Fermi's golden rule – derivation and application

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Fermi's Golden Rule is a simple formula for the constant transition rate from one energy eigenstate of a quantum system into other ennergy eigenstates in a continuum, effected by a perturbation. It is always used calculating lifetime.

1 Derivation of Fermi's Golen Rule

Consider the system to begin in an eigenstate, $|i\rangle$, of a given Hamiltonian, H_0 . Consider the effect of a (possibly time-dependent) perturbing Hamiltonian, H'. If H' is time-independent, the system goes only into those states in the continuum that have the same energy as the initial state. If H' is oscillating as a function of time with an angular frequency ω , the transition is into states with energies that differ by $\hbar\omega$ from the energy of the initial state.

1.1 Time dependent perturbation theory

Hamiltonian with perturbation is like

$$H = H_0 + H'(t) \tag{1}$$

The unperturbed Time independent Schrödinger equation is satisfied

$$H_0|\phi_n\rangle = E_n|\phi_n\rangle \tag{2}$$

The time dependent wave function can be expressed as

$$|\Psi(t)\rangle = |\phi_n\rangle e^{-iE_n t/\hbar} \tag{3}$$

Some derivation

$$\begin{split} H|\Psi(t)\rangle &= [H_0 + H^{'}(t)]|\Psi(t)\rangle = i\hbar\frac{\partial|\Psi(t)|}{\partial t} \\ |\Psi(t)\rangle &= \Sigma_n c_n(t)|\psi_n(t)\rangle = \Sigma_n c_n(t)\phi_n\rangle e^{-iE_nt/\hbar} \\ H_0\Sigma_k c_k(t)|\phi_k\rangle e^{-iE_kt/\hbar} + H^{'}(t)\Sigma_k c_k(t)|\phi_k\rangle e^{-iE_kt/\hbar} &= \\ &i\hbar\frac{\partial}{\partial t}\Sigma_k c_k(t)|\phi_k\rangle e^{-iE_kt/\hbar} \\ \Sigma c_k(t)E_k|\phi_k\rangle e^{-iE_kt/\hbar} + \Sigma c_k(t)H^{'}(t)|\phi_k\rangle e^{-iE_kt/\hbar} &= \\ &i\hbar\Sigma\frac{\partial c_k(t)}{\partial t}|\phi_k\rangle e^{-iE_kt/\hbar} + \Sigma_k c_k(t)|\phi_k\rangle (-\frac{iE_k}{\hbar})e^{-iE_kt/\hbar} \\ \Sigma_k c_k(t)W_{nk}(t)e^{-iE_kt/\hbar} &= i\hbar\frac{\partial c_n(t)}{\partial t}e^{-iE_nt/\hbar} \end{split}$$

where $W_{nk}(t) = \langle \phi_n | H' | \phi_k \rangle$. At last, we got the equation.

$$\frac{\partial c_n(t)}{\partial t} = \frac{1}{i\hbar} c_i(t) W_{ni}(t) e^{i\omega_{ni}t} \tag{5}$$

In which, i represents the initial state $|i\rangle$, and $\omega = (E_n - E_i)/\hbar$. Solving this, we can get the final result.

$$c_{f}(t) = \frac{1}{i\hbar} \int_{0}^{t} W_{fi}(t') e^{i\omega_{fi}t'} dt'$$
 (6)

The probability of finding the system in the eigenstate $|\phi_f|$ is

$$\mathcal{P}(t)_{if} = |\langle \phi_f | \psi(t) |^2$$

$$= \frac{1}{\hbar^2} |\int_0^t e^{i\omega_{fi}(t')} dt' |^2$$
(7)

1.2 High frequency harmonic perturbation

We could define a time dependent perturbation,

$$H'(t) = 2H\cos(\omega t) = H(e^{i\omega t} + e^{-i\omega t})$$
(8)

In this case, the probability becomes

$$\mathscr{P}_{if}(t) = \frac{W_{fi}^2}{\hbar^2} \left| \frac{e^{i(\omega_{fi} + \omega)t} - 1}{i(\omega_{fi} + \omega)} + \frac{e^{i(\omega_{fi} - \omega)t} - 1}{i(\omega_{fi} - \omega)} \right|^2 \tag{9}$$

Assuming that the oscilating angular frequency of the perturbation has a value near the Bohr angular frequency of the initial and final eigenstates, $\omega \sim \omega_{fi}$. The first term in Eq.9 becomes negliable, and the second term

$$A_{-} = \frac{e^{i(\omega_{fi} - \omega)t} - 1}{i(\omega_{fi} - \omega)}$$

$$= e^{i(\omega_{fi} - \omega)t/2} \frac{e^{i(\omega_{fi} - \omega)t/2} - e^{-i(\omega_{fi} - \omega)t/2}}{i(\omega_{fi} - \omega)}$$

$$= e^{i(\omega_{fi} - \omega)t/2} \frac{\sin[(\omega_{fi} - \omega)t/2]}{(\omega_{fi} - \omega)/2}$$
(10)

The probability becomes

$$\mathscr{P}_{fi}(t) = \frac{W_{fi}^2}{\hbar^2} \frac{\sin^2[(\omega_{fi} - \omega)t/2]}{[(\omega_{fi} - \omega)/2]^2}$$
(11)

when $\omega \sim \omega_{fi}$, the probability sharply increases. This is call resonant point. In A_+ , the resonant point is located on $\omega = -\omega_{fi}$. The resonant approximation is justified when $|A_+|^2$ and $|A_-|^2$ is far apart. This means that the matrix elements of the perturbation must be much smaller than the energy separation between the initial and final states.

1.3 Continuum

$$\mathscr{P}(t) = \int \mathscr{P}_{fi}(t)\rho(E)dE \tag{12}$$

Because the probability is very sharp at the resonant point just like a delta function, the density $\rho(E)$ can be considered as a constant.

$$\mathcal{P}(t) = \frac{W_{fi}^2}{\hbar^2} \rho(E_{fi}) \int \frac{\sin^2[(\omega_{fi} - \omega)t/2]}{[(\omega_{fi} - \omega)/2]^2} \hbar d\omega$$

$$= \frac{2\pi}{\hbar} W_{fi}^2 \rho(E_{fi}) t$$
(13)

the transition rate is

$$\mathcal{W}(t) = \frac{d\mathcal{P}(t)}{dt}$$

$$= \frac{2\pi}{\hbar} W_{fi}^2 \rho(E_{fi})$$
(14)

This is called Fermi's Golden Rule.