

Lecture Notes on Interband Transitions

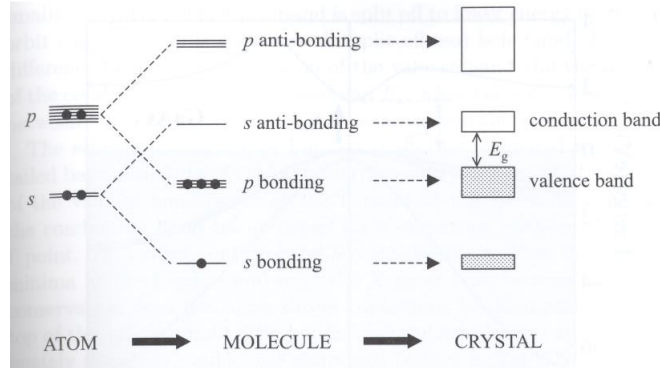
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1 Review of Band Structure

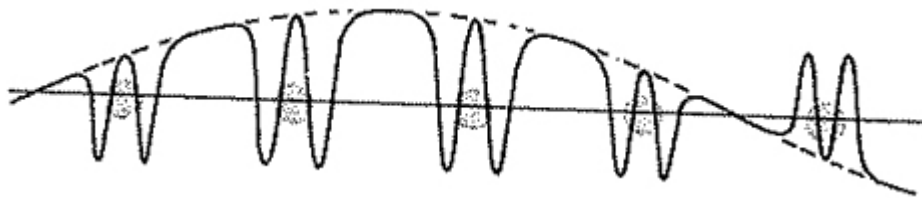
The "high school" view of band structure is illustrated in figure 1. The idea is that in atoms there are discrete degenerate energy levels such as s or p states, and then in molecules these energy levels get split based on symmetry/anti-symmetry and form bonding/anti-bonding pairs. These pairs are normally half filled as shown again are discrete but degenerate. Then in solids this idea is generalized to being bands that themselves are discrete, but inside the degeneracy is so high they appear continuous. Again only half of the states are filled and this divides valence and conduction bands.

Figure 1: The High School View of Band Structure [1]



A more sophisticated view on band structure comes from Quantum Mechanics, and specifically from Bloch's Theorem. The theorem states that in a periodic potential $\Psi(x+a) = \Psi(x)e^{i\kappa a}$. This leads to Bloch wave functions that are like plane-waves except they are locally modified by atomic potentials. One such example in 1-Dimension is shown in figure 2.

Figure 2: A Bloch Wave Function [2]



When solving for Bloch wave functions it becomes apparent that only certain values of k , called the reciprocal lattice vector, are allowed. The relation between k and the energy E is shown in Figure 3. The top plot shows the unfolded solution to this problem. The folding occurs because physically k can't be greater than π/a and so the allowed Energies fold onto themselves as suggested by the second plot in figure 3. This zone folding in k -space leads to only certain areas in x -space where the wave function is allowed, called Brillouin Zones. Further in these wave functions the particles (electrons) behave as though they had an effective mass proportional to $\frac{d^2}{dx^2} \frac{k}{E}$. Graphically the curvature of the E - k diagram is proportional to the inverse of the mass. Finally the energy gaps in between come about because of level repulsion, a common feature of nearly degenerate quantum systems.

Figure 3: A Visual Representation of How Energy Bands Come About



2 Interband Absorption

Absorption of photons in solids commonly occurs between bands and conduction to valence is one of the most common. This scenario is depicted in figure 4. Of note, absorption can happen across a wide range of frequencies because the electron does not need to start at the top of the conduction band or end at the bottom of the valence band.

Figure 4: An Energy Diagram of Interband Absorption [1]

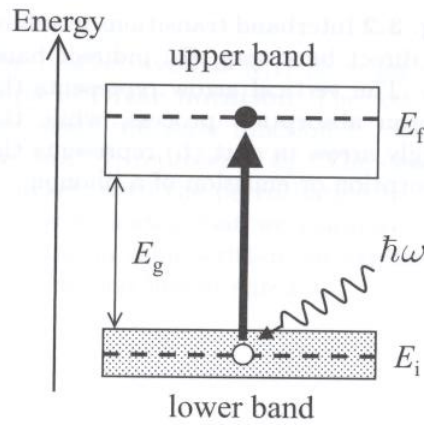
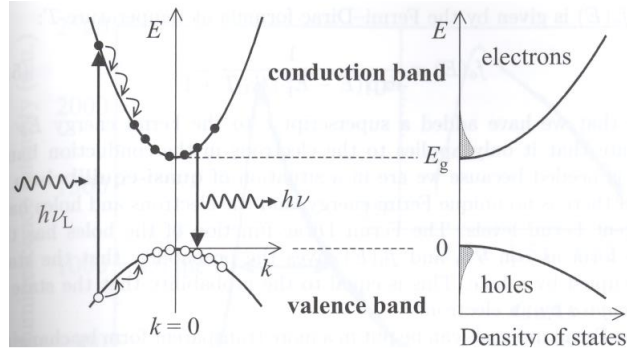


Figure 5 looks at interband absorption and emission in more detail. Although the electrons may not begin or end near the band edges, as shown in figure 5, they quite quickly relax to be at the band edges. Further the density of states shows the relative transition strengths of a sort; simply put transitions between the maxima in the density of states are most likely.

Figure 5: Absorption and Emission in Band Gap Solids [1]

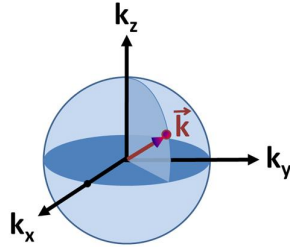


The transition rates between any two states is given by Fermi's Golden Rule: $W_{12} = \frac{2\pi}{\hbar} |M_{12}|^2 g(\hbar\omega)$ where $g(\hbar\omega)$ is the density of states and M_{12} is the matrix element between the two states defined as $M_{12} = \langle 2|H|1\rangle$ where the Hamiltonian is $H = \vec{p} \bullet E_0$.

3 Density of States

This derivation is done for 3-D parabolic bands. The total number of states is $g(E)dE = g(k)dk$ and $g(k)dk$ can be easily calculated. The number of states enclosed between $[k, k + dk]$ is $4\pi k^2 dk$ then $g(k)dk$ is $4\pi k^2 dk * \frac{abc}{(2\pi)^3} * \frac{1}{abc}$. The terms $\frac{abc}{(2\pi)^3}$ and $\frac{1}{abc}$ are the degeneracy per volume again divided by the total volume enclosed to make it unit less. Thus $g(E) = g(k) \frac{dk}{dE} = \frac{k^2}{2\pi^2} \frac{dk}{dE}$. Using the known information that our dispersion relation is $E = \frac{\hbar^2 k^2}{2m^*}$ so putting it all together $g(E) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}$.

Figure 6: K-Space Constant K-Surface in 3-D [3]



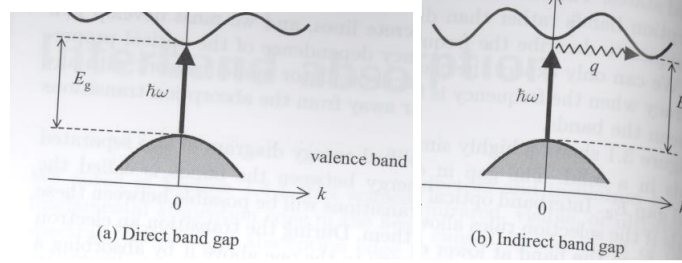
4 Direct and Indirect Absorption

Direct and indirect band gap semiconductors behave quite differently when exposed to light. As seen in figure 7, the key difference is that for indirect band gap materials to absorb photons they need to have a phonon interact as well. This is because $\frac{\pi}{a} \gg \frac{2\pi}{\lambda} = \vec{k}_{photon}$ so all optical transitions occur vertically in E-k space and for indirect band gap materials a phonon is required to give the electron the necessary momentum kick. Because of this key difference the absorption rates are different. For direct band gap materials, the absorption rate $a \sim (\hbar\omega - E_g)^{\frac{1}{2}}$ while indirect band gap materials $a \sim (\hbar\omega - E_g \pm \hbar\omega)^2$.

5 The 4 Band Model

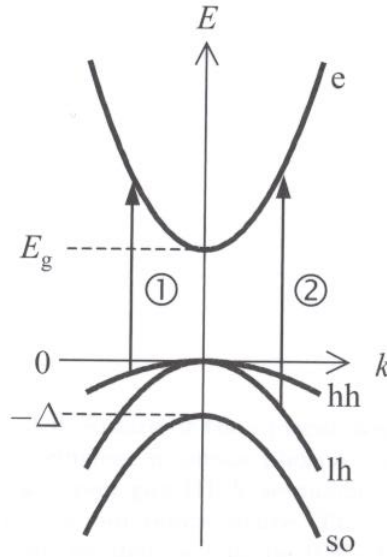
So far the only model discussed for the E-k relation has been a parabolic model, and this is primarily for simplicity. Real materials are not so simple. Near the

Figure 7: Direct and Indirect Band Gap Semiconductors [1]



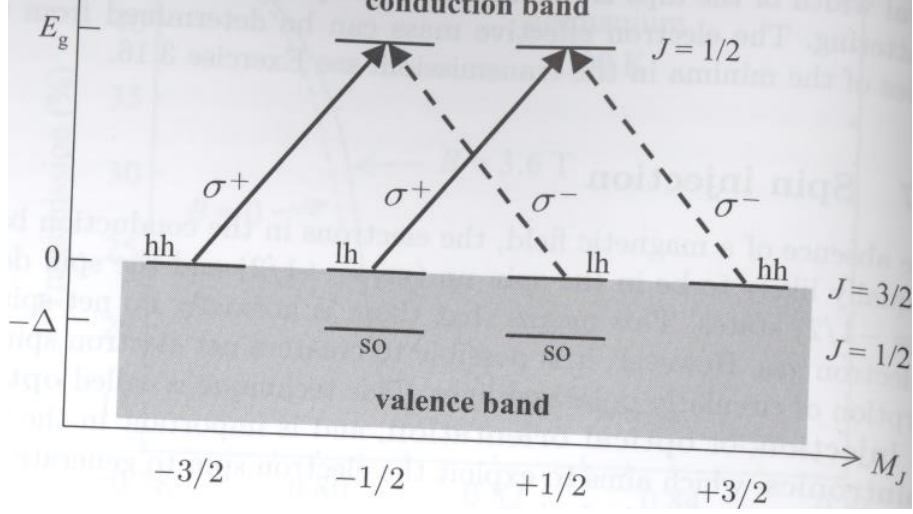
band edges they do behave parabolically, but there is often the complication of multiple conduction bands. This model is shown in figure 8. For the most part this model is a straight forward extension of the basic model. One complication is the different conduction bands have different spin quantum numbers. The valence band noted as e has $J = \frac{1}{2}$, the heavy hole band noted as hh has $J = \frac{3}{2}$, the light hole band noted as lh has $J = \frac{1}{2}$ and finally the spin-off hole band noted as so has $J = \frac{1}{2}$.

Figure 8: The 4 Band Model [1]



The difference in spin quantum numbers leads to spin injection, shown in detail in figure 9. The reason spin injection is important is that $|M_{12}|^2 \sim M_J$. This leads to heavy hole transitions being three times as likely as light hole transitions and generally dominating the dynamics.

Figure 9: Spin Injection[1]



References

- [1] Fox, Optical Properties of Solids
- [2] Wikipedia, Bloch Wave
- [3] Wikipedia, Density of States