1}{2} \left(\cos\frac{(n+2)\pi x}{2L} - \cos\frac{(n-2)\pi x}{2L} \right) \right|^2 \\
&= \frac{1}{2L^2} \left| \left[\frac{2L}{(n+2)\pi} \sin\frac{(n+2)\pi x}{2L} - \frac{2L}{(n-2)\pi} \sin\frac{(n-2)\pi x}{2L} \right]_0^L \right|^2 \\
&= \frac{2}{\pi^2} \left| \sin\frac{(n+2)\pi}{2} \frac{1}{(n+2)} - \sin\frac{(n-2)\pi}{2} \frac{1}{(n-2)} \right|^2 \\
&= \left[\begin{array}{ll} 0 & n = \text{even}, n \neq 2 \\ \frac{1}{2} & n = 2 \\ 32/\left(\pi^2 (n+2)^2 (n-2)^2\right) & n = \text{odd.} \end{array} \right.
\end{aligned}
$$

Note that

$$
\begin{aligned}
\sum_n |\langle \psi_f(n) \mid \psi_i\rangle|^2 &= \underbrace{\frac{1}{2}}_{n=2} + \frac{32}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+3)^2 (2n-1)^2} \\
&= \frac{1}{2} + \frac{32}{\pi^2} \sum_{n=0}^{\infty} \left[\frac{1}{(2n+3)^2} - \frac{1}{(2n-1)^2} \right] \frac{1}{(-8)(2n+1)} \\
&= \frac{1}{2} + \frac{4}{\pi^2} \sum_{n=0}^{\infty} \left(\frac{1}{(2n-1)^2 (2n+1)} - \frac{1}{(2n+3)^2 (2n+1)} \right) \\
&= \frac{1}{2} + \frac{4}{\pi^2} \sum_{n=0}^{\infty} \left\{ \frac{1}{(2n-1)} \left(\frac{1}{(2n-1)} - \frac{1}{2n+1} \right) \frac{1}{2} \right. \\
&\qquad \left. - \frac{1}{(2n+3)} \left(\frac{1}{(2n+1)} - \frac{1}{2n+3} \right) \frac{1}{2} \right\} \\
&= \frac{1}{2} + \frac{2}{\pi^2} \sum_{n=0}^{\infty} \left\{ \frac{1}{(2n-1)^2} + \frac{1}{(2n+3)^2} + \left(\frac{1}{(2n-1)} - \frac{1}{2n+1} \right) \left(-\frac{1}{2} \right) \right. \\
&\qquad \left. + \left(\frac{1}{(2n+1)} - \frac{1}{2n+3} \right) \left(-\frac{1}{2} \right) \right\} \\
&= \frac{1}{2} + \frac{2}{\pi^2} \sum_{n=0}^{\infty} \left\{ \frac{1}{(2n+1)^2} - \frac{1}{2(2n-1)} \right) + \frac{1}{2} \frac{1}{2n+3} \right\} \\
&= \frac{1}{2} + \frac{4}{\pi^2} \cdot \frac{\pi^2}{8} = \frac{1}{2} + \frac{1}{2} = 1
\end{aligned}
$$

so $\sum_f P_{f\leftarrow i} = 1$ as it must!