Fermi's golden rule & sudden approximation

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

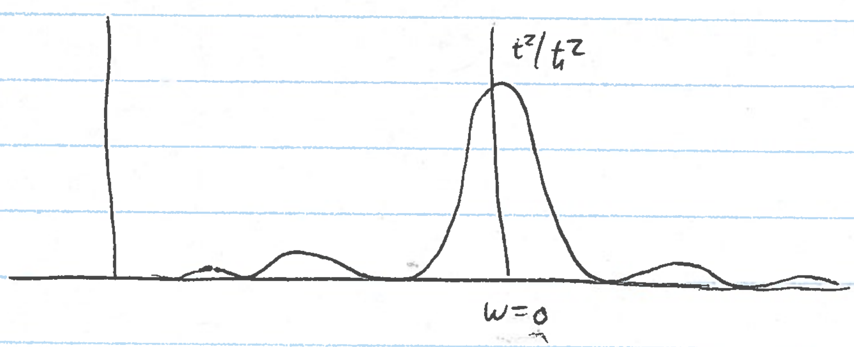
$$P_{n\leftarrow m}(t) = \frac{1}{\hbar^2} \left| \int_{t_0}^{t} dt_1\, e^{i\omega_{nm}(t_1-t_0)}\, V_{nm}(t_1) \right|^2$$

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

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

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

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



It is always positive. As $t\to\infty$ $f(\omega)\to c\, t\, \delta(\omega)$
But $\int_{-\infty}^{+\infty} d\omega\, f(\omega)\, d\omega = \frac{2\pi t}{\hbar^2} \Rightarrow c = \frac{2\pi}{\hbar^2}$

So $$\lim_{t\to\infty} P_{n\leftarrow m}(t) \to \frac{|V_{nm}|^2}{\hbar^2}\, 2\pi t\, \delta\left(\frac{E_n^{(0)}-E_m^{(0)}}{\hbar}\right) = \frac{2\pi}{\hbar}\, t\, \delta(E_n^{(0)}-E_m^{(0)})\, |V_{nm}|^2$$

The <u>rate</u> at which P increases is then

$$\frac{dP_{n\leftarrow m}(t)}{dt} = \dot{P}_{n\leftarrow m}(t) = \frac{2\pi}{\hbar}\,\delta\left(E_n^{(1)} - E_m^{(0)}\right) |V_{nm}|^2$$

In the continuum, all energy levels are allowed, so we drop the superscript (0) let n = f = final m = i = initial to get

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

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

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

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

In this case, the probability will always be bounded.

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

electron (r, p, m) muon (R, P, M) $M \gg m$

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{Ze^2}{r} + \frac{\hat{P}^2}{2M} - \frac{Ze^2}{R} + \frac{e^2}{|\vec{r} - \vec{R}|}$$

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

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

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

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

$$H_0 |\Psi(r,R)\rangle = E|\Psi(r,R)\rangle$$

$$|\Psi(r,R)\rangle_{n\ell m; n'\ell' m'} = \underset{\uparrow \text{ Helium field}}{U_{n'\ell'm'}(R)} \; \underset{\uparrow \text{ Hydrogen field}}{u_{n\ell m}(r)}$$

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

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

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

$$E_{12} - E_{gs} = \frac{3M e^4}{2\hbar^2}$$

Suppose system starts in excited state and drops to GS. 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 $n=2$ $n=1$

What is the electron ejection rate at large t?

$$\text{Rate} = \frac{2\pi}{\hbar} |V_{fi}|^2 \delta(E_f - E_i)$$

$$E_i = -\frac{e^4}{2\hbar^2}[M+m] \qquad E_f = -\frac{e^4}{2\hbar^2}[4M] + \frac{\hbar^2 k^2}{2m}$$

↑ assume e^- is a free particle since at such high energy.

$$|\psi_i\rangle = U_{2\ell m_\ell}(R)\, U_{100}(r)$$

$$|\psi_f\rangle = U_{100}(R)\, e^{ik\cdot r}$$

Sum over all final momenta to get the rate

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

$$\text{Rate} = \int \frac{d^3k}{(2\pi)^3} \frac{2\pi}{\hbar} |V_{fi}(k)|^2 \delta(E_f - E_i)$$

$$d^3k = k^2\, dk\, d\Omega = k\, \frac{dk^2}{2}\, d\Omega \qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

$$= \left(\frac{2m\varepsilon_k}{\hbar^2}\right)^{1/2} \frac{m}{\hbar^2}\, d\varepsilon_k\, d\Omega \qquad d\varepsilon_k = d\varepsilon_f$$

$$R = \int \frac{d\varepsilon_F\, d\Omega}{(2\pi)^3} \left(\frac{2m\,\varepsilon_k}{\hbar^2}\right)^{1/2} \frac{m}{\hbar^2} \frac{2\pi}{\hbar} |U_{fi}(k)|^2 \delta(E_f - E_i)$$

$$= \int \frac{d\Omega}{(2\pi)^3} \left(\frac{2m\, \frac{e^4}{2\hbar^2}(3M-m)}{\hbar^2}\right)^{1/2} \frac{m}{\hbar^2} \frac{2\pi}{\hbar} |U_{fi}(\vec{k})|^2$$

$$= \frac{1}{(2\pi)^2\hbar^5} e^2 m \sqrt{m(3M-m)} \int d\Omega\, |U_{fi}(\vec{k})|^2$$

$$|U_{fi}(k)|^2 = \int d^3R\, U_{2\ell m_\ell}(R)\, U_{100}(R) \int d^3r\, e^{-ik\cdot r}\, U_{100}(r) * \left[\frac{e^2}{|\vec{R}-\vec{r}|} - \frac{e^2}{r}\right]$$

will be nonzero only if $m_\ell = 0$

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?

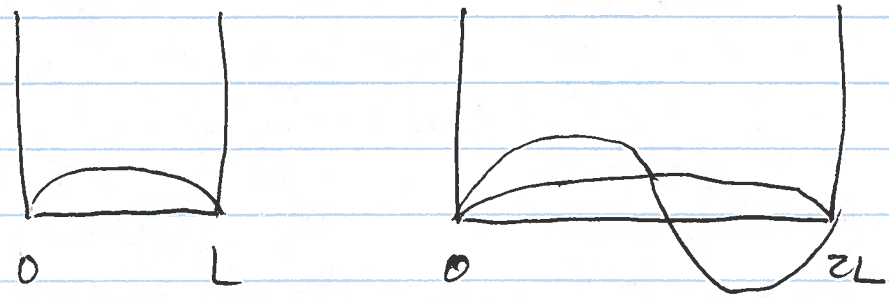
In practice, no potential changes instantly but these changes can be very fast (like in radioactive decay) In these cases the sudden approximation is valid

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 if 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.

Example: particle in 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?



The wave functions for a particle in a box are

$$|\psi_n\rangle = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad n = 1, 2, \ldots$$

$$\text{so } |\psi_i\rangle = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \qquad 0 < x < L$$

$$= 0 \qquad x > L$$

$$|\psi_f(n)\rangle = \frac{1}{\sqrt{L}} \sin \frac{n\pi x}{2L} \qquad n = 1, 2, \ldots$$

$$P_{f\leftarrow i} = |\langle \psi_f(n) | \psi_i \rangle|^2$$

$$= \left| \int_0^L dx \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \sqrt{\frac{1}{L}} \sin \frac{n\pi x}{2L} \right|^2$$

$$= \frac{2}{L^2} \left| \int_0^L dx \, \frac{1}{2}\left(\cos \frac{(n+2)\pi x}{2L} - \cos \frac{(n-2)\pi x}{2L} \right) \right|^2$$

$$= \frac{1}{2L^2} \left| \frac{2L}{(n+2)\pi} \sin \frac{(n+2)\pi x}{2L} - \frac{2L}{(n-2)\pi} \sin \frac{(n-2)\pi x}{2L} \Big|_0^L \right|^2$$

$$= \frac{2}{\pi^2} \left| \sin \frac{(n+2)\pi}{2} \frac{1}{(n+2)} - \sin \frac{(n-2)\pi}{2} \frac{1}{(n-2)} \right|^2$$

$$= \begin{cases} 0 & n = \text{even}, \; n \neq 2 \\ \frac{1}{2} & n = 2 \\ 32 / \left(\pi^2 (n+2)^2 (n-2)^2\right) & n = \text{odd} \end{cases}$$

$n=2$

Note that

$$\sum_n \left|\langle \psi_f(n)|\psi_i\rangle\right|^2 = \frac{1}{2} + \frac{32}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+3)^2(2n-1)^2}$$

$$= \frac{1}{2} + \frac{32}{\pi^2}\sum_{n=0}^{\infty}\left[\frac{1}{(2n+3)^2} - \frac{1}{(2n-1)^2}\right]\frac{1}{(-8)(2n+1)}$$

$$= \frac{1}{2} + \frac{4}{\pi^2}\sum_{n=0}^{\infty}\left(\frac{1}{(2n-1)^2(2n+1)} - \frac{1}{(2n+3)^2(2n+1)}\right)$$

$$= \frac{1}{2} + \frac{4}{\pi^2}\sum_{n=0}^{\infty}\left\{\frac{1}{(2n-1)}\left(\frac{1}{(2n-1)} - \frac{1}{2n+1}\right)\frac{1}{2} - \frac{1}{(2n+3)}\left(\frac{1}{(2n+1)} - \frac{1}{2n+3}\right)\frac{1}{2}\right\}$$

$$= \frac{1}{2} + \frac{8}{\pi^2}\sum_{n=0}^{\infty}\left\{\frac{1}{(2n-1)^2} + \frac{1}{(2n+3)^2} + \left(\frac{1}{(2n-1)} - \cancel{\frac{1}{2n+1}}\right)\left(-\frac{1}{2}\right) + \left(\cancel{\frac{1}{(2n+1)}} - \frac{1}{(2n+3)}\right)\left(-\frac{1}{2}\right)\right\}$$

$$= \frac{1}{2} + \frac{2}{\pi^2}\sum_{n=0}^{\infty}\left\{\frac{2}{(2n+1)^2} - \cancel{\frac{1}{2(2n-1)}} + \frac{1}{2}\cancel{\frac{1}{(2n+3)}}\right\}$$

$$= \frac{1}{2} + \frac{4}{\pi^2}\cdot\frac{\pi^2}{8} = \frac{1}{2} + \frac{1}{2} = 1$$

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