

Fermi's golden rule

Find the transition rate $\Gamma_{1 \rightarrow 2}$ by deriving Fermi's golden rule.

Let the perturbing Hamiltonian be

$$H_1(x, t) = 2V(x) \cos(\omega t + \phi)$$

Let $\Psi(x, t)$ be the following linear combination of the two eigenstates.

$$\Psi(x, t) = c_1(t)\psi_1(x) \exp(-i\omega_1 t) + c_2(t)\psi_2(x) \exp(-i\omega_2 t)$$

We need to solve for $c_2(t)$ to find the transition rate.

From the time-dependent Schrodinger equation we have

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = H_0(x)\Psi(x, t) + H_1(x, t)\Psi(x, t)$$

Expand the left-hand side.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Psi(x, t) &= i\hbar \frac{\partial c_1(t)}{\partial t} \psi_1(x) \exp(-i\omega_1 t) + \boxed{\hbar\omega_1 c_1(t) \psi_1(x) \exp(-i\omega_1 t)} \\ &\quad + i\hbar \frac{\partial c_2(t)}{\partial t} \psi_2(x) \exp(-i\omega_2 t) + \boxed{\hbar\omega_2 c_2(t) \psi_2(x) \exp(-i\omega_2 t)} \end{aligned}$$

Noting that $\hbar\omega_1 = E_1$ and $\hbar\omega_2 = E_2$, the boxed terms cancel with $H_0(x)\Psi(x, t)$ leaving

$$i\hbar \frac{\partial c_1(t)}{\partial t} \psi_1(x) \exp(-i\omega_1 t) + i\hbar \frac{\partial c_2(t)}{\partial t} \psi_2(x) \exp(-i\omega_2 t) = H_1(x, t)\Psi(x, t)$$

Substitute for $H_1(x)\Psi(x, t)$.

$$\begin{aligned} i\hbar \frac{\partial c_1(t)}{\partial t} \psi_1(x) \exp(-i\omega_1 t) + i\hbar \frac{\partial c_2(t)}{\partial t} \psi_2(x) \exp(-i\omega_2 t) \\ = 2 \cos(\omega t + \phi) \left[c_1(t)V(x)\psi_1(x) \exp(-i\omega_1 t) + c_2(t)V(x)\psi_2(x) \exp(-i\omega_2 t) \right] \end{aligned}$$

Take the inner product of $\psi_2^*(x)$ with the above equation to obtain

$$i\hbar \frac{\partial c_2(t)}{\partial t} \exp(-i\omega_2 t) = 2 \cos(\omega t + \phi) \left[c_1(t)M_{21} \exp(-i\omega_1 t) + c_2(t)M_{22} \exp(-i\omega_2 t) \right]$$

where M_{21} and M_{22} are the matrix elements

$$\begin{aligned} M_{21} &= \int \psi_2^*(x)V(x)\psi_1(x) dx \\ M_{22} &= \int \psi_2^*(x)V(x)\psi_2(x) dx \end{aligned}$$

Multiply both sides by $\exp(i\omega_2 t)$.

$$i\hbar \frac{\partial c_2(t)}{\partial t} = 2 \cos(\omega t + \phi) \left[c_1(t) M_{21} \exp(i(\omega_2 - \omega_1)t) + 2c_2(t) M_{22} \right]$$

Let the initial state be $\Psi(x, 0) = \psi_1(x)$ hence the initial conditions are

$$c_1(0) = 1, \quad c_2(0) = 0$$

Then for time t near the origin we can use the approximation

$$i\hbar \frac{\partial c_2(t)}{\partial t} = 2 \cos(\omega t + \phi) M_{21} \exp(i(\omega_2 - \omega_1)t)$$

Solve for $c_2(t)$ by integrating.

$$c_2(t) = \frac{2M_{21}}{i\hbar} \int_0^t \cos(\omega t' + \phi) \exp(i(\omega_2 - \omega_1)t') dt'$$

The solution is

$$c_2(t) = -\frac{M_{21}}{\hbar} \left(\frac{\exp(i(\omega_2 - \omega_1 - \omega)t) - 1}{\omega_2 - \omega_1 - \omega} \right) \exp(-i\phi) - \frac{M_{21}}{\hbar} \left(\frac{\exp(i(\omega_2 - \omega_1 + \omega)t) - 1}{\omega_2 - \omega_1 + \omega} \right) \exp(+i\phi) \quad (1)$$

For ω such that $\omega \approx \omega_2 - \omega_1$ the first term dominates so discard the second term and write

$$c_2(t) = -\frac{M_{21}}{\hbar} \left(\frac{\exp(i(\omega_2 - \omega_1 - \omega)t) - 1}{\omega_2 - \omega_1 - \omega} \right) \exp(-i\phi)$$

Rewrite using a sinc function.

$$c_2(t) = -\frac{it}{\hbar} M_{21} \exp\left(i \frac{\omega_2 - \omega_1 - \omega}{2} t - i\phi\right) \text{sinc}\left(\frac{\omega_2 - \omega_1 - \omega}{2} t\right) \quad (2)$$

Hence the transition probability is

$$P(1 \rightarrow 2) = |c_2(t)|^2 = \frac{t^2}{\hbar^2} |M_{21}|^2 \text{sinc}^2\left(\frac{\omega_2 - \omega_1 - \omega}{2} t\right) \quad (3)$$

Integrate $P(1 \rightarrow 2)$ to obtain the total transition probability $P_{tot}(1 \rightarrow 2)$.

$$P_{tot}(1 \rightarrow 2) = \frac{t^2}{\hbar^2} |M_{21}|^2 \int_{E-\epsilon}^{E+\epsilon} \text{sinc}^2\left(\frac{E'/\hbar - \omega}{2} t\right) g(E') dE'$$

where

$$E = \hbar(\omega_2 - \omega_1)$$

and $g(E')$ is the density of photon states for energy E' .

Use the approximation $g(E') \approx g(\hbar\omega)$ to obtain

$$P_{tot}(1 \rightarrow 2) = \frac{t^2}{\hbar^2} |M_{21}|^2 g(\hbar\omega) \int_{E-\epsilon}^{E+\epsilon} \text{sinc}^2 \left(\frac{E'/\hbar - \omega}{2} t \right) dE'$$

Let

$$y = \frac{E'/\hbar - \omega}{2} t$$

It follows that

$$E' = \frac{2\hbar y}{t} + \hbar\omega$$

and

$$dE' = \frac{2\hbar}{t} dy$$

The integration limits transform as

$$E \pm \epsilon \rightarrow \frac{(E \pm \epsilon)/\hbar - \omega}{2} t = \frac{Et}{2\hbar} - \frac{\omega t}{2} \pm \frac{\epsilon t}{2\hbar} \approx \pm \frac{\epsilon t}{2\hbar}$$

Hence

$$P_{tot}(1 \rightarrow 2) = \frac{2t}{\hbar} |M_{21}|^2 g(\hbar\omega) \int_{-\epsilon t/2\hbar}^{\epsilon t/2\hbar} \text{sinc}^2 y dy$$

Use the approximation

$$\int_{-\epsilon t/2\hbar}^{\epsilon t/2\hbar} \text{sinc}^2 y dy \approx \int_{-\infty}^{\infty} \text{sinc}^2 y dy = \pi$$

to obtain

$$P_{tot}(1 \rightarrow 2) = \frac{2\pi t}{\hbar} |M_{21}|^2 g(\hbar\omega)$$

The transition rate is the derivative of $P_{tot}(1 \rightarrow 2)$.

$$\Gamma_{1 \rightarrow 2} = \frac{d}{dt} P_{tot}(1 \rightarrow 2) = \frac{2\pi}{\hbar} |M_{21}|^2 g(\hbar\omega)$$