

---

## Assignment 4

EE 80724, Wide Bandgap Device Physics, Fall 2009

Debdeep Jena (djena@nd.edu), Department of Electrical Engineering, University of Notre Dame

---

### 1 Interband Optical transitions: Allowed and Forbidden Absorption

We derived the absorption coefficient for ALLOWED transitions for a 2-band direct-bandgap semiconductor. We found that the absorption coefficient to be (in  $cm^{-1}$ )

$$\alpha_{allowed} = 2.7 \times 10^5 \left(\frac{2m_r}{m}\right)^{\frac{3}{2}} \frac{f}{\eta} \sqrt{\hbar\omega - E_g} \quad (1)$$

Here  $f \approx 1 + m/m_h$  is the dimensionless oscillator strength, and  $\eta$  is the refractive index of the semiconductor.

In this problem, you will derive the absorption coefficient for a FORBIDDEN transition in a direct bandgap semiconductor. Follow the handouts closely for this problem.

- Find the matrix element  $W_{k'k}$  for absorption of a photon whose vector potential is given by  $\mathbf{A} = \hat{e}A_0e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$ . Use Bloch-functions as eigenstates for electrons in the initial (valence band) and final (conduction band) states. Show that it is composed of two terms, one leading to direct, and the other to indirect transitions.
- Show that the probability of forbidden transition is proportional to  $|\mathbf{a} \cdot \mathbf{k}|^2$ , where  $\mathbf{k}$  is the wavevector of the electron in the valence band. Since  $\mathbf{a}$  is a constant unit vector, show that the average value of  $|\mathbf{a} \cdot \mathbf{k}|^2$  over the Brillouin Zone is  $k^2/3$ .
- Show that the resulting absorption coefficient  $\alpha = r/\Phi$  where  $r$  is the rate of forbidden absorption per unit volume of the semiconductor, and  $\Phi = \langle \mathbf{S} \rangle / \hbar\omega$  is the photon flux is given by (Eq. 7.70)

$$\alpha = \frac{q^2(2m_r)^{\frac{5}{2}} f'}{6\pi\epsilon_0\eta cm^2\hbar^2} f_0(1 - f_0) \frac{(\hbar\omega - E_g)^{3/2}}{\hbar\omega}. \quad (2)$$

- There is a printing error in Equation 7.68 (in the handouts on optical properties) in the derivation of the absorption coefficient for forbidden transitions. Confirm this by dimensional analysis. What is the error?

### 2 Optical gain

In class, we discussed that a negative absorption coefficient implies emission, and optical gain. The absorption coefficient of a bulk semiconductor under non-equilibrium conditions is given by  $\alpha(\hbar\omega) = \alpha_0(\hbar\omega) \times [f_v(k_0) - f_c(k_0)]$ , where  $\alpha_0(\hbar\omega)$  is the equilibrium absorption coefficient,  $f(\dots)$  are the non-equilibrium Fermi-Dirac distribution functions of the valence and conduction bands, and  $k_0 = \sqrt{2m_r^*(\hbar\omega - E_g)/\hbar^2}$  is the wavevector of electron states that allow interband transition of energy  $\hbar\omega$ . The Bernard-Duraffourg conditions for optical gain were discussed.

Following up on the discussion, choosing GaN as an example and assuming a separation of quasi-Fermi levels larger than the bandgap by 0.2 eV ( $F_c - F_v = E_g + 0.2$  eV), make quantitative

plots the following as a function of photon energy  $\hbar\omega$  at room temperature :

- a) The equilibrium absorption coefficient  $\alpha_0(\hbar\omega)$ ,
- b) The Fermi difference function  $f_v(k_0) - f_c(k_0)$ ,
- c) The net absorption coefficient  $\alpha(\hbar\omega)$ , and
- d) The gain spectrum.

Give a numerical estimate of the maximum gain (in  $\text{cm}^{-1}$ ), and the energy at which it occurs. Look up reports of GaN-based lasers (they typically always involve quantum wells!) and compare numbers with your simple calculations.

### 3 Gain in Quantum Wells

Instead of bulk semiconductors, if we have a quantum well of thickness  $L_z$ , the absorption coefficient still follows the joint density of states feature. To derive this, do the following: assume an infinite barrier height (this approximation can be relaxed in a numerical approach, we keep things analytical here). Then,

a) Write down the wavefunctions of electron states in the  $n_c^{\text{th}}$  state of the conduction band  $|n_c, \mathbf{k}_c\rangle$  as a product of the quantized wavefunction  $C(n_c, z)$  along the confinement ( $z$ -)direction, a free electron wavefunction  $t_c(x, y, \mathbf{k}_c)$  in the transverse ( $x - y$ -)direction, and a Bloch function  $u_c(\mathbf{r})$ . Do the same for the valence band states  $|n_v, \mathbf{k}_v\rangle$ , choosing the functions  $V(n_v, z)$ ,  $t_v(x, y, \mathbf{k}_v)$ , and  $u_v(\mathbf{r})$ .

b) Argue why the transverse parts of the wavefunctions  $t_c(x, y, \mathbf{k}_c)$  and  $t_v(x, y, \mathbf{k}_v)$  must be the same for optical transitions.

c) The optical matrix element is given by  $W_{op} = \langle n_c, \mathbf{k}_c | -\frac{e}{m_0} \mathbf{A} \cdot \mathbf{p} | n_v, \mathbf{k}_v \rangle$ . Show that this can be written as the product  $W_{op} = \frac{eA_0}{m_0} \times \hat{e} \cdot \underbrace{\langle u_c | \mathbf{p} | u_v \rangle}_{\mathbf{p}_{cv}} \times \delta_{\mathbf{k}_c, \mathbf{k}_v} \times I_{v, n_v}^{c, n_c}$ , where the optical transition rules

are dictated by the integral  $I_{v, n_v}^{c, n_c} = \int_{-\infty}^{+\infty} C^*(n_c, z) V(n_v, z) dz$ .

d) Show that for infinite barrier quantum wells, the selection rule is  $I_{v, n_v}^{c, n_c} = \delta_{n_v, n_c}$ , i.e., the only transitions from valence band quantized states to conduction band quantized states that are allowed follow the selection rule  $\Delta n = n_v - n_c = 0$  (for example,  $1 \rightarrow 1, 2 \rightarrow 2 \dots$ ).

e) Based on part (d), show that the *equilibrium* absorption coefficient is then given by

$$\alpha_0(\hbar\omega) = \underbrace{\frac{\pi e^2}{n_r c \epsilon_0 m_0^2 \omega}}_{\text{same-coeff-as-3D}} |\hat{e} \cdot \mathbf{p}_{cv}|^2 \times \underbrace{\frac{m_r^*}{\pi \hbar^2 L_z}}_{\rho_r^{2D}} \times \underbrace{\sum_n \theta[\hbar\omega - (E_g + E_n^c + E_n^v)]}_{\text{staircase-function}}, \quad (3)$$

where  $E_n^c, E_n^v$  are the conduction and valence band quantization energies and  $n = n_c = n_v$ .

f) Plot a representative equilibrium absorption spectrum for an AlN/GaN quantum well of thickness  $L_z = 2$  nm, neglecting the built-in polarization field. Then qualitatively discuss the effect of polarization field on the spectrum you plotted.

### 4 Intersubband Absorption

Following similar arguments as in problem 3, discuss intersubband optical absorption as quantitatively as you can. Specifically, discuss why light of only a certain polarization can be absorbed in an intersubband process.