Chapter 3. Fermi Golden Rule

Fermi's Golden Rule provides Selection Rules and Lineshapes in the weak field limit, and can be derived from time dependent perturbation theory in the interaction picture.

For a system with total Hamiltonian $\hat{H}$, the state at time t in the Schrodinger picture is given by

$$|\alpha;t\rangle = \hat{U}(t)|\alpha;0\rangle \qquad \text{where} \qquad \hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

$$\langle\alpha;t|\hat{A}|\alpha;t\rangle = \langle\alpha;0|\hat{U}^{\dagger}(t)\hat{A}\hat{U}(t)|\alpha;0\rangle = \langle\alpha;0|\hat{A}_H(t)|\alpha;0\rangle$$

Operator in Heisenberg Picture ↑

When the total Hamiltonian is time dependent, the expression for the time evolution operator becomes complicated. Often, it is better to consider in the Interaction Picture - the Heisenberg picture of a reference Hamiltonian.

Interaction Picture

For time dependent Hamiltonian, $\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$

define $\hat{U}_0(t) = e^{-i\hat{H}_0 t/\hbar}$

Then,

$$\langle\alpha;t|\hat{A}|\alpha;t\rangle = \langle\alpha;t|\hat{U}_0(t)\hat{U}_0^\dagger(t)\hat{A}\hat{U}_0(t)\hat{U}_0^\dagger(t)|\alpha;t\rangle = {}_I\langle\alpha;t|\hat{A}_I(t)|\alpha;t\rangle_I$$

Schrodinger equation in the interaction picture

$$\frac{\partial}{\partial t}|\alpha;t\rangle_I = -\frac{i}{\hbar}\hat{H}_{1,I}(t)|\alpha;t\rangle_I$$

$$\longrightarrow \quad |\alpha;t\rangle_I = |\alpha;0\rangle_I - \frac{i}{\hbar}\int_0^t dt'\hat{H}_{1,I}(t')|\alpha;t'\rangle_I$$

First order time dependent perturbation theory in the Interaction Picture

$$|\alpha;t\rangle_I^{(1)} = |\alpha;0\rangle_I - \frac{i}{\hbar}\int_0^t dt'\hat{H}_{1,I}(t')|\alpha;0\rangle_I$$

In the Schrodinger Picture

$$|\alpha;t\rangle^{(1)} = |\alpha;t\rangle^{(0)} - \frac{i}{\hbar}\int_0^t dt' e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{H}_1(t')|\alpha;t'\rangle^{(0)}$$

Assume that $|\alpha;0\rangle = |n\rangle$

$$|\alpha;t\rangle^{(1)} = e^{-\frac{i}{\hbar}E_n t}|n\rangle - \frac{i}{\hbar}\int_0^t dt' e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{H}_1(t')e^{-\frac{i}{\hbar}E_n t'}|n\rangle$$

Probability for the state to make transition from $|n\rangle$ to $|m\rangle$

$$\begin{aligned} P_{n\to m}(t) &= \left|\langle m|\alpha;t\rangle^{(1)}\right|^2 \\ &= \frac{1}{\hbar^2}\int_0^t dt'\int_0^t dt'' e^{\frac{i}{\hbar}(E_m-E_n)(t'-t'')}\langle m|\hat{H}_1(t')|n\rangle\langle n|\hat{H}_1(t'')|m\rangle \end{aligned}$$

Transition rate: $\Gamma_{n\to m}(t) \equiv \frac{d}{dt}P_{n\to m}(t)$

Fermi Golden Rule: $\Gamma_{n\to m} = \lim_{t\to\infty}\Gamma_{n\to m}(t)$

For $\hat{H}(t) = \hat{H}_0 + \hat{V}_1 e^{-i\omega t} + \hat{V}_1 e^{i\omega t}$

$$\Gamma_{n\to m} = \frac{2\pi}{\hbar}|\langle m|\hat{V}_1|n\rangle|^2\left\{\delta(E_m - E_n - \hbar\omega) + \delta(E_m - E_n + \hbar\omega)\right\}$$

↑ Absorption ↑ Emission