Absorption / Gain Spectra

Regardless of the specific structure of interest, the gain spectrum can be obtained from Fermi's Golden Rule:

$$W_{ab} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega) + \frac{2\pi}{\hbar}\left|\mathcal{H}'^{+}_{ba}\right|^2 \delta(E_a - E_b + \hbar\omega)$$

It is important to recognize that this gives the rate of change of the probability that the higher Energy state $|b\rangle$ is occupied. To determine the absorption, we need to recognize that W_{ab} is the sum of the transition rates from a→b and from b→a:

$$W_{ab} = R_{a\to b} + R_{b\to a}$$

The absorption rate, however, is he difference between the rate from a→b and b→a:

$$R_{tot} = R_{a\to b} - R_{b\to a}$$

since $\delta(-x) = \delta(x)$

Where

$$R_{a\to b} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)$$

$$R_{b\to a} = \frac{2\pi}{\hbar}\left|\mathcal{H}'^{+}_{ba}\right|^2 \delta(E_a - E_b + \hbar\omega) = \frac{2\pi}{\hbar}\left|\mathcal{H}'^{+}_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)$$

This is the starting point for the gain spectrum of bulk semiconductors and quantum-confined structures alike! We consider each case individually.

Bulk Semiconductor:

In a bulk semiconductor, transitions occur between the parabolic valence band and conduction band. The energies E_a and E_b are given by:

$$E_a = E_v - \frac{\hbar^2 k^2}{2m_h} \quad ; \quad E_b = E_c + \frac{\hbar^2 k^2}{2m_e}$$

In a bulk Semiconductor. there are many different values for k. To get the total rate, we must sum over all of the possible $\bar{k}$ vectors:

$$R_{a\to b} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \sum_{k_x}\sum_{k_y}\sum_{k_z} \delta\left(E_c + \frac{\hbar^2k^2}{2m_e} - E_v + \frac{\hbar^2k^2}{2m_h} - \hbar\omega\right) \times 2/V$$

The $2/V$ term accounts for the 2 electron spins an normalization by volume. Note that this is not quite complete; we still need to account for the fact that transitions can only occur from states that are occupied to unoccupied states. The occupancy is given by fermi-dirac statistics. The full transition rate is:

$$R_{a\to b} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \frac{2}{V}\sum_{k_x}\sum_{k_y}\sum_{k_z} \delta\left(E_g + \frac{\hbar^2k^2}{2m_r} - \hbar\omega\right) f_v(E_a)\left[1 - f_c(E_b)\right]$$

Consider the summation. For sufficiently closely spaced k's, we can take the sum to an integral:

$$\sum_{k_x}\sum_{k_y}\sum_{k_z} \longrightarrow \int \frac{d^3\bar{k}}{(2\pi)^3/V}$$

Thus the summation becomes

$$\frac{2}{V}\int \frac{d^3\bar{k}}{(2\pi)^3/V}\,\delta\left(E_g - \hbar\omega + \frac{\hbar^2k^2}{2m_r}\right) f_v(E_a)\left[1 - f_c(E_b)\right]$$

$$= \quad 2\int \frac{4\pi k^2 dk}{(2\pi)^3}\,\delta\left(E_g - \hbar\omega + \frac{\hbar^2k^2}{2m_r}\right) f_v\left(E_c + \frac{\hbar^2k^2}{2m_e}\right)\left[1 - f_c\left(E_v - \frac{\hbar^2k^2}{2m_h}\right)\right]$$

let $u = \frac{\hbar^2k^2}{2m_r} \Rightarrow k = \sqrt{\frac{2m_r u}{\hbar^2}} \Rightarrow dk = \sqrt{\frac{m_r}{\hbar^2}}\,\frac{1}{\sqrt{2u}}\,du$

$$= \int \frac{du}{\pi^2} \frac{2m_r u}{\hbar^2} \sqrt{\frac{m_r}{\hbar^2}} \frac{1}{\sqrt{u}} \delta\left(u - (\hbar\omega - E_g)\right) f_v\left(E_c + \frac{m_r}{m_e} u\right)\left[1 - f_c\left(E_v - \frac{m_r}{m_h} u\right)\right]$$

$$= \int du \frac{2}{\pi^2}\left(\frac{m_r}{\hbar^2}\right)^{3/2} \sqrt{u}\, \delta\left(u - (\hbar\omega - E_g)\right) f_v\left(E_c + \frac{m_r}{m_e} u\right)\left[1 - f_c\left(E_v - \frac{m_r}{m_h} u\right)\right]$$

$$= \frac{2}{\pi^2}\left(\frac{m_r}{\hbar^2}\right)^{3/2} \sqrt{\hbar\omega - E_g}\, f_v\left(E_c + \frac{m_r}{m_e}(\hbar\omega - E_g)\right)\left[1 - f_c\left(E_v - \frac{m_r}{m_h}(\hbar\omega - E_g)\right)\right]$$

We can write this more simply by recognizing that the first 3 terms are the joint density of states:

$$= \rho_r^{3D}(\hbar\omega - E_g) f_v \left[1 - f_c\right]$$

It follows that the absorption rate from a→b is:

$$R_{a\to b} = \frac{2\pi}{\hbar} |H'_{ba}|^2 \rho_r^{3D}(\hbar\omega - E_g) f_v \left[1 - f_c\right]$$

Following an identical process yields the emission rate from b→a:

$$R_{b\to a} = \frac{2\pi}{\hbar} |H'^{+}_{ba}|^2 \rho_r^{3D}(\hbar\omega - E_g) f_c \left[1 - f_v\right]$$

For the sake of simplicity, assume $|H'^{+}_{ba}|^2 = |H'_{ba}|^2$. The net absorption rate is thus:

$$R_{net} = \frac{2\pi}{\hbar} |H'_{ba}|^2 \rho_r^{3D}(\hbar\omega - E_g) \left[f_v - f_c\right]$$

Defining $f_g = f_c - f_v$ and using $\alpha(\hbar\omega) = R_{net}$, we have:

$$\boxed{\alpha(\hbar\omega) = \frac{-2\pi}{\hbar} |H'_{ba}|^2 \rho_r^{3D}(\hbar\omega - E_g) f_g(\hbar\omega - E_g)}$$

where $f_g(\hbar\omega - E_g) = f_c\left(E_c + \frac{m_r}{m_h}(\hbar\omega - E_g)\right) - f_v\left(E_v - \frac{m_r}{m_e}(\hbar\omega - E_g)\right)$

↑ Fermi Inversion factor

Interband Transitions in 2D quantum wells

Absoption in 2D quantum wells for interband transitions can be demonstrated in exactly the same way as 3D bulk semiconductors. We begin w/ the transition rate (per unit volume) from a state a in the valence band to a state b in the conduction band:

$$R_{a\to b} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \sum_{k_x}\sum_{k_y} \delta\left(E_b - E_a - \hbar\omega\right) \times \frac{2}{V} \times f_v(E_a)\left[1 - f_c(E_b)\right]$$

⚠ Technically also need to sum over all m

We have only summed over k_x & k_y since there is confinement in the z direction. The energies E_b & E_a for a quantum well are:

$$E_a = E_v - E_m - \frac{\hbar^2 k_t^2}{2m_h} \quad ; \quad E_b = E_c + E_n + \frac{\hbar^2 k_t^2}{2m_e}$$

Where $k_t = |\bar{k}_t| = k_x\hat{x} + k_y\hat{y}$ (the "transverse" k vecter) and E_m and E_n are the quantized energy levels of the well:

$$E_m = \frac{\hbar^2\pi^2}{2m_h}\left(\frac{m}{L_z}\right)^2 \quad ; \quad E_n = \frac{\hbar^2\pi^2}{2m_e}\left(\frac{n}{L_z}\right)^2$$

The transition rate becomes:

$$\frac{1}{m_r} = \frac{1}{m_e} + \frac{1}{m_h}$$

$$R_{a\to b} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \frac{2}{V}\sum_{k_x}\sum_{k_y} \delta\left(E_g + E_n + E_m + \frac{\hbar^2 k_t^2}{2m_r} - \hbar\omega\right) f_v(E_a)\left[1 - f_c(E_b)\right]$$

$$\to \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \frac{2}{L_xL_yL_z}\int \frac{d^2\bar{k}_t}{(2\pi)^2/L_xL_y}\, \delta\left(E_g + E_n + E_m + \frac{\hbar^2 k_t^2}{2m_r} - \hbar\omega\right) f_v(E_a)\left[1 - f_c(E_b)\right]$$

$$= \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \frac{2}{L_xL_yL_z}\int \frac{2\pi k_t\, dk_t}{4\pi^2/L_xL_y}\, \delta\left(E_g + E_n + E_m + \frac{\hbar^2 k^2}{2m_r} - \hbar\omega\right) f_v(E_a)\left[1 - f_c(E_b)\right]$$

let $u = \frac{\hbar^2 k_t^2}{2m_r} \Rightarrow k = \sqrt{\frac{2m_r u}{\hbar^2}} \Rightarrow dk = \sqrt{\frac{m_r}{2\hbar^2}}\frac{1}{\sqrt{u}}$

So

$$R_{a\to b} = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \int du\, \frac{1}{\pi L_z}\frac{m_r}{\hbar^2}\, \delta\left(E_g + E_n + E_m + u - \hbar\omega\right) f_v(E_a)\left[1 - f_c(E_b)\right]$$

Completing the integral, we have:

$$R_{a\to b} = \frac{2\pi}{\hbar}|\mathcal{H}_{ba}'|^2 \frac{m_r}{\pi\hbar^2 L_z} f_v\left(E_v - E_m - \frac{m_r}{m_h}(\hbar\omega - E_g')\right)\left[1 - f_c\left(E_c + E_n + \frac{m_r}{m_e}(\hbar\omega - E_g')\right)\right]$$

$$= \frac{2\pi}{\hbar}|\mathcal{H}_{ba}'|^2 \rho_r^{2D} f_v[1-f_c]$$

where $E_g' = E_g + E_n + E_m$. As w/ the bulk case, the rate of stimulated emission follows in the same manner:

$$R_{b\to a} = \frac{2\pi}{\hbar}|\mathcal{H}_{ba}'^{+}|^2 \rho_r^{2D} f_c[1-f_v]$$

Once again, assume that $|\mathcal{H}_{ba}'^{+}|^2 \simeq |\mathcal{H}_{ba}'|^2$. It follows that the absorption spectrum, given by $\alpha_{2D}(\hbar\omega) = R_{a\to b} - R_{b\to a}$ is:

$$\boxed{\alpha_{2D}(\hbar\omega) \simeq -\frac{2\pi}{\hbar}|\mathcal{H}_{ba}'|^2 \rho_r^{2D} f_g(\hbar\omega - E_g')}$$

Where

$$f_g(\hbar\omega - E_g') = f_c\left(E_c + E_n + \frac{m_r}{m_e}(\hbar\omega - E_g')\right) - f_v\left(E_v - E_m - \frac{m_r}{m_h}(\hbar\omega - E_g')\right)$$

Intersubband Transitions in 2D Quantum wells (conduction band)

The transition rate from a→b when both $|a\rangle$ and $|b\rangle$ are in the same band has a very different behavior than interband transitions. As w/ the interband transition, the intersubband transition rate from a→b is given by

$$R_{a\to b} = \frac{2\pi}{\hbar}|\mathcal{H}_{ba}'|^2 \cancel{\frac{2}{V}} \sum_{k_x}\sum_{k_y} \delta(E_a - E_b - \hbar\omega) \times \frac{2}{V} \times f_c(E_a)[1 - f_c(E_b)]$$

Intersubband transitions are distinguished from inter band transitions by the Energies E_a & E_b which are given by

$$E_a = E_c + E_m + \frac{\hbar^2 k_t^2}{2m_e} \quad ; \quad E_b = E_c + E_n + \frac{\hbar^2 k_t^2}{2m_e}$$

Notice that the dependence on k_t is the same in both energies. Plugging this in, we have

$$R_{a\to b} = \frac{2\pi}{\hbar} |\mathcal{H}'_{ba}|^2 \frac{2}{V} \sum_{k_x} \sum_{k_y} \underbrace{\delta(E_n - E_m - \hbar\omega)}_{\text{independent of } k} f_c(E_a)\left[1 - f_c(E_b)\right]$$

$$= \frac{2\pi}{\hbar} |\mathcal{H}'_{ba}|^2 \delta(E_n - E_m - \hbar\omega) \sum_{k_x} \sum_{k_y} f_c(E_a)\left[1 - f_c(E_b)\right] \frac{2}{V}$$

Before simplifying the sum, notice that the transition rate from $b \to a$ takes a similar form:

$$R_{b\to a} = \frac{2\pi}{\hbar} |\mathcal{H}'^{+}_{ba}|^2 \delta(E_n - E_m - \hbar\omega) \sum_{k_x} \sum_{k_y} \frac{2}{V} f_c(E_b)\left[1 - f_c(E_a)\right]$$

The net Absorption rate is thus (assuming $|\mathcal{H}'_{ba}| \simeq |\mathcal{H}'^{+}_{ba}|$)

$$\alpha(\hbar\omega) = \frac{2\pi}{\hbar} |\mathcal{H}'_{ba}|^2 \delta(E_n - E_m - \hbar\omega) \sum_{k_x} \sum_{k_y} \frac{2}{V} \left\{ f_c(E_a) - f_c(E_b) \right\}$$

Next, notice that the summation is just the difference in electron concentration of the two levels:

$$\sum_{k_x} \sum_{k_y} \frac{2}{V} f_c(E_{a/b}) \to \frac{2}{V} \int \frac{d^2 \bar{k}}{(2\pi)^2 / L_x L_y} f_c(E_{a/b}) = \int dk\, \rho_{2D}(k) f_c(E_{a/b}) = N_{a/b}$$

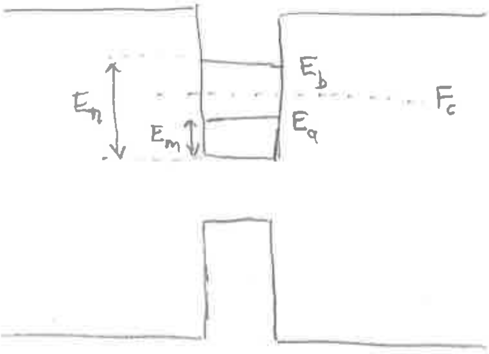
Thus,

$$\boxed{\alpha(\hbar\omega) = \frac{2\pi}{\hbar} |\mathcal{H}'_{ba}|^2 \delta(E_n - E_m - \hbar\omega) \left[N_a - N_b\right]}$$

We can take this analysis a bit further and consider two specific situations of interest: ① $F_c < E_n + E_c$ ② $F_c > E_n + E_c$

For simplicity, let us define $E_{em} = E_c + E_m$ and $E_{en} = E_c + E_n$

Consider first the case in which $F_c < E_{en}$ Graphically:



It can be shown that the 2D electron concentration is

$$N_m^{2D} = \int dE \, \rho^{2D}(E) f_n(E|E_{em})$$

$$= \frac{m_e^* k_B T}{\pi \hbar^2 L_z} \ln\left[1 + e^{\frac{F_c - E_{em}}{k_B T}}\right]$$

Using this expression, we can write a general expression for the absorption coefficient:

$$\alpha(\hbar\omega) = \frac{2\pi}{\hbar} |\mathcal{H}_{ba}'|^2 \delta(E_n - E_m - \hbar\omega) \frac{m_e^* k_B T}{\pi \hbar^2 L_z} \left\{ \ln\left[1 + e^{\frac{F_c - E_{em}}{k_B T}}\right] - \ln\left[1 + e^{\frac{F_c - E_{en}}{k_B T}}\right] \right\}$$

Notice that for F_c sufficiently less than E_{en}, this expression reduces to:

Note: $\ln[1+x] \sim x$

$$\alpha(\hbar\omega) \simeq \frac{2\pi}{\hbar} |\mathcal{H}_{ba}'|^2 \delta(E_n - E_m - \hbar\omega) \frac{m_e^*}{\pi \hbar^2 L_z} (F_c - E_{em})$$

$$\simeq \frac{2\pi}{\hbar} |\mathcal{H}_{ba}'|^2 \delta(E_n - E_m - \hbar\omega) N_1$$

Let us consider, specifically, a transition between the lowest two energy levels of the quantum well:

$$\boxed{\alpha(\hbar\omega) \simeq \frac{2\pi}{\hbar} |\mathcal{H}_{ba}'|^2 \delta(E_{e2} - E_{e1} - \hbar\omega) N_1}$$

Because these two levels are close to the conduction band edge, the absorption will depend rather strongly doping concentration of the well. In particular, if doped N-type, the absorption coefficient will be:

$$\boxed{\alpha(\hbar\omega) \simeq \frac{2\pi}{\hbar} |\mathcal{H}_{ba}'|^2 \delta(E_{e2} - E_{e1} - \hbar\omega) N_d \qquad F_c < E_{e2}}$$

since $N \simeq N_d$

Next, consider the 2nd case in which $F_c > E_{e2}$

In this case, we can simplify our logarithmic expression by noting that the exponential term in each log is $\gg 1$. This simplification leads to an absorption coefficient given by:

$$\boxed{\alpha(\hbar\omega) \simeq \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \delta(E_n - E_m - \hbar\omega)\frac{m_e^*}{\pi\hbar^2 L_z}\left(E_{e2} - E_{e1}\right)}$$

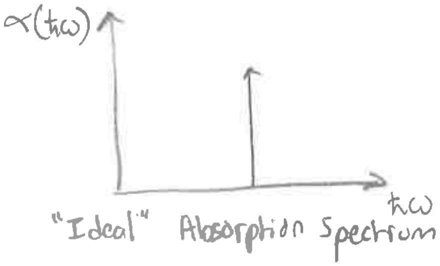
Notice that this is (for the most part) independent of doping concentration.

Some other stuff

Recall our most general expression for the intersubband transitions:

$$\alpha(\hbar\omega) = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \delta(E_n - E_m - \hbar\omega)\left[N_a - N_b\right]$$

Notice that we assumed that the energy levels were perfectly sharp. As a result, only a single wavelength $\hbar\omega = E_n - E_m$ would be absorbed (And it would be absorbed completely).



"Ideal" Absorption Spectrum

In reality, quantum wells are never completely decoupled from the outside world. As a result, electrons have a finite lifetime in any given state which leads to an effective blurring of energy levels.

Because of this, the δ-function is not truely appropriate. Instead a finite-width function w/ a normalized area is more physical. A common model for level broadening is the Lorentzian:

$$g(E) = \frac{1}{\pi}\frac{\Gamma/2}{E^2 + (\Gamma/2)^2} \quad ☆$$

where Γ is he full width at half maximum and a measure of line width broadening. The new general expression for the absorption coefficient is thus:

$$\alpha(\hbar\omega) = \frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 g(E_n - E_m - \hbar\omega)\left[N_a - N_b\right]$$

Next, the matrix element can be predicted if he assume that the well is an infinite square well:

dipole moment

Infinite square well wavefunctions

$$\boxed{\frac{2\pi}{\hbar}\left|\mathcal{H}'_{ba}\right|^2 \simeq \frac{\pi\omega}{n_r c \varepsilon_0}\left|\mu_{ba}\right|^2} \quad \text{where } \mu_{ba} = \int \varphi_b(z)\, z\, \varphi_a(z)\, dz$$

Assuming $a=1$ and $b=2$ we find:

$$\frac{2\pi}{\hbar}\left|\mathcal{H}'_{21}\right|^2 \simeq \frac{\pi\omega}{n_r c \varepsilon_0}\left(\frac{16}{9} e L_z\right)^2$$

Hence the general expression for $\alpha(\hbar\omega)$ becomes:

$$\alpha(\hbar\omega) \simeq \frac{\pi\omega}{n_r c \varepsilon_0}\left(\frac{16}{9} e L_z\right)^2 g(E_{e2} - E_{e1} - \hbar\omega)\left[N_1 - N_2\right]$$

Notice that he maximum possible absorption occurs when $F_c < E_{e2}$ and $\hbar\omega = E_{e2} - E_{e1}$. The value is:

$$\boxed{\alpha_{max} \simeq \frac{\pi\omega}{n_r c \varepsilon_0}\left(\frac{16}{9} e L_z\right)^2 \frac{2}{\pi\Gamma} N}$$