EE 232: Lightwave Devices
Lecture #10 – Absorption in quantum wells

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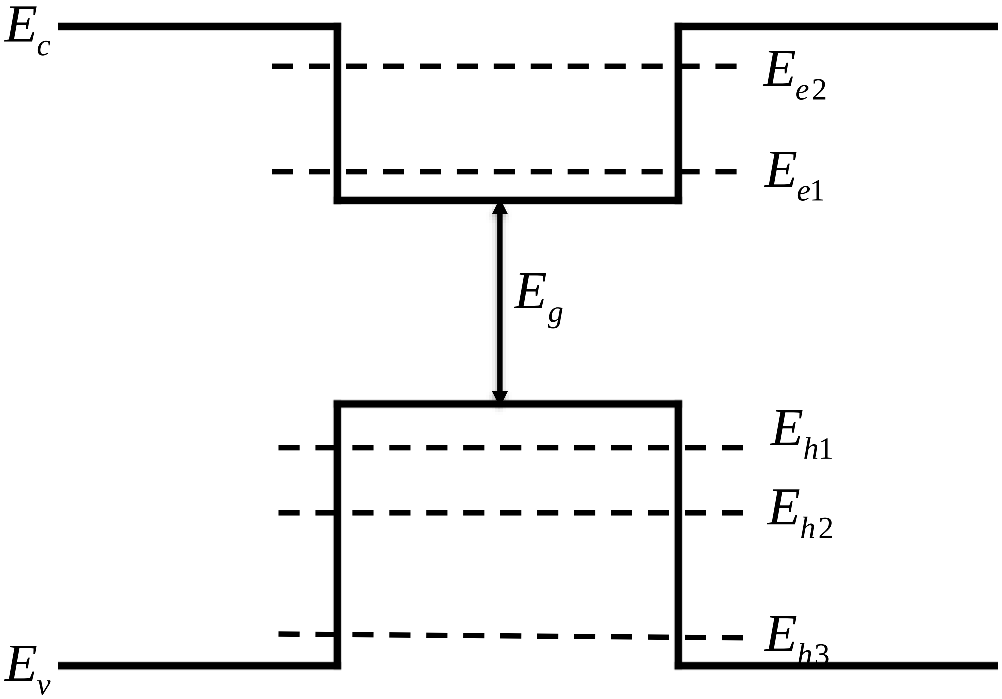
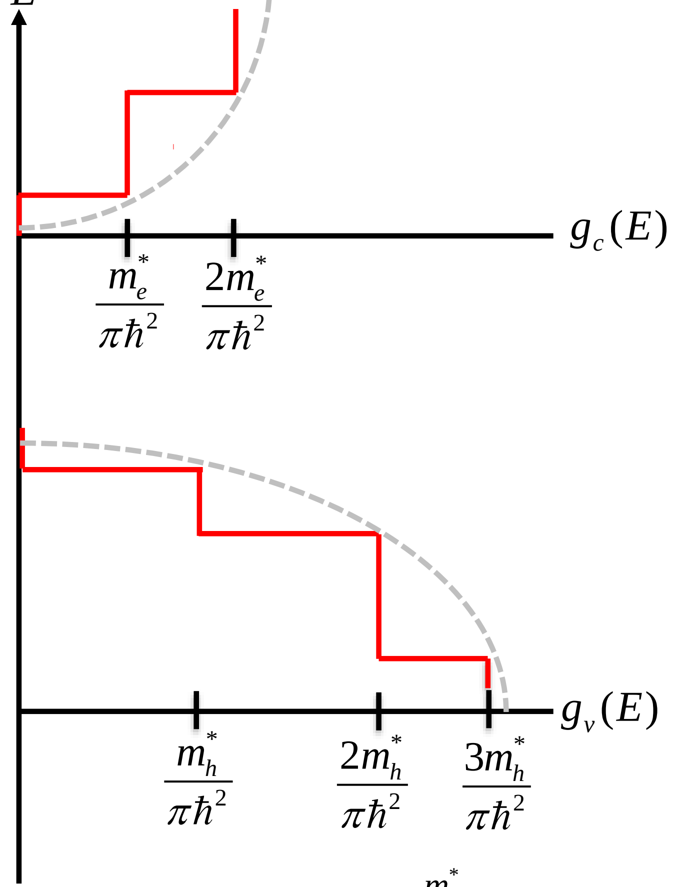
Semiconductor quantum well



$$g_c(E) = \frac{m_e^*}{\pi\hbar^2}\sum_n H(E - E_g - E_{en})$$



$$g_v(E) = \frac{m_h^*}{\pi\hbar^2}\sum_m H(E_{hm} - E)$$

Absorption coefficient

$$\alpha = C_0 \frac{2}{V} \sum_{k_z} \sum_{k_t} |\hat{e} \cdot \mathbf{p}_{cv}|^2 \ \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c \right)$$

$$2\sum_{k_t} \rightarrow A \int_{-\infty}^{\infty} \frac{2d^2 k_t}{(2\pi)^2} = A \int_{-\infty}^{\infty} \frac{2(2\pi k_t) dk_t}{(2\pi)^2} = A \int_{-\infty}^{\infty} \frac{k_t dk_t}{\pi}$$

Note that here,

$$\mathbf{p}_{cv} = \langle \psi_c | \mathbf{p} | \psi_v \rangle$$

ψ_c and ψ_v are bloch states

$$E_e = E_g + E_{en} + \frac{\hbar^2 k_t{}^2}{2m_e^*}$$

$$E_h = E_{hm} - \frac{\hbar^2 k_t{}^2}{2m_h^*}$$

$$E_e - E_h = E_{hm}^{en} + \frac{\hbar^2 k_t{}^2}{2m_r^*} \quad \text{where} \quad \frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

$$\text{Let } E = \frac{h^2 k_t{}^2}{2m_r^*} \rightarrow k_t = \sqrt{\frac{2m_r^* E}{\hbar^2}} \qquad \frac{dk_t}{dE} = \frac{m_r^*}{\hbar^2} \sqrt{\frac{\hbar^2}{2m_r^* E}}$$

Absorption coefficient

$$2\sum_{k_t} \rightarrow A\int_{-\infty}^{\infty} \frac{2d^2k_t}{(2\pi)^2} = A\int_{-\infty}^{\infty} \frac{2(2\pi k_t)dk_t}{(2\pi)^2} = A\int_{-\infty}^{\infty} \frac{k_t dk_t}{\pi}$$

$$= A\int_{0}^{\infty} \frac{m_r^*}{\pi\hbar^2} dE$$

$$= A\int_{-\infty}^{\infty} \frac{m_r^*}{\pi\hbar^2} H(E)dE = A\int_{-\infty}^{\infty} \rho_{r,2D} H(E)dE$$

$$\alpha = C_0 \frac{2}{V} \sum_{k_z}\sum_{k_t} |\hat{e}\cdot\mathbf{p}_{cv}|^2 \, \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right)$$

$$= C_0 \frac{1}{L_z} \sum_{n,m} \int_{-\infty}^{\infty} |\hat{e}\cdot\mathbf{p}_{cv}|^2 \, \rho_{r,2D} H(E)\delta(E + E_{hm}^{en} - \hbar\omega)\left(f_v(E) - f_c(E)\right)dE$$

$$= C_0 \frac{1}{L_z} \sum_{n,m} |\hat{e}\cdot\mathbf{p}_{cv}|^2 \, \rho_{r,2D} H(\hbar\omega - E_{hm}^{en})\left[f_v(E = \hbar\omega - E_{hm}^{en}) - f_c(E = \hbar\omega - E_{hm}^{en})\right]$$

$$\boxed{\alpha(\hbar\omega) = C_0 \frac{1}{L_z} \sum_{n,m} |\hat{e}\cdot\mathbf{p}_{cv}|^2 \, \rho_{r,2D} H(\hbar\omega - E_{hm}^{en})\left[f_v(E = \hbar\omega - E_{hm}^{en}) - f_c(E = \hbar\omega - E_{hm}^{en})\right]}$$

Absorption with inclusion of other valence bands

$$\alpha_{hh}(\hbar\omega) = C_0 \frac{1}{L_z} \sum_{n,m} |\hat{e}\cdot\mathbf{p}_{cv,hh}|^2 \rho_{r,hh,2D} H(\hbar\omega - E_{hm}^{en}) \left[f_v(E = \hbar\omega - E_{hm}^{en}) - f_c(E = \hbar\omega - E_{hm}^{en}) \right]$$

(heavy hole)

$$\alpha_{lh}(\hbar\omega) = C_0 \frac{1}{L_z} \sum_{n,m} \underbrace{|\hat{e}\cdot\mathbf{p}_{cv,lh}|^2 \rho_{r,lh,2D} H(\hbar\omega - E_{hm}^{en})}_{\text{Valence band dependent}} \left[f_v(E = \hbar\omega - \underset{\uparrow}{E_{hm}^{en}}) - f_c(E = \hbar\omega - \underset{\uparrow}{E_{hm}^{en}}) \right]$$

(light hole)

Valence band dependent

$$\boxed{\alpha(\hbar\omega) = \alpha_{lh} + \alpha_{hh}}$$

Total absorption coefficient
is the summation of absorption
between the conduction and each
valence band.

Fermi factor

$$f_c(E_e) = \frac{1}{1 + \exp[(E_e - F_c)/kT]}$$

$$f_v(E_h) = \frac{1}{1 + \exp[(E_h - F_v)/kT]}$$

We need a change of variables from $E_e, E_h \to E = \frac{\hbar^2 k^2}{2m_r^*}$

Because of the delta function, $E = \hbar\omega - E_{hm}^{en} = \frac{\hbar^2 k^2}{2m_r^*} \to k = \sqrt{\frac{2m_r^*}{\hbar^2}(\hbar\omega - E_{hm}^{en})}$

$$E_e = E_g + E_{en} + \frac{\hbar^2 k^2}{2m_e^*}$$

$$= E_g + E_{en} + \left(\hbar\omega - E_{hm}^{en}\right)\frac{m_r^*}{m_e^*}$$

$$E_h = E_{hm} - \frac{\hbar^2 k^2}{2m_h^*}$$

$$= E_{hm} - (\hbar\omega - E_{hm}^{en})\left(\frac{m_r^*}{m_h^*}\right)$$

$$\boxed{f_c(\hbar\omega) = \frac{1}{1 + \exp\left[(E_g + E_{en} + \left(\hbar\omega - E_{hm}^{en}\right) m_r^* / m_e^* - F_c)/kT)\right]}}$$

$$\boxed{f_v(\hbar\omega) = \frac{1}{1 + \exp\left[(E_{hm} - (\hbar\omega - E_{hm}^{en}) m_r^* / m_h^* - F_v)/kT\right]}}$$

Optical matrix element

Optical matrix element

$$\hat{H}_{cv} = \left\langle \psi_c \middle| \frac{-qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0} \hat{e}\cdot\mathbf{p} \middle| \psi_v \right\rangle$$

Bloch states

$$\psi_c = \underset{\uparrow}{u_c(\mathbf{r})} \underbrace{\frac{e^{i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{A}} \phi_n(z)}_{\uparrow} \qquad \psi_v = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{A}} g_m(z)$$

periodic with lattice

envelope function

$$\hat{H}_{cv} = \left\langle u_c(\mathbf{r}) \frac{e^{i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{A}} \phi_n(z) \middle| \frac{-qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0} \hat{e}\cdot\mathbf{p} \middle| u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{A}} g_m(z) \right\rangle$$

$$= \int u_c^*(\mathbf{r}) \frac{e^{-i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{A}} \phi_n^*(z) \frac{-qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0} \hat{e}\cdot\mathbf{p} u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{A}} g_m(z) d^3\mathbf{r}$$

Optical matrix element

$$\hat{H}_{cv} = \int u_c^*(\mathbf{r}) \frac{e^{-i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{A}} \phi_n^*(z) \frac{-qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0} \hat{e}\cdot\mathbf{p}u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{A}} g_m(z) d^3\mathbf{r}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\int_V e^{i(-\mathbf{k}_c+\mathbf{k}_v+\mathbf{k}_{op})\cdot\mathbf{r}} \phi_n^*(z) g_m(z) \frac{d^3\mathbf{r}}{A} \int_\Omega u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r}) \frac{d^3\mathbf{r}}{\Omega}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\mathbf{p}_{cv}\int_V e^{i(-\mathbf{k}_c+\mathbf{k}_v+\mathbf{k}_{op})\cdot\mathbf{r}} \phi_n^*(z) g_m(z) \frac{d^3\mathbf{r}}{A}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\mathbf{p}_{cv}\int_A e^{i(-\mathbf{k}_c+\mathbf{k}_v+\mathbf{k}_{op,t})\cdot(x\hat{x}+y\hat{y})} \frac{\mathbf{dxdy}}{A} \int_{L_z} e^{i\mathbf{k}_{op,z}\cdot z\hat{z}} \phi_n^*(z) g_m(z) d\mathbf{z}$$

$$\simeq \frac{-qA_0}{2m_0}\hat{e}\cdot\mathbf{p}_{cv}\delta_{\mathbf{k}_c,\mathbf{k}_v} \int_{L_z} \phi_n^*(z) g_m(z) dz$$

$$\boxed{= \frac{-qA_0}{2m_0}\hat{e}\cdot\mathbf{p}_{cv}\delta_{\mathbf{k}_c,\mathbf{k}_v} I_{hm}^{en}}$$

Note that here,

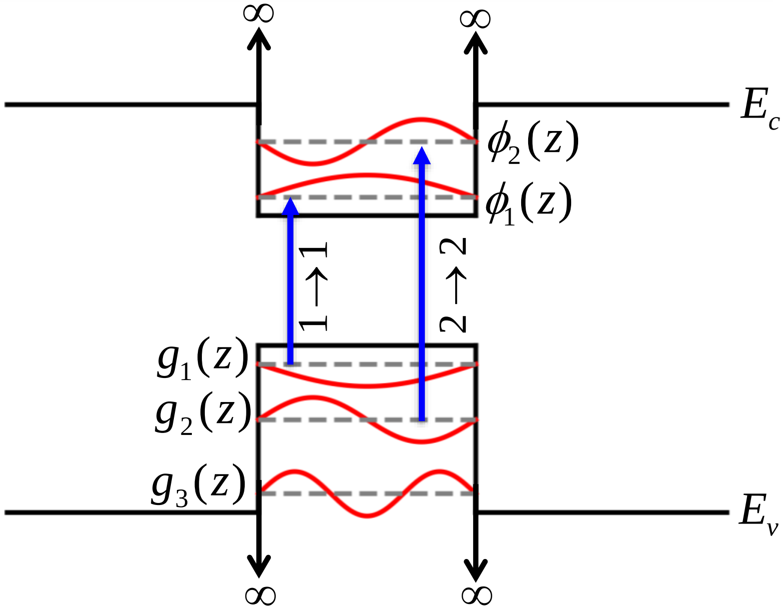
$$\mathbf{p}_{cv} = \langle u_c|\mathbf{p}|u_v\rangle$$

u_c and u_v are bloch functions

Overlap integral

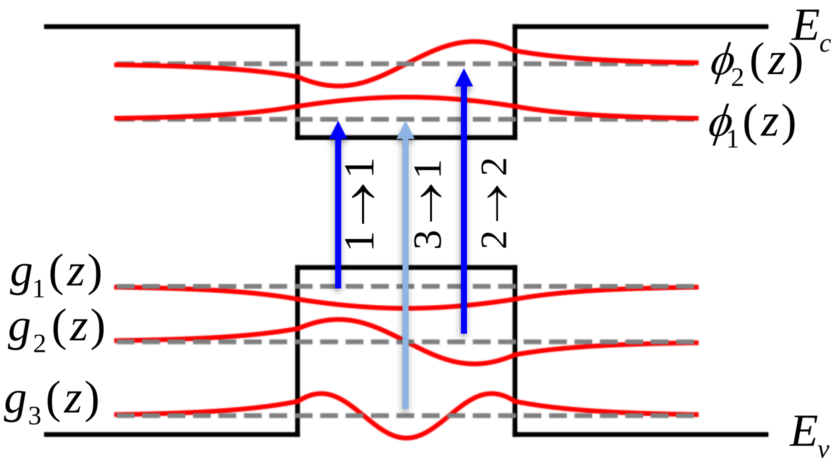
$$\hat{H}_{cv} = \frac{-qA_0}{2m_0}\hat{e}\cdot\mathbf{p}_{cv}\delta_{\mathbf{k}_c,\mathbf{k}_v}\int_{L_z}\phi_n^*(z)g_m(z)dz \qquad I_{hm}^{en} = \int_{L_z}\phi_n^*(z)g_m(z)dz$$

Infinite barrier well (approximation)



$$I_{hm}^{en} = \begin{cases} 0 & \text{for n} \neq \text{m} \\ 1 & \text{for n=m} \end{cases}$$

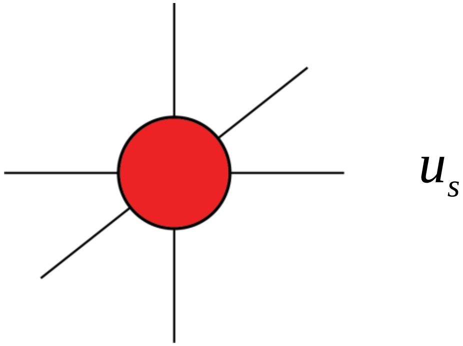
Finite barrier well



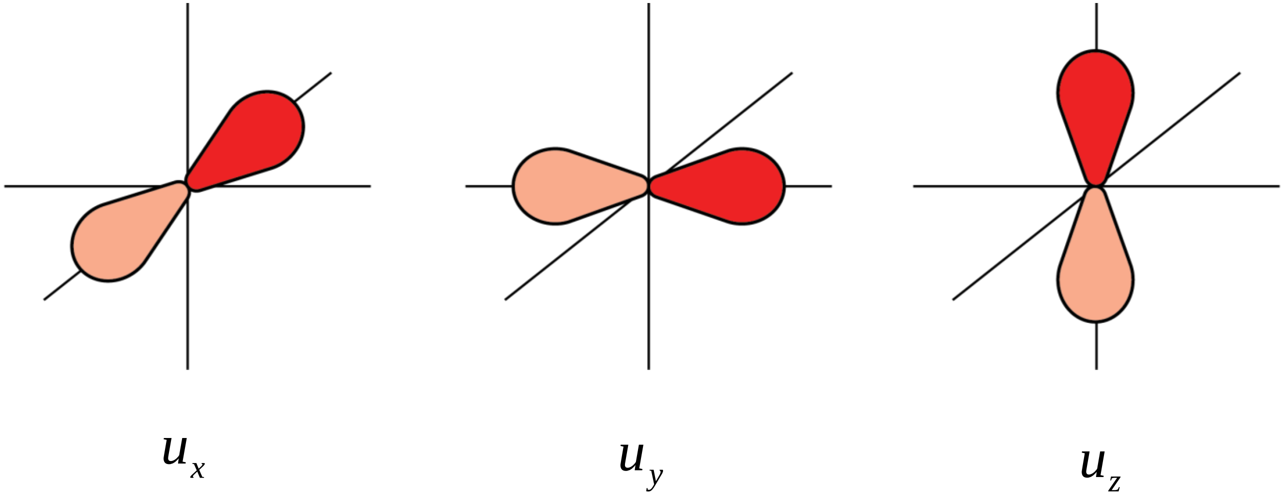
$$I_{hm}^{en} = \begin{cases} 0 & \text{for n,m different parity} \\ \sim 1 & \text{for n=m} \\ \sim 0 & \text{for n} \neq \text{m and n,m same parity} \end{cases}$$

Bloch functions u_c and u_v

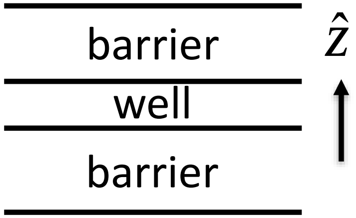
Conduction band
Basis function



Valence band
Basis functions



Bloch functions u_c and u_v



barrier

well

barrier

$\hat{z}$

Near the bandedge the electron/hole wavevector is primarily directed in the z-direction

$$\mathbf{k}_c = \mathbf{k}_v = k_z \hat{z}$$

Below are the Bloch functions for electron wavevector in the z-direction as derived from Kane's $k \cdot p$ model for the band structure

Conduction band Bloch functions

$$u_c = i u_s \qquad \bar{u}_c = i \bar{u}_s$$

Valence band Bloch functions

$$u_{hh} = -\frac{1}{\sqrt{2}}\left(u_x + i u_y\right) \qquad \bar{u}_{hh} = \frac{1}{\sqrt{2}}\left(\bar{u}_x - i \bar{u}_y\right)$$

$$u_{lh} = -\frac{1}{\sqrt{6}}(\bar{u}_x + i \bar{u}_y - 2u_z) \qquad \bar{u}_{lh} = \frac{1}{\sqrt{6}}(u_x - i u_y + 2\bar{u}_z)$$

$$u_{so} = -\frac{1}{\sqrt{3}}(\bar{u}_x + i \bar{u}_y + u_z) \qquad \bar{u}_{so} = \frac{1}{\sqrt{3}}(u_x - i u_y - \bar{u}_z)$$

Note: bar denotes spin-down

Reference: Chuang 4.2, Coldren App 8

Polarization dependent matrix element

Let's calculate $\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2$ for the **conduction band to <u>heavy-hole</u> band transition**

$$
\begin{aligned}
\hat{e}\cdot\mathbf{p}_{cv} &= \hat{e}\cdot\langle u_c|\mathbf{p}|u_v\rangle \\
&= \hat{e}\cdot\langle u_c|-i\hbar\nabla|u_v\rangle \\
&= \hat{e}\cdot\left\langle u_c\left|-i\hbar\left(\frac{\partial}{\partial x}\hat{x}+\frac{\partial}{\partial y}\hat{y}+\frac{\partial}{\partial z}\hat{z}\right)\right|u_v\right\rangle \\
&= \hat{e}\cdot\langle u_c|\mathbf{p}_x+\mathbf{p}_y+\mathbf{p}_z|u_v\rangle \\
&= \hat{e}\cdot\left\langle iu_s\left|\mathbf{p}_x+\mathbf{p}_y+\mathbf{p}_z\right|-\frac{1}{\sqrt{2}}\left(u_x+iu_y\right)\right\rangle
\end{aligned}
$$

<u>for $\hat{e}=\hat{x}$</u>

$$\hat{x}\cdot\mathbf{p}_{cv}=\left\langle iu_s\left|\mathbf{p}_x\right|-\frac{1}{\sqrt{2}}\left(u_x+iu_y\right)\right\rangle$$

$$\left|\hat{x}\cdot\mathbf{p}_{cv}\right|^2=\frac{1}{2}\left|\langle u_s|\mathbf{p}_x|u_x\rangle\right|^2=\frac{3}{2}M_b{}^2$$

<u>for $\hat{e}=\hat{y}$</u>

$$\hat{y}\cdot\mathbf{p}_{cv}=\left\langle iu_s\left|\mathbf{p}_y\right|-\frac{1}{\sqrt{2}}\left(u_x+iu_y\right)\right\rangle$$

$$\left|\hat{y}\cdot\mathbf{p}_{cv}\right|^2=\frac{1}{2}\left|\langle u_s|\mathbf{p}_y|u_y\rangle\right|^2=\frac{3}{2}M_b{}^2$$

Polarization dependent matrix element

Let's calculate $\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2$ for the **conduction band to <u>heavy-hole</u> band transition**

$$\begin{aligned}
\hat{e}\cdot\mathbf{p}_{cv} &= \hat{e}\cdot\langle u_c|\mathbf{p}|u_v\rangle \\
&= \hat{e}\cdot\langle u_c|-i\hbar\nabla|u_v\rangle \\
&= \hat{e}\cdot\langle u_c|-i\hbar\left(\frac{\partial}{\partial x}\hat{x}+\frac{\partial}{\partial y}\hat{y}+\frac{\partial}{\partial z}\hat{z}\right)|u_v\rangle \\
&= \hat{e}\cdot\langle u_c|\mathbf{p}_x+\mathbf{p}_y+\mathbf{p}_z|u_v\rangle \\
&= \hat{e}\cdot\left\langle iu_s\middle|\mathbf{p}_x+\mathbf{p}_y+\mathbf{p}_z\middle|-\frac{1}{\sqrt{2}}\left(u_x+iu_y\right)\right\rangle
\end{aligned}$$

$$\underline{\text{for } \hat{e}=\hat{z}}$$

$$\hat{z}\cdot\mathbf{p}_{cv} = \left\langle iu_s\middle|\mathbf{p}_z\middle|-\frac{1}{\sqrt{2}}\left(u_x+iu_y\right)\right\rangle = 0$$

$$\left|\hat{z}\cdot\mathbf{p}_{cv}\right|^2 = 0$$

Light with polarization in the z-direction will not cause a transition between the conduction and heavy hole band!
(Reminder: this is at the bandedge)

Polarization dependent matrix element

Let's calculate $\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2$ for the **conduction band to <u>light-hole</u> band transition**

$$\hat{e}\cdot\mathbf{p}_{cv} = \hat{e}\cdot\left\langle iu_s\left|\mathbf{p}_x+\mathbf{p}_y+\mathbf{p}_z\right|-\frac{1}{\sqrt{6}}(\bar{u}_x+i\bar{u}_y-2u_z)\right\rangle$$

for $\hat{e}=\hat{x}$

$$\hat{x}\cdot\mathbf{p}_{cv} = \left\langle iu_s\left|\mathbf{p}_x\right|-\frac{1}{\sqrt{6}}(\bar{u}_x+i\bar{u}_y-2u_z)\right\rangle$$

$$\left|\hat{x}\cdot\mathbf{p}_{cv}\right|^2 = \frac{1}{6}\left|\left\langle u_s\left|\mathbf{p}_x\right|u_x\right\rangle\right|^2 = \frac{1}{2}M_b{}^2$$

for $\hat{e}=\hat{y}$

$$\hat{y}\cdot\mathbf{p}_{cv} = \left\langle iu_s\left|\mathbf{p}_y\right|-\frac{1}{\sqrt{6}}(\bar{u}_x+i\bar{u}_y-2u_z)\right\rangle$$

$$\left|\hat{y}\cdot\mathbf{p}_{cv}\right|^2 = \frac{1}{6}\left|\left\langle u_s\left|\mathbf{p}_y\right|u_y\right\rangle^2\right| = \frac{1}{2}M_b{}^2$$

for $\hat{e}=\hat{z}$

$$\hat{z}\cdot\mathbf{p}_{cv} = \left\langle iu_s\left|\mathbf{p}_z\right|-\frac{1}{\sqrt{6}}(\bar{u}_x+i\bar{u}_y-2u_z)\right\rangle$$

$$\left|\hat{z}\cdot\mathbf{p}_{cv}\right|^2 = \frac{2}{3}\left|\left\langle u_s\left|\mathbf{p}_z\right|u_z\right\rangle\right|^2 = 2M_b{}^2$$

Momentum matrix element (bandedge)

TE polarization $\hat{e} = \hat{x}$ or $\hat{e} = \hat{y}$

$$\left|\hat{e}\cdot\mathbf{p}_{c-hh}\right|^2 = \frac{3}{2}M_b^2$$ (heavy hole, bandedge)

$$\left|\hat{e}\cdot\mathbf{p}_{c-lh}\right|^2 = \frac{1}{2}M_b^2$$ (light hole, bandedge)

TM polarization $\hat{e} = \hat{z}$

$$\left|\hat{e}\cdot\mathbf{p}_{c-hh}\right|^2 = 0$$ (heavy hole, bandedge)

$$\left|\hat{e}\cdot\mathbf{p}_{c-lh}\right|^2 = 2M_b^2$$ (light hole, bandedge)

Momentum matrix element (general)

$\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2$ can also be calculated “away from the bandedge” (i.e. $k_t \neq 0$)

TE polarization $\hat{e}=\hat{x}$ or $\hat{e}=\hat{y}$

$$\left|\hat{e}\cdot\mathbf{p}_{c-hh}\right|^2 = \frac{3}{4}(1+\cos^2\theta)M_b^2$$ (heavy hole)

$$\left|\hat{e}\cdot\mathbf{p}_{c-lh}\right|^2 = \left[\frac{5}{4}-\frac{3}{4}\cos^2\theta\right]M_b^2$$ (light hole)

Note: $\cos^2\theta = \dfrac{E_{en}}{E_{en}+\dfrac{\hbar^2k_t^2}{2m_e^*}}$

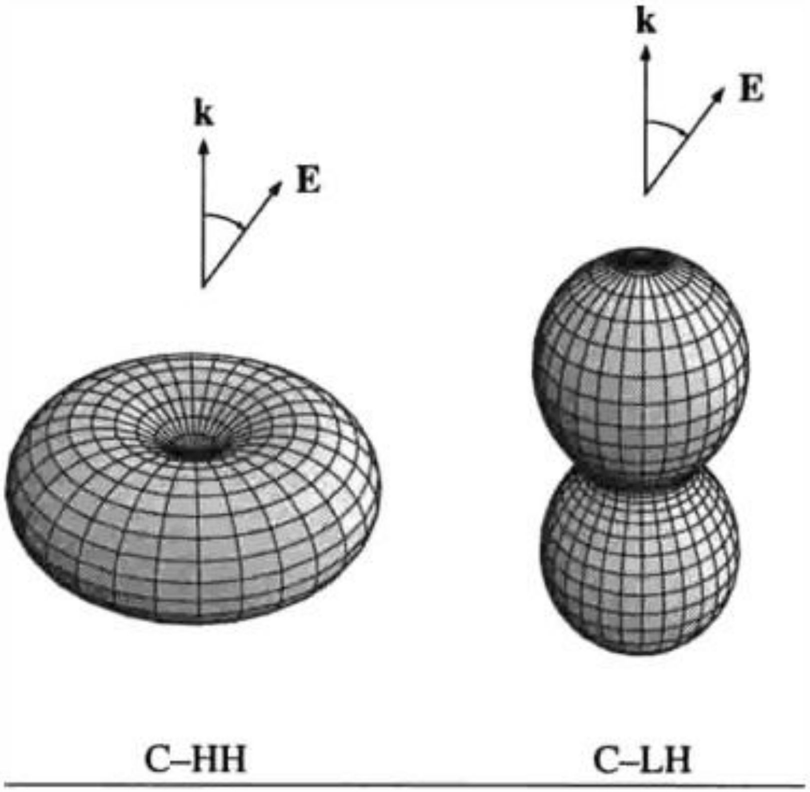
TM polarization $\hat{e}=\hat{z}$

$$\left|\hat{e}\cdot\mathbf{p}_{c-hh}\right|^2 = \frac{3}{2}\sin^2\theta M_b^2$$ (heavy hole)

$$\left|\hat{e}\cdot\mathbf{p}_{c-lh}\right|^2 = \frac{1}{2}(1+3\cos^2\theta)M_b^2$$ (light hole)

Momentum matrix element (general)

$\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2$ can also be calculated “away from the bandedge” (i.e. $k_t \neq 0$)



Relative magnitude of M_b^2 for conduction to heavy hole and light hole transitions.

Source: Zory. Quantum Well Lasers

Summary

$$\boxed{\alpha(\hbar\omega) = C_0 \frac{1}{L_z} \sum_{hh,lh} \sum_{n,m} \left| I_{hm}^{en} \right|^2 \, |\hat{e}\cdot\mathbf{p}_{cv}|^2 \, \rho_{r,2D} H(\hbar\omega - E_{hm}^{en}) \left[f_v(E=\hbar\omega - E_{hm}^{en}) - f_c(E=\hbar\omega - E_{hm}^{en}) \right]}$$

$$\rho_{r,2D} = \frac{m_r^*}{\pi\hbar^2}$$

$$I_{hm}^{en} = \int_{L_z} \phi_n^*(z) g_m(z) dz$$

$$\mathbf{p}_{cv} = \langle u_c | \mathbf{p} | u_v \rangle$$

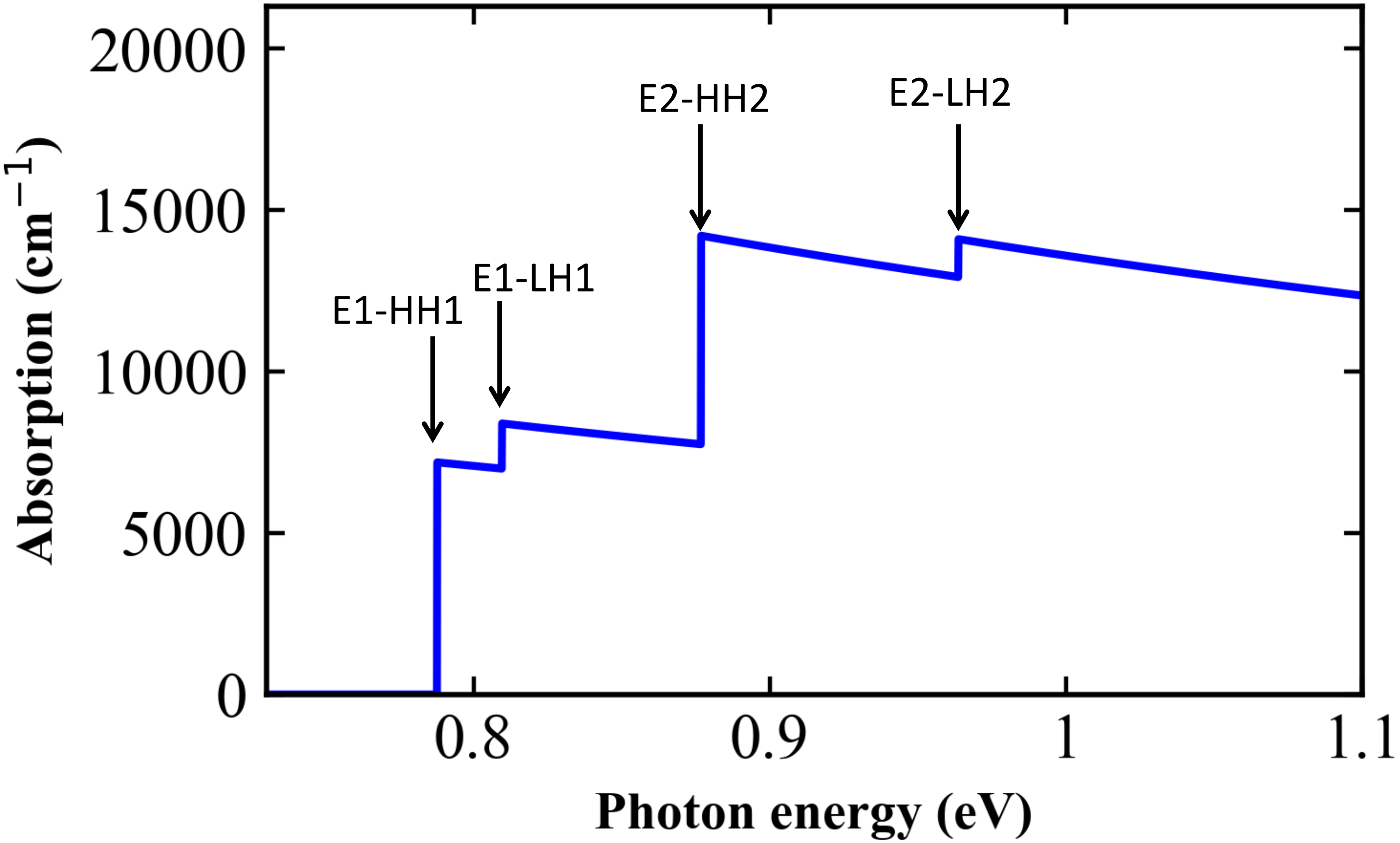
u_c and u_v are bloch functions

$$C_0 = \frac{\pi q^2}{n c \epsilon_0 \omega m_0^2}$$

$$f_c(\hbar\omega) = \frac{1}{1+\exp\left[(E_g + E_{en} + \left(\hbar\omega - E_{hm}^{en}\right) m_r^* / m_e^* - F_c \right] / kT]}$$

$$f_v(\hbar\omega) = \frac{1}{1+\exp\left[(E_{hm} - (\hbar\omega - E_{hm}^{en}) m_r^* / m_h^* - F_v) / kT \right]}$$

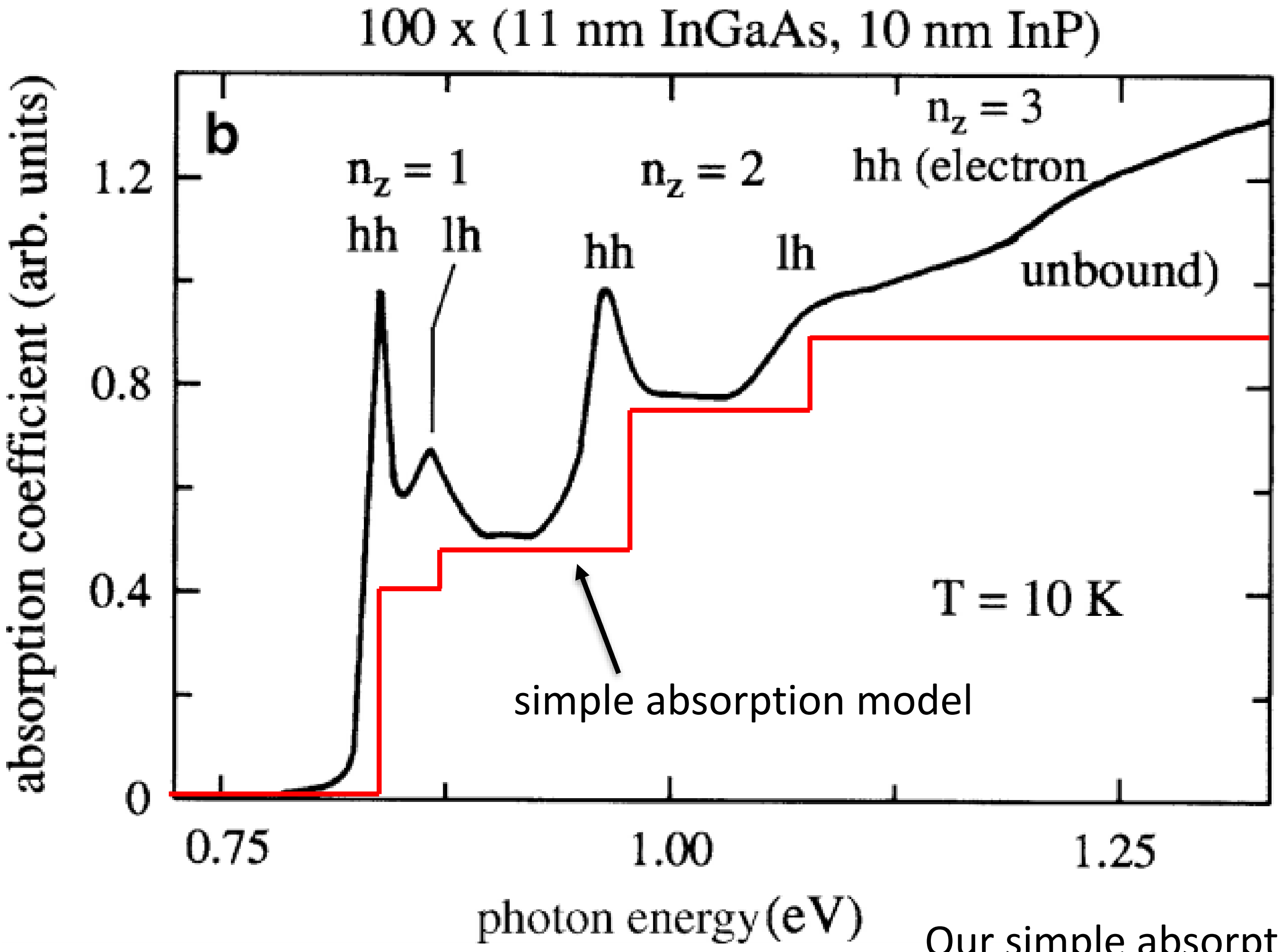
Calculated absorption spectrum



InP/InGaAs quantum well (L_z= 11nm) T=10K

TE bandedge matrix elements are used

Comparison with experimental data



simple absorption model

Our simple absorption model does not include excitonic effects or transitions to unbound states.

Source: Klingshirn. Semiconductor Optics.