FERMI'S GOLDEN RULE (1st Derived by P.A.M. Dirac)

A (Brief) Review of Time-Dependent Perturbation Theory

Say initially we have an eigenstate ϕ_n of an unperturbed Hamiltonian, $\hat{H}_0$.

The time-dependent eigenstates of this Hamiltonian are of the form

$$\psi_n(\bar{r},t) = \phi_n(\bar{r})\, e^{-i\omega_n t} \quad , \text{ where}$$

$$\hat{H}_0 \phi_n = E_n \phi_n \equiv \hbar\omega_n \phi_n$$

Now, there appears a perturbation to the Hamiltonian, $\hat{H}'(t)$.

The total Hamiltonian is now:

(1) $$\hat{H}(\bar{r},t) = \hat{H}_0(\bar{r}) + \lambda \hat{H}'(\bar{r},t)$$

The $\psi_n(\bar{r},t)$ form a complete set. So, at a time t (after the perturbation has begun) the system is in a state

(2) $$\psi(\bar{r},t) = \sum_n c_n(t)\, \psi_n(\bar{r},t)$$

If we could determine the c_n, we could identify the probability that the system is in state ψ_n as $|c_n|^2$. So how do we go about doing this?

The wavefunction $\psi(\bar{r},t)$ is a solution of the time-dependent Schrödinger equation:

(3) $$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi = (\hat{H}_0 + \lambda \hat{H}')\psi$$

Inserting Eq. (2) into the above, followed by an inner product w/ $\psi_k(\bar{r},t)$ we have (dropping arguments)

(4) $$i\hbar \frac{dc_k}{dt} = \lambda \sum_n \langle \psi_k | H' | \psi_n \rangle c_n$$

We notice two things about the above equation. First, it is an infinite series of coupled equations for the c_k. Second, in the limit $\lambda \to 0$, the c_k are constant.

We therefore seek a series solution of the form

(5) $$c_k(t) = c_k^{(0)} + \lambda c_k^{(1)} + \lambda^2 c_k^{(2)} + \cdots$$

Substituting this into eq. (4) and denoting the matrix elements $\langle \psi_k | H' | \psi_n \rangle$ as H'_{kn} we have;

(6) $$\begin{aligned} i\hbar \dot{c}_k^{(0)} &= 0 \\ i\hbar \dot{c}_k^{(1)} &= \sum_n H'_{kn} c_n^{(0)} \\ &\;\vdots \\ i\hbar \dot{c}_k^{(s+1)} &= \sum_n H'_{kn} c_n^{(s)} \end{aligned}$$

If the initial state was in a definite eigenstate of $\hat{H}_0$, say $\psi_\ell(\bar{r},t)$, eq. (2) requires $c_n^{(0)}(t=t_0) = \delta_{n\ell}$

We can substitute this value into eq. (6) to get (w/ dropped superscripts)

(7) $$i\hbar \dot{c}_k(t) = \sum_n H'_{kn} c_n(t_0) = H'_{k\ell}$$

Thus, the 1^{st} order solution is

(8) $$c_k(t) = (i\hbar)^{-1} \int_{t_0}^{t} H'_{k\ell}(\bar{r},t')\,dt' \qquad k \neq \ell$$

If we assume the time dependence of $\hat{H}'(\bar{r},t)$ is factorable; that is:

(9) $$\hat{H}'(\bar{r},t) = \hat{V}(\bar{r}) f(t)$$

$H_{k\ell}$ becomes:

(10) $$H'_{k\ell} \equiv \langle \psi_k | H' | \psi_\ell \rangle = \langle \psi_k | \hat{V}(\bar{r}) | \psi_\ell \rangle e^{i(\omega_k - \omega_\ell)t} f(t)$$

Substituting this back into eq. (8) we can determine the transition probability from state ψ_ℓ to state ψ_k as;

(11) $$P_{\ell k} = |c_k|^2 = \left| \frac{V_{k\ell}}{\hbar} \right|^2 \left\{ \int_{t_0}^{t} e^{i(\omega_k - \omega_\ell)t'} f(t')\,dt' \right\}^2$$

Harmonic Perturbation

Consider a perturbation that is monochromatically harmonic in time that 'turns on' at $t=0$;

(12) $$\hat{H}'(\vec{r},t) = 2\hat{V}(\vec{r})\cos\omega t \qquad t \geq 0$$

Substituting this into the final equation for $c_k(t)$ $[\text{eq } 11]^{1/2}$ we find:

$$c_k(t) = \frac{\hat{V}_{k\ell}}{i\hbar}\int_0^t e^{i(\omega_k-\omega_\ell)t'}\left(e^{-i\omega t'} + e^{i\omega t'}\right)dt'$$

using $e^{i\theta}-1 = 2ie^{i\theta/2}\sin(\theta/2)$ we obtain

(13) $$c_k(t) = -\frac{2i\hat{V}_{k\ell}}{\hbar}\left[\frac{e^{i(\omega_{k\ell}-\omega)t/2}\sin(\omega_{k\ell}-\omega)t/2}{\omega_{k\ell}-\omega} + \frac{e^{i(\omega_{k\ell}+\omega)t/2}\sin(\omega_{k\ell}-\omega)t/2}{\omega_{k\ell}+\omega}\right]$$

where $\omega_{k\ell} \equiv \omega_k - \omega_\ell$ has been used.

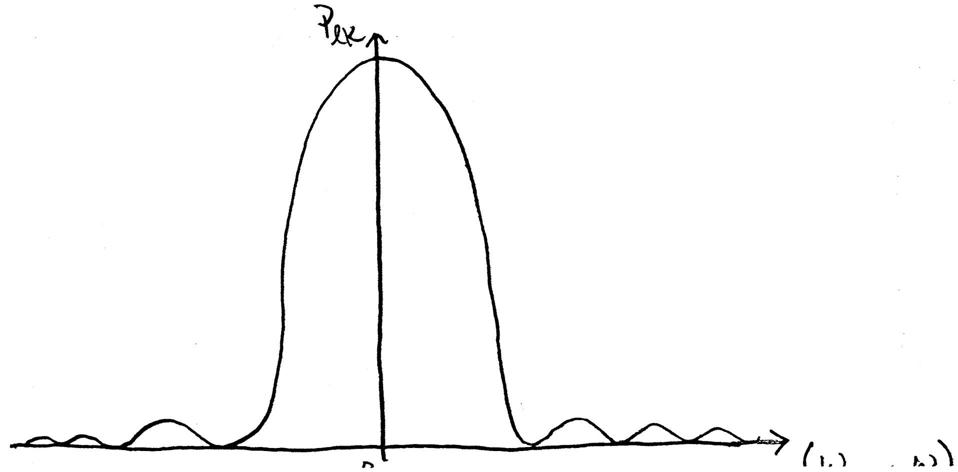
The dominant contributions to eq. (13) arise when $\pm\omega_{k\ell} \simeq \omega$.

For $\omega_{k\ell} > 0$, $E_k > E_\ell$ and the system absorbs energy equal to $\hbar\omega$.

$\omega_{k\ell} < 0$ $E_k < E_\ell$ and the system radiates a photon away. (Stimulated emission)

In the case where resonant absorbtion occurs, the first term in brackets in eq. (13) dominates and the probability of a transiti[on] to the k^{th} state is;

(14) $$P_{\ell k} = |c_k|^2 = \frac{4|\hat{V}_{k\ell}^2|}{\hbar^2(\omega_{k\ell}-\omega)^2}\sin^2\left[\frac{1}{2}(\omega_{k\ell}-\omega)\right]$$



THE GOLDEN RULE

Consider the situation in which the final excited state lies in a band of energies, such as ionization or free-particle scattering. These states comprise a continuum. For a density of these final states, $g(E_k)$, then

(15) $$dN = g(E_k)\, dE_k$$

represents the number of states from E_k to $E_k + dE_k$.

The probability that a transition occurs in a width of 2Δ centered about E_k is:

(16) $$\bar{P}_{\ell k} = \int_{E_k-\Delta}^{E_k+\Delta} P_{\ell k}\, dN$$

Inserting eq. (14) into this we find that

(17)* $$\bar{P}_{\ell k} = \int_{E_k-\Delta}^{E_k+\Delta} dE_k'\, g(E_k') \left| \frac{\hat{V}_{k\ell}}{\hbar} \right|^2 \frac{\sin^2\beta}{\beta^2/t^2} \qquad \beta \equiv \frac{\hbar}{2}(\omega_{k\ell} - \omega)t = \frac{1}{2\hbar}(E_k' - E_\ell - \hbar\omega)t$$

Noting that, for constant E_ℓ, t & ω, $dE_k' = \frac{2\hbar}{t}\, d\beta$ and owing to the rapid decrease of eq. (14) we may write:

(18) $$\bar{P}_{\ell k} = \frac{2t}{\hbar}\, g(E_k)\, |V_{k\ell}|^2 \int_{-\infty}^{\infty} \frac{\sin^2\beta}{\beta^2}\, d\beta$$

$$= t\left[\frac{2\pi}{\hbar}\, g(E_k)\, |V_{k\ell}|^2\right]$$

Thus, the transition probability rate is

(19) $$\boxed{\bar{W}_{\ell k} = \frac{2\pi}{\hbar}\, g(E_k)\, |V_{k\ell}|^2}$$ FERMI'S GOLDEN RULE