Interband Transitions

While at low frequencies, the primary electronic and optical excitation mechanism is via free carrier conduction, as the photon energy approach the energy gap, a new conduction process can occur. An interband transition occurs when a photon excites a carrier from an occupied state in the valence band to an unoccupied state in the conduction band.

Points to consider:

1. We expect this process to have an energy threshold equal to the energy gap.
2. Transitions are either direct (i.e., conserve crystal momentum) or indirect (a phonon is involved, so $k_{\text{valence}} = k_{\text{conduction}} + q_{\text{phonon}}$). Note that $q_{\text{photon}} \ll G$, but $q_{\text{phonon}} \approx G$.

   Ex: Yellow light $-600 \text{ nm} = \lambda \Rightarrow k = \frac{2\pi}{\lambda} \approx 10^5 \text{ cm}^{-1}$, $G \approx 10^8 \text{ cm}^{-1}$.

3. The transition rate depends on the coupling between valence and conduction bands via the momentum matrix element:

   Electromagnetic Hamiltonian

   $$\mathcal{H} = \frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^2}{2m} + V(r) = \frac{p^2}{2m} + V(r) - \frac{e}{mc}\mathbf{A} \cdot \mathbf{p} + \frac{e^2\mathbf{A}^2}{2mc^2}$$

   Since optical fields usually represent a perturbation, we keep only the linear term, so

   $$\mathcal{H}' = -\frac{e}{mc}\mathbf{p} \cdot \mathbf{A}$$

4. The Pauli Exclusion Principle requires that an interband transition occurs from an occupied state below the Fermi level to an unoccupied state above the Fermi level.

5. Photons of a certain energy are more effective in producing interband transitions if the
energy separation between the bands is nearly constant over many $k$ values, where the two bands have a large joint density of state.

Large joint density of states from $E_c - E_v = \hbar \omega$ near $k = 0$

Large joint density of states from $A'$ to $A$.

Interband transitions contribute to the conductivity and to the dielectric constant. For a current density in the $\alpha$ direction due to a $\beta$-directed field.

Interband conductivity:

$$j_{\text{int}} = \sigma_{\text{int} \beta} E_{\beta}$$

where

$$\sigma_{\text{int} \beta} = -\frac{e^2}{m^2} \sum_{i,j} \frac{[f(E_i) - f(E_j)]}{E_i - E_j} \frac{\langle i | P_{\alpha} | i \rangle \langle j | P_{\beta} | j \rangle}{[-i\omega + \frac{1}{\epsilon} + \frac{1}{\hbar} (E_i - E_j)]}$$

sum over all valence and conduction states

The dielectric constant is then

$$\epsilon = \epsilon_{\text{core}} + \frac{4\pi i}{\alpha} \left[ \sigma_{\text{free carrier}} + \sigma_{\text{int}} \right]$$

Connection between Optical Transitions and Effective Mass: $k \cdot p$ Perturbation Theory
We will see that because of the connection between optical transition matrix elements between valence and conduction states $\langle \nu | p | c \rangle$ and the effective mass $\frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial k^2}$, band diagrams provide important information about optical properties. Conversely, experimental information about optical properties can provide information about $\mathcal{E}(k)$. If we have a Bloch solution to the Schrödinger equation

$$\psi_{nk}(r) = e^{ik \cdot r} u_{nk}(r)$$

and thus

$$\left[ \frac{p^2}{2m^*} + V(r) \right] e^{ik \cdot r} u_{nk}(r) = \mathcal{E}_n(k) e^{ik \cdot r} u_{nk}(r)$$

we also have

$$p e^{ik \cdot r} u_{nk}(r) = e^{ik \cdot r} (p + \hbar k) u_{nk}(r)$$

Therefore the equation for $u_{nk}(r)$ is

$$\left[ \frac{p^2}{2m^*} + V(r) + \frac{\hbar k \cdot p}{m} + \frac{\hbar^2 k^2}{2m} \right] u_{nk}(r) = \mathcal{E}_n(k) u_{nk}(r)$$

or

$$\left[ \frac{p^2}{2m} + V(r) + \frac{\hbar k \cdot p}{m} \right] u_{nk}(r) = \left[ \mathcal{E}_n(k) - \frac{\hbar^2 k^2}{2m} \right] u_{nk}(r)$$

$$[\mathcal{H}_0 + \mathcal{H}'] u_{nk}(r) = \mathcal{E}_n(k) u_{nk}(r)$$

If we know the solution at a point $k = k_0$, $k \cdot p$ perturbation theory allows us to find the $\mathcal{E}(k)$ for states near $k_0$. Let’s set $k = k_0 = 0$

$$\mathcal{E}_n(k) = \mathcal{E}_n(0) + \langle u_{n,0} | \mathcal{H}' | u_{n,0} \rangle + \sum_{n' \neq n} \frac{\langle u_{n,0} | \mathcal{H}' | u_{n',0} \rangle \langle u_{n',0} | \mathcal{H}' | u_{n,0} \rangle}{\mathcal{E}_n(0) - \mathcal{E}_{n'}(0)}$$

The first order term vanishes by inversion symmetry. ($\mathcal{H}'$ is odd, $u_{n,0}$ is either even or odd). Since

$$\mathcal{H}' = \frac{\hbar k \cdot p}{m}$$

the matrix element is

$$\langle u_{n,0} | \mathcal{H}' | u_{n',0} \rangle = \frac{\hbar}{m} k \cdot \langle u_{n,0} | p | u_{n',0} \rangle$$

Now assume

1. The bands $n$ and $n'$ are strongly coupled (close to each other and far away from other bands)
2. Interband transitions occur across an energy gap $\mathcal{E}_g$

n.b., again:

$$\mathcal{E}_n(k) = \mathcal{E}_n(0) - \frac{\hbar^2 k^2}{2m^*}$$

$$\mathcal{E}_n(k) = \mathcal{E}_n(0) + \frac{\hbar^2}{m^2} k_a k_\beta \frac{|\langle v | p_\alpha | c \rangle \langle c | p_\beta | v \rangle|}{\mathcal{E}_g}$$

$$\mathcal{E}_n(k) = \mathcal{E}_n(0) + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} k_a k_\beta$$

define effective mass by

$$\mathcal{E}_n(k) = \frac{\hbar^2 k^2}{2m^*} + \mathcal{E}_n(0)$$

then

$$\frac{1}{m_{\alpha \beta}^*} = \frac{\delta_{\alpha \beta}}{m} + \frac{2}{m^2} \frac{|\langle v | p_\alpha | c \rangle \langle c | p_\beta | v \rangle|}{\mathcal{E}_g}$$