

and

$$H' = \frac{ie\hbar}{mc} \mathbf{A} \cdot \nabla. \quad (15.88)$$

In some cases, especially for forbidden transitions, the higher order term needs to be included. We will first address the problem assuming simple plane wave states for the electronic unperturbed problem. Later we will discuss the effect of Bloch central cell terms on the photon emission and absorption. The central cell terms play a crucial role in optical interactions in semiconductors, and, among other things, determine the selection rules.

The first order time dependent perturbation theory gives us the transition rates from the initial electron state  $|i\rangle$  to the final state  $|f\rangle$  by the golden rule

$$W(i) = \frac{2\pi}{\hbar} \sum_f \left| \langle f | H' | i \rangle \right|^2 \delta(E_f - E_i \mp \hbar\omega) \quad (15.89)$$

where the upper sign is for photon absorption and the lower one is for emission. For the scattering rate to have physical significance, we need to define the final state as having either a spread in the electronic states or a spread in the photonic states.

In case of absorption process, the final electronic states have a spread given by the concept of the density of states. For emission of photons, the spread is in the photon spectra. If we assume that the photons are spread over a range of frequency with width  $d\omega$ , we can write the photon density as

$$N_{\text{ph}} = n \rho(\hbar\omega) d(\hbar\omega) \quad (15.90)$$

where  $n$  is the photon occupation and  $\rho(\hbar\omega)$  is the photon density of states for a 3-dimensional volume of space is given by

$$\rho(\hbar\omega) = \frac{\omega^2}{2\pi^2 \hbar v^3} \quad (15.91)$$

where

$$v = c \text{ if } \epsilon = 1.$$

The vector potential is then given from Equation 15.18 by

$$\begin{aligned} |\mathbf{A}_0|^2 &= \frac{2\pi\hbar N_{\text{ph}} c^2}{\omega\epsilon} \\ &= \frac{2\pi\hbar c^2 n \rho(\omega) d\omega}{\omega\epsilon}. \end{aligned} \quad (15.92)$$

Expressing the final state density of states in terms of photon density of states we then get the absorption rate, after substituting for  $H'$  and  $\mathbf{A}_0$  in the Fermi golden rule

$$W_{\text{abs}}(\omega) = \frac{4\pi^2 e^2 n \rho(\omega)}{m^2 \omega \epsilon} \left| \int \psi_{\mathbf{k}'}^* \exp(i\mathbf{k}_{\text{ph}} \cdot \mathbf{r}) p_a \psi_{\mathbf{k}} d^3r \right|^2 \quad (15.93)$$

where  $\psi_{\mathbf{k}}$  and  $\psi_{\mathbf{k}'}$  represent the initial and final states of the electron and  $\mathbf{k}_{\text{ph}}$  is the photon wavevector.  $p_a$  is the momentum operator in the direction of the vector  $\mathbf{A}$ . We note that the photon intensity  $I(\omega)$  per unit frequency interval is

$$I(\omega) = V \hbar^2 \omega n \rho(\omega), \quad (15.94)$$

so that the absorption rate can also be written as

$$W_{\text{abs}} = \frac{4\pi^2 e^2 I(\omega)}{m^2 V \omega^2 \hbar^2 \epsilon} \left| \int \psi_{\mathbf{k}'}^* \exp(i\mathbf{k}_{\text{ph}} \cdot \mathbf{r}) p_a \psi_{\mathbf{k}} d^3r \right|^2 \quad (15.95)$$

In a similar manner, the emission rate is given by

$$W_{\text{em}} = \frac{4\pi^2 e^2 n \rho(\omega)}{m^2 \omega \epsilon} \left| \int \psi_{\mathbf{k}'}^* \exp(i\mathbf{k}_{\text{ph}} \cdot \mathbf{r}) p_a \psi_{\mathbf{k}} d^3r \right|^2. \quad (15.96)$$

The transition rates can be written in terms of final state electron density of states  $N(E_f)$  instead of photonic density of states  $\rho(\omega)$ , giving the transition rates

$$W_{\text{abs}} = \frac{4\pi^2 e^2 \hbar}{m^2 \epsilon} \frac{1}{\hbar\omega} n |a \cdot p_{if}|^2 N(E_f) \quad (15.97)$$

$N(E_f)$  is the reduced density of states since the transition energy is governed by ( $\mathbf{k}_{\text{ph}} \sim 0$  making the transitions "vertical")

$$\begin{aligned} \hbar\omega &= \frac{\hbar^2 k^2}{2} \left( \frac{1}{m_e^*} + \frac{1}{m_h^*} \right) \\ &= \frac{\hbar^2 k^2}{2m_r^*}. \end{aligned} \quad (15.98)$$

The quantity  $p_{if}$  is the momentum matrix element between the initial and final states. A similar term for emission of photons can be written.

In the expressions derived above, the emission and absorption theory are both proportional to  $n$ , the photon occupation. This result is modified when a proper quantum theory for the perturbation theory is used. As in the case of phonons, the general approach goes as follows:

Perturbation	$e\mathbf{A} \cdot \rho/mc$
Quantization of EM field	$\mathbf{A} \rightarrow a^\dagger + a$
	$a^\dagger =$ creation operator for photons
	$a =$ destruction operator of photon
Emission matrix element	$\langle n+1   a^\dagger   n \rangle \rightarrow (n+1)^{1/2}$
Absorption matrix element	$\langle n-1   a   n \rangle \rightarrow n^{1/2}$ .

With this approach we get the following rates written in terms of either photon or electron final state density of states. The main difference is that as with phonon emission, the emission process has a factor  $(n+1)$  instead of  $n$ . Thus,

photons can be emitted (spontaneous emission) even if there are no photons already present.

Final photon density of states

$$\begin{aligned} W_{\text{abs}} &= \frac{4\pi^2 e^2 \hbar}{m^2 \epsilon} \frac{1}{\hbar \omega} n |\mathbf{a} \cdot \mathbf{p}_{if}|^2 \rho(\hbar \omega) \\ W_{\text{em}} &= \frac{4\pi^2 e^2 \hbar}{m^2 \epsilon} \frac{1}{\hbar \omega} (n+1) |\mathbf{a} \cdot \mathbf{p}_{if}|^2 \rho(\hbar \omega) \\ \rho(\hbar \omega) &= \frac{\omega^2}{2\pi^2 \hbar v^3} \\ v &= \frac{c}{\sqrt{\epsilon}} \end{aligned} \quad (15.99)$$

Final electron density of states

$$\begin{aligned} W_{\text{abs}} &= \frac{4\pi^2 e^2 \hbar}{m^2 \epsilon} \frac{1}{\hbar \omega} n |\mathbf{a} \cdot \mathbf{p}_{if}|^2 N(E_f) \\ W_{\text{em}} &= \frac{4\pi^2 e^2 \hbar}{m^2 \epsilon} \frac{1}{\hbar \omega} (n+1) |\mathbf{a} \cdot \mathbf{p}_{if}|^2 N(E_f). \end{aligned} \quad (15.100)$$

The electronic density of states depends upon the material bandstructure and dimensionality, as we have discussed several times.

It may seem from the discussions above that the absorption or emission rates could be very different depending upon whether the photon or electron density of states are used. These two densities are obviously very different leading to very different rates. However, as shown in Figure 15.7, there is no inconsistency between these two rates. In a scattering process involving electrons and photons, we may be interested in the transition rate of either a particular photon or a particular electronic state. For example, in discussing absorption coefficient we are interested in the rate at which *photons* at a particular energy are absorbed. We do not care which electronic states are involved in the absorption process. Thus, we integrate over the electronic density of states. On the other hand, in emission processes we focus on the rate at which an electron in a given state in the conduction band recombines with a hole. In this case, we do not care about the particular nature of the photon emitted and, therefore, integrate over the final photon density of states. Of course, this is the usual way of defining absorption and emission process. One is perfectly free to use alternate descriptions, but one has to be careful to compare these rates with experimental results.

## 15.6 SELECTION RULES FOR OPTICAL PROCESSES

A number of selection rules which determine whether or not electron-photon interactions will take place can be derived by using simple symmetry arguments. We will examine these selection rules by examining the matrix element

$$|\mathbf{a} \cdot \mathbf{p}_{if}|^2 = \left| \int \psi_j^* p_a \psi_i e^{i\mathbf{q} \cdot \mathbf{r}} d^3 r \right|^2 \quad (15.101)$$

### ELECTRON - PHOTON SYSTEM

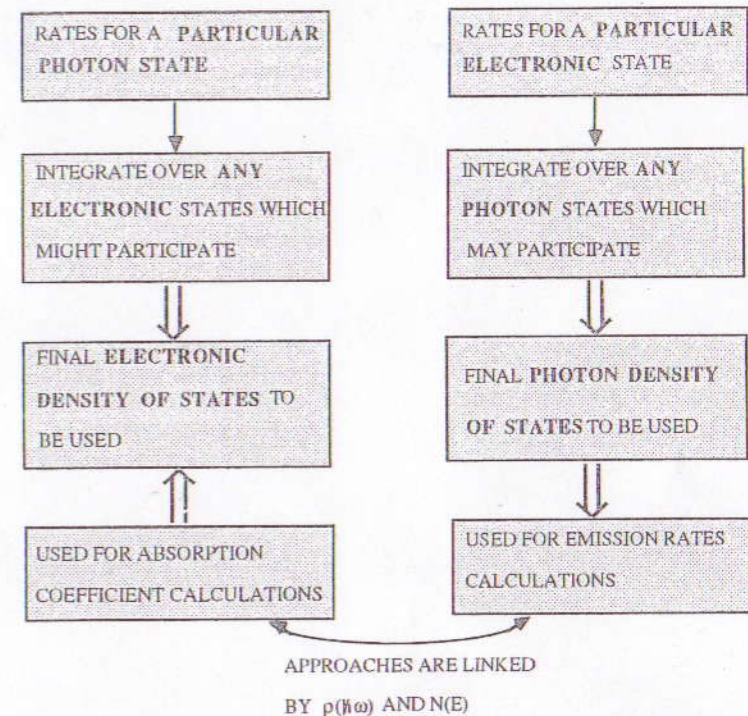


Figure 15.7: Final states used in scattering rates in the Fermi golden rule.

where  $p_a$  is the momentum component along the polarization direction. In most problems the relevant dimensions of the integration are such that  $\exp(i\mathbf{q} \cdot \mathbf{r})$  can be taken as a constant (= unity) in the integral. This approximation is called the dipole approximation. We can write

$$\frac{1}{m} \langle f | \mathbf{p} | i \rangle = \frac{d}{dt} \langle f | \mathbf{r} | i \rangle. \quad (15.102)$$

The time dependence of the initial and final states can be written as

$$|i(t)\rangle = |i(0)\rangle e^{iE_i t/\hbar} \quad (15.103)$$

$$|f(t)\rangle = |f(0)\rangle e^{iE_f t/\hbar} \quad (15.104)$$