Chapter 10

Optical Transitions in Semiconductor Quantum Wells

10.1 Introduction

10.1.1 Optical Transition in Bulk Semiconductors:

In Chapter 3 we calculated the transition rate due to stimulated absorption in bulk semiconductors and the results was,

$$R_{\uparrow}(\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega n n_{g}^{M} \varepsilon_{o}}\right) 2 \times \int_{\mathsf{FBZ}} \frac{d^{3}\vec{k}}{(2\pi)^{3}} \left|\vec{p}_{cv}(\vec{k}).\hat{n}\right|^{2} f_{v}(\vec{k}) \left[1 - f_{c}(\vec{k})\right] \delta\left(E_{c}(\vec{k}) - E_{v}(\vec{k}) - \hbar\omega\right)$$

The momentum matrix element was defined as,

$$\vec{P}_{cv}(\vec{k}).\,\hat{n} = \left\langle \psi_{c,\vec{k}} \middle| \,\hat{\vec{p}} .\,\hat{n} \middle| \psi_{v,\vec{k}} \right\rangle$$

The momentum matrix element is a function of the electron wavevector \vec{k} and also of the polarization direction of the electric field given by the unit vector \hat{n} . In III-V semiconductors with cubic symmetry (SC, FCC, or BCC) and spin-orbit coupling, near a band extremum the momentum matrix element is a strong function of the direction of the wavevector \vec{k} and a weak function of the magnitude of \vec{k} . When the integral over k-space is performed in calculating $R_{\uparrow}(\omega)$, and the electron and hole distributions are both symmetric in k-space, the result is independent of the polarization direction of the electric field. It is therefore convenient to assume an average value for the momentum matrix element and bring it out of the integral sign. This was what was done in Chapter 3 and the result was,

$$R_{\uparrow}(\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega \ln g^{M} \varepsilon_{o}}\right) \left\langle \left| \vec{p}_{cv} \cdot \hat{n} \right|^{2} \right\rangle 2 \times \int_{\text{FBZ}} \frac{d^{3}\vec{k}}{(2\pi)^{3}} f_{v}\left(\vec{k}\right) \left[1 - f_{c}\left(\vec{k}\right)\right] \delta\left(E_{c}\left(\vec{k}\right) - E_{v}\left(\vec{k}\right) - \hbar\omega\right)$$

The average value of the momentum matrix element is described in terms of the energy E_p ,

$$\left\langle \left| \vec{p}_{cv} \cdot \hat{n} \right|^2 \right\rangle = \frac{mE_p}{6}$$

In lower dimensional semiconductors, such as in semiconductor quantum wells, the electron occupation in k-space is not symmetric and therefore the average value of the momentum matrix element becomes dependent on the polarization direction of the electric field.

10.2 Optical Interband Transition in Quantum Wells

10.2.1 Introduction:

Consider a quantum well structure shown in the Figure below. We assume the following bulk energy dispersion relations for each material,

$$E_{c1}(k) = E_{c1} + \frac{\hbar^2}{2m_{e1}} \left(k_x^2 + k_y^2 + k_z^2 \right)$$
$$E_{c2}(k) = E_{c2} + \frac{\hbar^2}{2m_{e2}} \left(k_x^2 + k_y^2 + k_z^2 \right)$$
$$E_{v1}(k) = E_{v1} - \frac{\hbar^2}{2m_{h1}} \left(k_x^2 + k_y^2 + k_z^2 \right)$$
$$E_{v2}(k) = E_{v2} - \frac{\hbar^2}{2m_{h2}} \left(k_x^2 + k_y^2 + k_z^2 \right)$$



The energy dispersion for the conduction band states in the quantum well can be written as,

$$E_c(s, \vec{k}_{||}) = E_{c2} + E_s^c + \frac{\hbar^2 k_{||}^2}{2m_{e2}}$$
 { { s = 1, 2, 3

The dispersion relation for the valence band states in the quantum well is,

$$E_{v}(p,\vec{k}_{||}) = E_{v2} - E_{p}^{v} - \frac{\hbar^{2}k_{||}^{2}}{2m_{h2}} \qquad \{p = 1, 2, 3...\}$$

The corresponding wavefunctions in the effective mass approximation for the conduction and valence band states near the wavevector \vec{k}_0 can be written as,

$$\psi_{\boldsymbol{c},\boldsymbol{s},\vec{k}_{\parallel}}(\vec{r}) = \frac{e^{i\boldsymbol{k}_{\parallel}.\vec{\rho}}}{\sqrt{A}} \phi_{\boldsymbol{s}}^{\boldsymbol{c}}(\boldsymbol{z}) \sqrt{V} \psi_{\boldsymbol{c},\vec{k}_{o}}(\vec{r})$$
(1)
$$\psi_{\boldsymbol{v},\boldsymbol{p},\vec{k}_{\parallel}}(\vec{r}) = \frac{e^{i\vec{k}_{\parallel}.\vec{\rho}}}{\sqrt{A}} \phi_{\boldsymbol{p}}^{\boldsymbol{v}}(\boldsymbol{z}) \sqrt{V} \psi_{\boldsymbol{v},\vec{k}_{o}}(\vec{r})$$
(2)

Here, the position vector in the plane of the quantum well is $\vec{\rho} = x\hat{x} + y\hat{y}$ and A is the area of the quantum well and V is the volume of the entire crystal. The wavevector \vec{k}_0 deserves a bit more scrutiny. Generally it is taken to be the wavevector corresponding to the band extremum. For example, in III-Vs \vec{k}_0 could be assumed to be zero. This strategy works because Bloch functions are not strongly dependent on the magnitude of the wavevector near band extrema. In III-V semiconductors with cubic symmetry (SC, FCC, or BCC) and spin-orbit coupling, Bloch functions are strongly dependent on the direction of

the wavevector near band extrema. A much better strategy is to choose the wavevector \vec{k}_o such that its magnitude is approximately zero but its direction is the direction of the wavevector of the Bloch function closest to the quantum state under consideration. For example, consider the state $\psi_{c,s,\vec{k}_{\parallel}}(\vec{r})$. Noting that the z-dependent part of the envelope function will have the approximate form $\sin(k_z z)$ or $\cos(k_z z)$, where k_z is $s\pi/L$, the best choice for the direction of the wavevector \vec{k}_o is either one of the directions given by the two wavevectors $(\pm s\pi/L)\hat{z} + \vec{k}_{\parallel}$ and both these choices give the same result as far as optical transition rate is concerned. The wavevector \vec{k}_o is therefore a function of the wavevector \vec{k}_{\parallel} . Also note that since $|\vec{k}_{\parallel}| \ll \pi/L$, the wavevector \vec{k}_o is almost parallel to the z-axis.

We assume the proper normalization of the Bloch functions,

$$\int d^{3}\vec{r} \left| \psi_{\boldsymbol{c},\vec{k}_{o}}\left(\vec{r}\right) \right|^{2} = \int d^{3}\vec{r} \left| \psi_{\boldsymbol{v},\vec{k}_{o}}\left(\vec{r}\right) \right|^{2} = 1$$

This implies that the periodic part of the Bloch functions are normalized such that,

$$\frac{V}{\Omega}\int_{\Omega}d^{3}\vec{r}\left|u_{c,\vec{k}_{o}}\left(\vec{r}\right)\right|^{2}=\frac{V}{\Omega}\int_{\Omega}d^{3}\vec{r}\left|u_{v,\vec{k}_{o}}\left(\vec{r}\right)\right|^{2}=1$$

The integral above is over one primitive cell of volume Ω . Unity normalizations of the states $\psi_{c,s,\vec{k}_{\parallel}}(\vec{r})$ and $\psi_{v,p,\vec{k}_{\parallel}}(\vec{r})$ then require,

$$\int_{-\infty}^{+\infty} \left| \phi_{s}^{c}(z) \right|^{2} dz = 1 \qquad \qquad \int_{-\infty}^{+\infty} \left| \phi_{p}^{v}(z) \right|^{2} dz = 1$$

The proof is given below.

$$\int d^{3}\vec{r} \left| \psi_{c,s,\vec{k}_{\parallel}}(\vec{r}) \right|^{2} = 1$$

$$\Rightarrow \int d^{3}\vec{r} \left| \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \sqrt{V} \psi_{c,\vec{k}_{0}}(\vec{r}) \right|^{2} = 1$$

$$\Rightarrow V \int d^{3}\vec{r} \left| \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \right|^{2} \left| \psi_{c,\vec{k}_{0}}(\vec{r}) \right|^{2} = 1$$

$$\Rightarrow V \sum_{j} \left| \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \right|^{2}_{\vec{r}=\vec{R}_{j}} \int_{j-\text{th primitive cell}} d^{3}\vec{r} \left| \psi_{c,\vec{k}_{0}}(\vec{r}) \right|^{2} = 1$$

$$\Rightarrow \sum_{j} \Omega \left| \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \right|^{2}_{\vec{r}=\vec{R}_{j}} \frac{V}{\Omega} \int_{\text{one primitive cell}} d^{3}\vec{r} \left| u_{c,\vec{k}_{0}}(\vec{r}) \right|^{2} = 1$$

$$\Rightarrow \sum_{j} \Omega \left| \frac{e^{i\vec{k}_{\parallel} \cdot \vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \right|_{\vec{r} = \vec{R}_{j}}^{2} \frac{V}{\Omega} \int_{\Omega} d^{3}\vec{r} \left| u_{c,\vec{k}_{0}}(\vec{r}) \right|^{2} = 1$$
$$\Rightarrow \sum_{j} \Omega \left| \frac{e^{i\vec{k}_{\parallel} \cdot \vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \right|_{\vec{r} = \vec{R}_{j}}^{2} = 1$$
$$\Rightarrow \int d^{3}\vec{r} \left| \frac{e^{i\vec{k}_{\parallel} \cdot \vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \right|^{2} = 1$$
$$\Rightarrow \int_{-\infty}^{\infty} dz \left| \phi_{s}^{c}(z) \right|^{2} = 1$$

10.2.2 Momentum Matrix Elements:

In order to calculate the optical transition rates in quantum wells we will need momentum matrix element between the valence and conduction band states. We assume that the valence band and the conduction band states are,

$$\psi_{c,s,\vec{k}_{||}}(\vec{r}) = \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{s}^{c}(z) \sqrt{V} \psi_{c,\vec{k}_{o}}(\vec{r}) \qquad \psi_{v,p,\vec{k}_{||}}(\vec{r}) = \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{p}^{v}(z) \sqrt{V} \psi_{v,\vec{k}_{o}}(\vec{r})$$

This matrix element is calculated below,

$$\left\langle \psi_{c,s,\vec{k}_{||}} \middle| e^{i\vec{q}\cdot\hat{\vec{r}}}\hat{\vec{p}}\cdot\hat{n} \middle| \psi_{v,p,\vec{k}_{||}} \right\rangle = \int d^{3}\vec{r} \; \psi_{c,s,\vec{k}_{||}}^{*}(\vec{r}) \quad e^{i\vec{q}\cdot\vec{r}} \; \hat{\vec{p}}\cdot\hat{n} \; \psi_{v,p,\vec{k}_{||}}(\vec{r})$$

$$= V \int d^{3}\vec{r} \; \frac{e^{-i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} \; \psi_{c,\vec{k}_{0}}^{*}(\vec{r}) \quad e^{i\vec{q}\cdot\vec{r}} \; \hat{\vec{p}}\cdot\hat{n} \; \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{p}^{v}(z) \psi_{v,\vec{k}_{0}}(\vec{r})$$

$$= V \int d^{3}\vec{r} \; \frac{e^{-i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} \; e^{-i\vec{k}_{0}\cdot\vec{r}} u_{c,\vec{k}_{0}}^{*}(\vec{r}) \quad e^{i\vec{q}\cdot\vec{r}} \; \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} e^{i\vec{k}_{0}\cdot\vec{r}} \left(\hat{\vec{p}} + \hbar \left(\vec{k}_{0} + \vec{k}_{||} \right) \right) \cdot \hat{n} \; \phi_{p}^{v}(z) u_{v,\vec{k}_{0}}(\vec{r})$$

$$= V \int d^{3}\vec{r} \; \frac{e^{-i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} \; u_{c,\vec{k}_{0}}^{*}(\vec{r}) \quad e^{i\vec{q}\cdot\vec{r}} \; \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \; \hat{\vec{p}}\cdot\hat{n} \; \phi_{p}^{v}(z) u_{v,\vec{k}_{0}}(\vec{r})$$

Note that we have ignored the exponentials containing the wavevectors \vec{k}_0 and \vec{k}_0 since the magnitudes of these wavevectors are assumed to be close to zero. As in the bulk case, we will also assume that the photon wavevector \vec{q} is very small compared to the electronic wavevectors and can be ignored. We then have,

$$\left\langle \psi_{c,s,\vec{k}_{||}} \left| e^{i\vec{q}\cdot\vec{r}}\hat{\vec{p}}\cdot\hat{n} \right| \psi_{v,p,\vec{k}_{||}} \right\rangle$$

$$= V \int d^{3}\vec{r} \frac{e^{-i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} u_{c,\vec{k}_{o}}^{*}(\vec{r}) \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \hat{\vec{p}}\cdot\hat{n} \phi_{p}^{v}(z) u_{v,\vec{k}_{o}}(\vec{r})$$

$$= V \int d^{3}\vec{r} \frac{e^{-i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} u_{c,\vec{k}_{o}}^{*}(\vec{r}) \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{p}^{v}(z) \hat{\vec{p}}\cdot\hat{n} u_{v,\vec{k}_{o}}(\vec{r})$$

$$+ V \int d^{3}\vec{r} \frac{e^{-i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} u_{c,\vec{k}_{o}}^{*}(\vec{r}) \frac{e^{i\vec{k}_{||}\cdot\vec{\rho}}}{\sqrt{A}} u_{v,\vec{k}_{o}}(\vec{r}) p_{z}n_{z} \phi_{p}^{v}(z)$$

In the first term on the right hand side the momentum operator acts on the periodic part of the Bloch function, and in the second term the z-component of the momentum operator acts on the envelope function. In each term, the rapidly varying periodic part and the slowly varying envelope part can be separated to get,

$$\left\langle \psi_{c,s,\vec{k}_{\parallel}} \left| e^{i\vec{q}\cdot\vec{r}}\hat{\vec{p}}\cdot\hat{n} \right| \psi_{v,p,\vec{k}_{\parallel}} \right\rangle$$

$$= \int d^{3}\vec{r} \frac{e^{-i\vec{k}_{\parallel}\cdot\vec{p}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} \frac{e^{i\vec{k}_{\parallel}\cdot\vec{p}}}{\sqrt{A}} \phi_{p}^{v}(z) \frac{V}{\Omega} \int_{\Omega} d^{3}\vec{r} u_{c,\vec{k}_{0}}^{*}(\vec{r}) \hat{\vec{p}}\cdot\hat{n} u_{v,\vec{k}_{0}}(\vec{r})$$

$$+ \frac{V}{\Omega} \int_{\Omega} d^{3}\vec{r} u_{c,\vec{k}_{0}}^{*}(\vec{r}) u_{v,\vec{k}_{0}}(\vec{r}) \int d^{3}\vec{r} \frac{e^{-i\vec{k}_{\parallel}\cdot\vec{p}}}{\sqrt{A}} \frac{e^{i\vec{k}_{\parallel}\cdot\vec{p}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} p_{z}n_{z} \phi_{p}^{v}(z)$$

The second term on the right hand side is zero since the periodic parts of the valence and the conduction band Bloch functions are orthogonal. We finally get,

$$\left\langle \psi_{c,s,\vec{k}_{\parallel}} \middle| e^{i\vec{q}\cdot\vec{r}}\hat{\vec{p}}\cdot\hat{n} \middle| \psi_{v,p,\vec{k}_{\parallel}} \right\rangle$$

$$= \vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o})\cdot\hat{n} \int d^{3}\vec{r} \frac{e^{-i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{p}^{v}(z)$$

$$= \vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o})\cdot\hat{n} \int d^{2}\vec{\rho} \int dz \frac{e^{-i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \left[\phi_{s}^{c}(z) \right]^{*} \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \phi_{p}^{v}(z)$$

$$= \vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o})\cdot\hat{n} \int d^{2}\vec{\rho} \frac{e^{-i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} \int dz \left[\phi_{s}^{c}(z) \right]^{*} \phi_{p}^{v}(z)$$

$$= \delta_{\vec{k}_{\parallel},\vec{k}_{\parallel}} \quad \vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o})\cdot\hat{n} \int dz \left[\phi_{s}^{c}(z) \right]^{*} \phi_{p}^{v}(z)$$

The final result shows that the crystal momenta of the initial and final states must be equal and that the momentum matrix element is weighted by the overlap integral of the envelop functions of the conduction and valence band states in the direction of quantum confinement. This overlap integral will give us and important selection rule for optical transitions in quantum wells.

10.2.3 Calculation of the Optical Transition Rates:

The optical transition rates in quantum wells can be calculated using Fermi's golden rule. Assuming the photon density at the location of the quantum well to be n_p , the expressions for the rate of stimulated absorption $R_{\uparrow}(s, p, \omega)$ (units: transitions per unit area per second) and the rate of stimulated emission $R_{\downarrow}(s, p, \omega)$ (units: transitions per unit area per second) for the *s*-th conduction subband and the *p*-th valence subband are,

$$R_{\uparrow}(s,p,\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega \ln_{g}^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \times 2 \times \int \frac{d^{2}\vec{k}_{\parallel}}{(2\pi)^{2}} \left| \vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o}^{'}) \cdot \hat{n} \right|^{2} f_{v}(p,\vec{k}_{\parallel}) \left[1 - f_{c}(s,\vec{k}_{\parallel}) \right] \delta\left(E_{c}(s,\vec{k}_{\parallel}) - E_{v}(p,\vec{k}_{\parallel}) - \hbar\omega\right) \\ R_{\downarrow}(s,p,\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega \ln_{g}^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \times 2 \times \int \frac{d^{2}\vec{k}_{\parallel}}{(2\pi)^{2}} \left| \vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o}^{'}) \cdot \hat{n} \right|^{2} f_{c}(s,\vec{k}_{\parallel}) \left[1 - f_{v}(p,\vec{k}_{\parallel}) \right] \delta\left(E_{c}(s,\vec{k}_{\parallel}) - E_{v}(p,\vec{k}_{\parallel}) - \hbar\omega\right)$$



The above expressions are similar to the expressions obtained in Chapter 3 for bulk semiconductors. The main differences are the presence of the overlap integrals involving the envelope functions and the fact that the summations are performed over the two dimensional k-space relevant to a quantum well and not over a three dimensional k-space as in the case of bulk semiconductors.

10.2.4 Subband Selection Rule:

The integral $\left|\int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z)\right|^{2}$ appearing in the transition

rates allows optical transitions between conduction and valence band states whose envelope functions have the same parity; either both have odd symmetry or both have even symmetry with respect to spatial inversion in the z-dimension. Therefore, both s and p have to be either even or both have to be odd for $R_{\uparrow}(s, p, \omega) \neq 0$. This selection rule is relaxed if the confining

potential of the quantum well does not have inversion symmetry in the z-dimension, in which case the envelope functions do not have a definite parity.

10.2.5 Average Values of Squared Momentum Matrix Elements and Transition Rates:

The squared momentum matrix element $\left|\vec{p}_{cv}(\vec{k}_{o},\vec{k}_{o}),\hat{n}\right|^{2}$ is a function of the wavevector \vec{k}_{\parallel} . The electron and hole distributions in k-space for a bulk semiconductor and for a semiconductor quantum well are shown below.



Electron and hole distribution in a bulk semiconductor

Electron and hole distribution in a semiconductor quantum well

It can be seen that the carrier distribution in k-space is not symmetric in a quantum well. Consequently, the average value of $\left|\vec{p}_{cv}(\vec{k}_o, \vec{k}_o'), \hat{n}\right|^2$ is not independent of the polarization direction of the electric field. The average value of $\left|\vec{p}_{cv}(\vec{k}_o, \vec{k}_o'), \hat{n}\right|^2$ is also different for transitions between a heavy-hole subband and a conduction subband and for transitions between a light-hole subband and a conduction subband. The results are summarized below.

Transition involving a heavy-hole subband and a conduction subband:

$$\left\langle \left| \vec{p}_{cv} \left(\vec{k}_{o}, \vec{k}_{o} \right) \cdot \hat{n} \right|^{2} \right\rangle = \frac{m E_{p}}{4} \left(n_{x}^{2} + n_{y}^{2} \right)$$

The rates for stimulated emission and absorption can be written as,

$$R_{\uparrow}(\mathbf{s}, \mathbf{p}, \omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega n n_{g}^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \frac{m E_{p}}{4} \left(n_{x}^{2} + n_{y}^{2}\right) \times 2 \times \int \frac{d^{2} \vec{k}_{||}}{(2\pi)^{2}} f_{v}\left(p, \vec{k}_{||}\right) \left[1 - f_{c}\left(s, \vec{k}_{||}\right)\right] \delta\left(E_{c}\left(s, \vec{k}_{||}\right) - E_{v}\left(p, \vec{k}_{||}\right) - \hbar\omega\right)$$
$$R_{\downarrow}(s, p, \omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega n n_{g}^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \frac{m E_{p}}{4} \left(n_{x}^{2} + n_{y}^{2}\right) \times 2 \times \int \frac{d^{2} \vec{k}_{||}}{(2\pi)^{2}} f_{c}\left(s, \vec{k}_{||}\right) \left[1 - f_{v}\left(p, \vec{k}_{||}\right)\right] \delta\left(E_{c}\left(s, \vec{k}_{||}\right) - E_{v}\left(p, \vec{k}_{||}\right) - \hbar\omega\right)$$

The above expression shows that optical transitions between a heavy-hole subband and a conduction subband are only possible if the electric field has a component in the plane of the quantum well.

Transition involving a light-hole subband and a conduction subband:

$$\left\langle \left| \vec{p}_{cv} \left(\vec{k}_{o}, \vec{k}_{o} \right) \cdot \hat{n} \right|^{2} \right\rangle = \frac{mE_{p}}{4} \left[\frac{1}{3} \left(n_{x}^{2} + n_{y}^{2} \right) + \frac{4}{3} n_{z}^{2} \right]$$

The rates for stimulated emission and absorption can be written as,

$$\begin{aligned} R_{\uparrow}(s,p,\omega) &= \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega \ln g^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{m}^{v}(z) \right|^{2} \frac{mE_{p}}{4} \left[\frac{1}{3} \left(n_{x}^{2} + n_{y}^{2}\right) + \frac{4}{3} n_{z}^{2}\right] \times \\ & 2 \times \int \frac{d^{2}\vec{k}_{||}}{(2\pi)^{2}} f_{v}\left(p,\vec{k}_{||}\right) \left[1 - f_{c}\left(s,\vec{k}_{||}\right)\right] \delta\left(E_{c}\left(s,\vec{k}_{||}\right) - E_{v}\left(p,\vec{k}_{||}\right) - \hbar\omega\right) \\ & R_{\downarrow}(s,p,\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega \ln g^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \frac{mE_{p}}{4} \left[\frac{1}{3} \left(n_{x}^{2} + n_{y}^{2}\right) + \frac{4}{3} n_{z}^{2}\right] \times \\ & 2 \times \int \frac{d^{2}\vec{k}_{||}}{(2\pi)^{2}} f_{c}\left(s,\vec{k}_{||}\right) \left[1 - f_{v}\left(p,\vec{k}_{||}\right)\right] \delta\left(E_{c}\left(s,\vec{k}_{||}\right) - E_{v}\left(p,\vec{k}_{||}\right) - \hbar\omega\right) \end{aligned}$$

Optical transitions between a light-hole subband and a conduction subband are stronger (by about four times) if the electric field is polarized perpendicular to the plane of the quantum well.

Parameters at 300K	GaAs	AlAs	InAs	InP	GaP
Ep (eV)	25.7	21.1	22.2	20.7	22.2

10.2.6 Joint Density of States in Quantum Wells:

The integral,

$$2 \times \int \frac{d^2 \vec{k}_{||}}{(2\pi)^2} \,\delta\left(E_c\left(s, \vec{k}_{||}\right) - E_v\left(p, \vec{k}_{||}\right) - \hbar\omega\right)$$

represents the joint density of states for optical transitions. As an example, we consider the rate for stimulated absorption involving a heavy-hole subband and a conduction subband and assume that the valence subband is completely full and the conduction subband is completely empty,

$$R_{\uparrow}(s,p,\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega n n_{g}^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \frac{m E_{p}}{4} \left(n_{x}^{2} + n_{y}^{2}\right) \times 2 \times \int \frac{d^{2} \vec{k}_{||}}{(2\pi)^{2}} \delta\left(E_{c}\left(s,\vec{k}_{||}\right) - E_{v}\left(p,\vec{k}_{||}\right) - \hbar\omega\right)$$

We assume the following energy dispersions for the conduction subband and the heavy-hole subband,

$$E_{c}(s,\vec{k}_{||}) = E_{c2} + E_{s}^{c} + \frac{\hbar^{2}k_{||}^{2}}{2m_{e2}} \qquad \{s = 1, 2, 3 \dots \\ E_{v}(p,\vec{k}_{||}) = E_{v2} - E_{p}^{v} - \frac{\hbar^{2}k_{||}^{2}}{2m_{hh2}} \qquad \{p = 1, 2, 3 \dots \}$$

We define the reduced effective mass m_{r2} as follows,

$$E_{c}(s,\vec{k}_{||}) - E_{v}(p,\vec{k}_{||}) = E_{g2} + E_{s}^{c} + E_{p}^{v} + \frac{\hbar^{2}k_{||}^{2}}{2} \left(\frac{1}{m_{e2}} + \frac{1}{m_{hh2}}\right)$$
$$= E_{g2} + E_{s}^{c} + E_{p}^{v} + \frac{\hbar^{2}k^{2}}{2m_{r2}}$$

The joint density of states can be found by the methods described in Chapter 3 and the result is,

$$2 \times \int \frac{d^2 \vec{k}_{||}}{(2\pi)^2} \,\delta\left(\boldsymbol{E}_{c}\left(\boldsymbol{s}, \vec{k}_{||}\right) - \boldsymbol{E}_{v}\left(\boldsymbol{p}, \vec{k}_{||}\right) - \hbar\omega\right) = \frac{m_{r2}}{\pi \,\hbar^2} \,\theta\left(\hbar\omega - \boldsymbol{E}_{g2} - \boldsymbol{E}_{s}^{c} - \boldsymbol{E}_{p}^{v}\right)$$

The rate for stimulated absorption is then, $B_{\Delta}(s, p, w) =$

$$\left(\frac{q}{m}\right)^{2} \left(\frac{\pi n_{p}}{\omega n n_{g}^{M} \varepsilon_{o}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \frac{m E_{p}}{4} \left(n_{x}^{2} + n_{y}^{2}\right) \times \frac{m_{r2}}{\pi \hbar^{2}} \theta \left(\hbar \omega - E_{g2} - E_{s}^{c} - E_{p}^{v}\right)$$

10.2.7 Volume Rates for Stimulated Transitions:

The total rate of stimulated absorption $R_{\uparrow}(\omega)$ and of stimulated emission $R_{\downarrow}(\omega)$ (units: transitions per unit volume per second) can be obtained by summing the transition rates for each possible pair of conduction and valence subbands,

$$R_{\downarrow}(\omega) = \sum_{p,s} \frac{R_{\downarrow}(s, p, \omega)}{L}$$
$$R_{\uparrow}(\omega) = \sum_{p,s} \frac{R_{\uparrow}(s, p, \omega)}{L}$$

In the expressions above, the transition rates per unit area have been divided by the width of the quantum well to get the transition rates per unit volume.

10.2.8 Optical Absorption Coefficient:

The absorption (or loss) coefficient for the quantum well can be obtained as discussed in Chapter 3, $\sum R_{\downarrow}(s, p, \omega) - R_{\uparrow}(s, p, \omega)$

$$\alpha(\omega) = \frac{R_{\uparrow}(\omega) - R_{\downarrow}(\omega)}{n_{p} v_{g}^{M}} = \sum_{p,s} \frac{\sum_{p,s} R_{\downarrow}(s, p, \omega) - R_{\uparrow}(s, p, \omega)}{L n_{p} v_{g}^{M}}$$

In general, contributions from both heavy-hole and light-hole bands are included in the absorption coefficient, $\alpha(\omega) = \alpha_{hh}(\omega) + \alpha_{\ell h}(\omega)$

The Figure above shows the absorption coefficient plotted for the case of two heavy-hole subbands and two conduction subbands assuming that the heavy-hole subbands are all occupied and the conduction subbands are all empty.

10.2.9 Spontaneous Emission Rates:

The spontaneous emission rate into a single radiation mode is obtained from the corresponding stimulated emission rate assuming one photon in the mode. For example, the spontaneous emission rate $R_{sp}(s, p, \omega)$

(units: transitions per unit area per second) for the *s*-th conduction subband and the *p*-th valence subband is,

$$R_{\downarrow}(s,p,\omega) = \left(\frac{q}{m}\right)^{2} \left(\frac{\pi}{\omega n n_{g}^{M} \varepsilon_{o}}\right) \left(\frac{1}{V_{p}}\right) \left| \int dz \left[\phi_{s}^{c}(z)\right]^{*} \phi_{p}^{v}(z) \right|^{2} \times 2 \times \int \frac{d^{2}\vec{k}_{\parallel}}{(2\pi)^{2}} \left| \vec{p}_{cv}\left(\vec{k}_{o},\vec{k}_{o}\right) \cdot \hat{n} \right|^{2} f_{c}\left(s,\vec{k}_{\parallel}\right) \left[1 - f_{v}\left(p,\vec{k}_{\parallel}\right)\right] \delta\left(E_{c}\left(s,\vec{k}_{\parallel}\right) - E_{v}\left(p,\vec{k}_{\parallel}\right) - \hbar\omega\right)$$

The total spontaneous emission rate $R_{sp}(\omega)$ (units: transitions per unit volume per second) is obtained by including the contributions from each possible pair of conduction and valence subbands,

$$R_{sp}(\omega) = \sum_{p,s} \frac{R_{sp}(s, p, \omega)}{L}$$

The total spontaneous emission rate R_{Tsp} (per unit volume of the material) into all the radiation modes can be written, as in the case of bulk semiconductors, in terms of the absorption coefficient,

$$R_{Tsp} = \int_{0}^{\infty} R_{sp}(\omega) V_{p} g_{p}(\omega) d\omega$$
$$R_{Tsp} = \int_{0}^{\infty} V_{g}^{M} \alpha(\omega) \frac{g_{p}(\omega)}{e^{(\hbar\omega - qV)/KT} - 1} d\omega$$

10.2.10 Population Inversion and Optical Gain:

In the Figure below, the loss coefficient for one conduction subband and one heavy-hole subband is plotted as a function of the photon frequency for different values of the electron and hole densities assuming that electrons are taken from the valence band and placed in the conduction band thereby creating population inversion. Given a value for the Fermi level splitting, optical frequencies for which $E_{g2} + E_1^c + E_1^v < \hbar\omega < E_{fe} - E_{fh}$ experience optical gain and frequencies for which $\hbar\omega > E_{g2} + E_1^c + E_1^v$, $E_{fe} - E_{fh}$ experience optical loss.



Optical gain $g(\omega)$ is defined, as in the bulk semiconductors, to be equal to $-\alpha(\omega)$. The following relations useful for bulk semiconductors also hold for quantum wells,

$$R_{\downarrow}(\omega) - R_{\uparrow}(\omega) = v_g^M g(\omega) n_p$$
$$R_{\uparrow}(\omega) - R_{\downarrow}(\omega) = v_g^M \alpha(\omega) n_p$$
$$R_{sp}(\omega) = v_g^M g(\omega) \frac{n_{sp}(\omega)}{V_p}$$

10.3 Optical Intraband Processes in Quantum Wells

10.3.1 Free-Carrier Losses in Quantum Wells:

In Chapter 6 we discussed the contributions to the absorption coefficient coming from interband and intraband optical processes. The absorption coefficient can be written as,

 $\alpha(\omega) = \alpha(\omega)_{interband} + \alpha(\omega)_{intraband}$

In previous Sections, we discussed the contributions to the absorption coefficient from interband transitions. From the discussion in Chapter 3, we can write the intraband contribution to the absorption coefficient as,

$$\alpha(\omega)_{\text{intraband}} = \frac{1}{\varepsilon_{o} c n(\omega) L} \left[\frac{nq^{2}\tau_{e}/m_{e}}{\left(1 + \omega^{2}\tau_{e}^{2}\right)} + \frac{pq^{2}\tau_{h}/m_{h}}{\left(1 + \omega^{2}\tau_{h}^{2}\right)} \right]$$

Notice that in contrast to the expression given in Chapter 6, the width L of the quantum well is present in the denominator in the expression given above. This is because the units of the electron and hole densities in quantum wells is number per unit area and not number per unit volume. Dividing the areal carrier densities by the width of the quantum well gives the average volume density of carriers in the quantum well. The electron and the hole densities appearing in the expressions above are the total electron and hole densities in all the subbands.

10.4 Quantum Well Active Regions

10.4.1 Introduction:

Active regions of most active III-V optoelectronic devices, such as light emitting diodes, optical amplifiers, and lasers, generally consist of multiple quantum wells rather than bulk material. Quantum wells offer several advantages over bulk materials. A brief listing is as follows:

1) Quantum wells, being very thin, can be coherently strained (by as much as $\pm 1.5\%$) without generation of crystal dislocations. Strain allows one to modify the bandstructure. Bandstructure modification via strain can help in reducing the non-radiative recombination rates and in increasing the optical gain and the differential gain, which, as we will see, determines the modulation bandwidth (or speed) of semiconductor lasers. Strain also lifts the degeneracy between the heavy-hole and the light–hole bands and thereby helps in removing unwanted density of states.

2) The reduced density of states in quantum wells compared to bulk semiconductors results in smaller transparency carrier densities. Smaller transparency carrier densities imply reduced current densities in

optical amplifiers and lasers. The reduced density of states in quantum wells also helps in increasing the differential gain.

3) Quantum wells allow polarization sensitive optoelectronic devices to be realized.

4) Quantum wells help trap electrons and holes better than bulk heterostructures and reduce leakage currents.

The active regions of a bulk and a multiple quantum well (MQW) semiconductor optical amplifier are shown in the Figure below.

