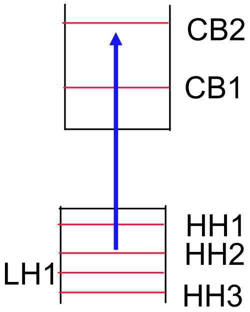
In This Lecture:

- Interband Transitions in Quantum Wells
- Intraband Transitions in Bulk & QWs

Interband Transitions in Quantum Wells

transitions between subbands derived from different bulk bands



Subband Wavefunctions

$$\psi_c^n = \frac{1}{\sqrt{AW}} e^{i\mathbf{k}_e\cdot\rho}\, g_c^n(z)\, u^n_{c\mathbf{k}_e}$$

$$\psi_v^m = \frac{1}{\sqrt{AW}} e^{i\mathbf{k}_h\cdot\rho} \boxed{\sum_\nu} g_\nu^{\nu m}(z)\, u^{\nu m}_{\nu\mathbf{k}_h}$$

Normalization area

Well width

Due to mixing in the VB

3D to 2D: Optical transitions are affected in two ways

- Form of JDOS
- Momentum matrix element; anisotropy is now genuine

Momentum Matrix Element in QWs

In going from 3D to 2D:

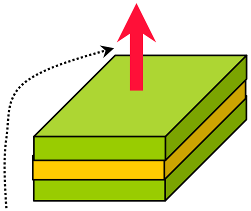
Cartesian component

$$p_{\mathrm{if}}^{\mathrm{3D}} = \frac{1}{V}\int e^{i(\mathbf{k}_e-\mathbf{k}_h)\cdot\mathbf{r}}\langle u_v^{\nu}|p_a|u_c\rangle\, d^3r$$

$$\rightarrow p_{\mathrm{if}}^{\mathrm{2D}} = \frac{1}{AW}\sum_{\nu}\underbrace{\langle g_v^{\nu m}|g_c^{n}\rangle}_{\text{env. fn. overlap along growth dir.}}\underbrace{\int e^{i(\mathbf{k}_e-\mathbf{k}_h)\cdot\rho}\,\langle u_v^{\nu m}|p_a|u_c\rangle\, d^2\rho}_{\text{in-plane overlap}}$$

[Other term, p_a acting on $g_c^n(z)$ leaves $\langle u_\upsilon^{\nu m}|u_c\rangle = 0$ at the same $\vec{k}$ state]

Unlike 3D, polarization dependence exists in 2D



Notation

- TE (to growth axis): Electric field in QW plane
- TM (to growth axis): Electric field along growth axis

Ref: Singh

Let the QW growth axis be *z* axis

TE (Optical electric field in *xy* plane)

Optical dipole matrix element is averaged over the azimuthal angle

From both **HH** bands to $\langle iS\uparrow'|$

$$|\hat{e}\cdot\mathbf{p}_{cv}|^2 \equiv \langle|\hat{e}\cdot\mathbf{M}_{c-hh}|^2\rangle = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,|\hat{x}\cdot\mathbf{M}_{c-hh}|^2$$

$$= \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi(\cos^2\theta\cos^2\phi + \sin^2\phi)\frac{P_x^2}{2}$$

$$= \frac{3}{4}(1+\cos^2\theta)M_b^2$$

Same results for the other CB spins not considered

From both **LH** bands to $\langle iS\downarrow'|$

$$\langle|\hat{e}\cdot\mathbf{M}_{c-lh}|^2\rangle = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\left(\left|\left\langle iS\downarrow'|p_x|\frac{3}{2},\frac{1}{2}\right\rangle\right|^2 + \left|\left\langle iS\downarrow'|p_x|\frac{3}{2},-\frac{1}{2}\right\rangle\right|^2\right)$$

$$= \left(\frac{2}{3}\sin^2\theta\langle\cos^2\phi\rangle + \frac{1}{6}\cos^2\theta\langle\cos^2\phi\rangle + \frac{1}{6}\langle\sin^2\phi\rangle\right)P_x^2$$

$$= \left[\sin^2\theta + \frac{1}{4}(\cos^2\theta + 1)\right]M_b^2$$

$$= \left(\frac{5}{4} - \frac{3}{4}\cos^2\theta\right)M_b^2$$

Same results for the other CB spins not considered

Ref: Chuang

TM (Optical electric field along *z* axis)

$$\langle|\hat{e}\cdot\mathbf{M}_{c-hh}|^2\rangle = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi|\hat{z}\cdot\mathbf{M}_{c-hh}|^2 = \frac{3}{2}\sin^2\theta M_b^2$$

$$\begin{aligned}\langle|\hat{e}\cdot\mathbf{M}_{c-lh}|^2\rangle &= \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\left(\left|\left\langle \mathrm{i}S\downarrow'|ez|\frac{3}{2},\frac{1}{2}\right\rangle\right|^2 + \left|\left\langle \mathrm{i}S\downarrow'|ez|\frac{3}{2},-\frac{1}{2}\right\rangle\right|^2\right)\\ &= \left(\frac{1}{6}\sin^2\theta + \frac{2}{3}\cos^2\theta\right)P_x^2\\ &= \frac{1+3\cos^2\theta}{2}M_b^2\end{aligned}$$

Table 9.1 Summary of the Momentum Matrix Elements in Parabolic Band Model ($|\hat{e}\cdot\mathbf{p}_{cv}|^2 = |\hat{e}\cdot\mathbf{M}|^2$)

Bulk $|\hat{x}\cdot\mathbf{p}_{cv}|^2 = |\hat{y}\cdot\mathbf{p}_{cv}|^2 = |\hat{z}\cdot\mathbf{p}_{cv}|^2 = M_b^2 = \frac{m_0}{6}E_p$

Quantum Well

TE Polarization ($\hat{e} = \hat{x}$ or $\hat{y}$)	**TM Polarization** ($\hat{e} = \hat{z}$)
$\langle|\hat{e}\cdot\mathbf{M}_{c-hh}|^2\rangle = \frac{3}{4}(1+\cos^2\theta)M_b^2$	$\langle|\hat{e}\cdot\mathbf{M}_{c-hh}|^2\rangle = \frac{3}{2}\sin^2\theta M_b^2$
$\langle|\hat{e}\cdot\mathbf{M}_{c-lh}|^2\rangle = (\frac{5}{4}-\frac{3}{4}\cos^2\theta)M_b^2$	$\langle|\hat{e}\cdot\mathbf{M}_{c-lh}|^2\rangle = \frac{1}{2}(1+3\cos^2\theta)M_b^2$

Conservation Rule

Sum Rules

$\langle|\hat{x}\cdot\mathbf{M}_{c-h}|^2\rangle + \langle|\hat{y}\cdot\mathbf{M}_{c-h}|^2\rangle + \langle|\hat{z}\cdot\mathbf{M}_{c-h}|^2\rangle = 3M_b^2, (h = hh \text{ or } lh)$

$\langle|\hat{e}\cdot\mathbf{M}_{c-hh}|^2\rangle + \langle|\hat{e}\cdot\mathbf{M}_{c-lh}|^2\rangle = 2M_b^2$

Ref: Chuang

Back to Absorption Rate in QWs

JDOS in 2D:

$$\frac{N_{cv}^{2D}(\hbar\omega)}{W} = \frac{m_r^*}{\pi\hbar^2 W}\sum_{nm}\langle g_v^m|g_c^n\rangle\,\theta(E_{nm}-\hbar\omega)$$

$$E_{nm} = E_{gap} + E_c^n + E_v^m$$

$$\alpha(\hbar\omega) = \frac{\pi e^2\hbar}{m_o^2 c n_r \epsilon_o}\,\frac{1}{(\hbar\omega)}\,|a\cdot p_{if}|^2\,\frac{N_{2D}(\hbar\omega)}{W}\sum_{n,m} f_{nm}\,\theta(E_{nm}-\hbar\omega)$$

$$f_{nm} = \left|\sum_{\nu}\langle g_v^{\nu m}|\,g_c^n\rangle\right|^2$$

Observe that even-odd parity transitions are not allowed due to vanishing of this overlap

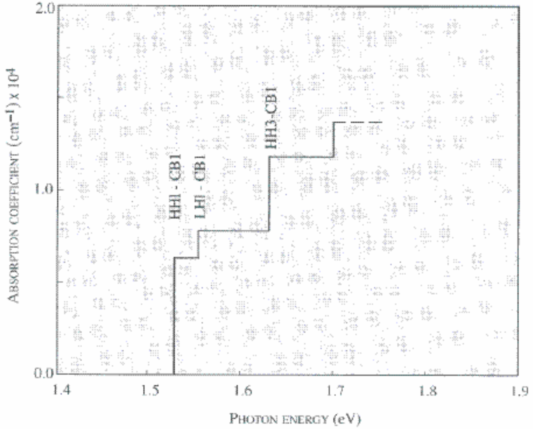


Figure 9.7: Calculated absorption coefficient in a 100 Å GaAs/Al$_{0.3}$Ga$_{0.7}$As quantum well structure for in-plane polarized light. The HH transition is about three times stronger than the LH transition in this polarization. In a real material excitonic transition dominate near the bandedges as disucssed in the next chapter.

Ref: Singh

Indirect Interband Transitions in Bulk

Common Indirect Se/c: Si, Ge, C, AlAs, GaP, AlP, SiC, AlN (zb)

No energy cons.

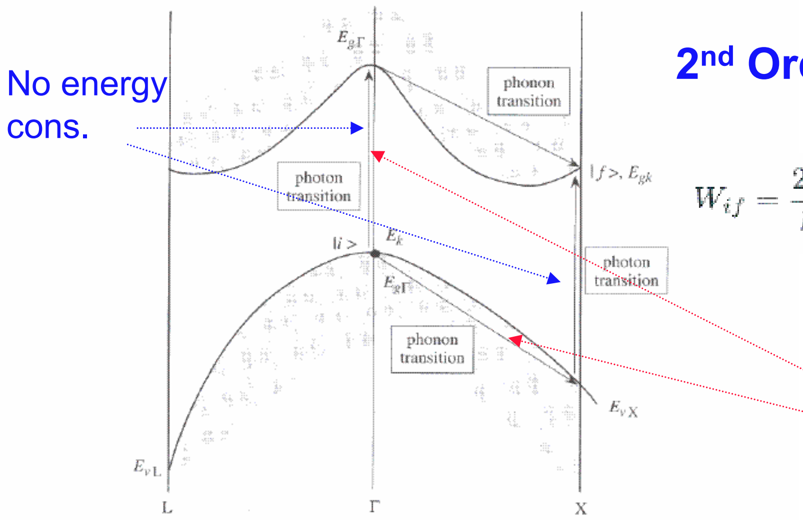


Figure 9.9: Two processes showing how a photon and a phonon can take an electron from state $|i\rangle$ to state $|f\rangle$. The photon energy need not be equal to the vertical energy, since the intermediate transitions are "virtual," i.e., the electron does not reside there for any length of time.

2nd Order Matrix Element:

Intermediate virtual state summed over

$$W_{if} = \frac{2\pi}{\hbar} \int \left| \frac{\sum \langle f|H_{\text{per}}|n\rangle \langle n|H_{\text{per}}|i\rangle}{E_i - E_n} \right|^2 \delta(E_f - E_i) \frac{d^3k}{(2\pi)^3}$$

$$H_{\text{per}} = H_{\text{ph}} + H_{\text{ep}}$$

Weight of these two pathways $\propto \dfrac{1}{|E_i - E_n|^2}$

With photon energies smaller than the direct band gap intermediate transitions can occur since energy need not be conserved

$$W_{if}(\boldsymbol{k}) = \frac{2\pi}{\hbar}\int_f \left\{|M_{\rm em}|^2 + |M_{\rm abs}|^2\right\}\delta(\boldsymbol{E}_f - \boldsymbol{E}_i)\frac{d^3k}{(2\pi)^3}$$

Pathways which require phonon emission/absorption

Form of the matrix elements:

$$M_{\rm abs} = \frac{\left|\langle c,\boldsymbol{k}+\boldsymbol{q}|H_{\rm ep}^{\rm abs}|c,\boldsymbol{k}\rangle\right|^2 \left|\langle c,\boldsymbol{k}|H_{\rm ph}^{\rm abs}|v,\boldsymbol{k}\rangle\right|^2}{(\boldsymbol{E}_{g\Gamma} - \hbar\omega)^2}$$

$$M_{\rm em} = \frac{\left|\langle c,\boldsymbol{k}-\boldsymbol{q}|H_{\rm ep}^{\rm em}|c,\boldsymbol{k}\rangle\right|^2 \left|\langle c,\boldsymbol{k}|H_{\rm ph}^{\rm em}|v,\boldsymbol{k}\rangle\right|^2}{(\boldsymbol{E}_{g\Gamma} - \hbar\omega)^2}$$

direct optical transitions

e-phonon scattering matrix elements
due to optical phonon intervalley scattering
with the associated matrix element:

$$M_q^2 = \frac{\hbar D_{ij}^2}{2\rho V\omega_{ij}}\left\{\begin{array}{l} n(\omega_{ij}) \longrightarrow \text{abs.} \\ n(\omega_{ij})+1 \longrightarrow \text{em.}\end{array}\right.$$

D_{ij} : Deformation potential

ρ : Mass density

ω_{ij} : Intervalley phonon frequency

$n(\omega_{ij})$: phonon occupancy (BE distr.)

For parabolic bands, the absorption rate results in:

equivalent valleys

$$
\begin{aligned}
W_{\rm abs}(\hbar\omega) &= \frac{M_{\rm ph}^2\, D_{ij}^2\, J_v\, (m_c m_v)^{3/2}}{8\pi^2 (E_{g\Gamma}-\hbar\omega)^2\, \hbar^6\, \rho\, \omega_{ij}} \\
&\times \left[n(\omega_{ij}) \left(\hbar\omega - E_{g\mathbf{k}'} + \hbar\omega_{ij}\right)^2 \right. \\
&+ \left. \{n(\omega_{ij})+1\} \left(\hbar\omega - E_{g\mathbf{k}'} - \hbar\omega_{ij}\right)^2 \right]
\end{aligned}
$$

Photon-related matrix element

$$
M_{\rm ph}^2 = \frac{e^2 \hbar n_{\rm ph}\, |a \cdot p_{\rm if}|^2}{2 m_o^2 \epsilon \omega}
$$

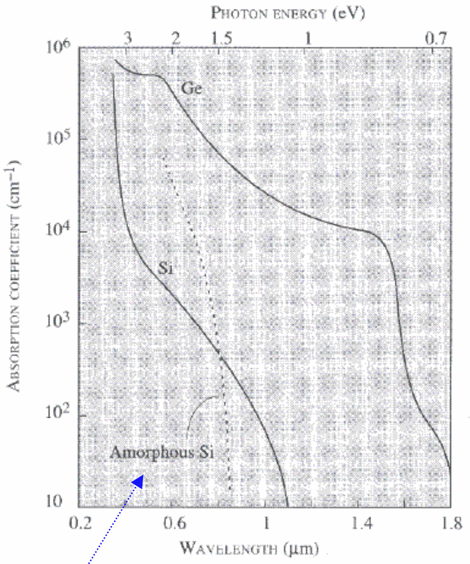


Figure 9.10: Absorption coefficient of Si and Ge. Also shown is absorption coefficient for amorphous silicon which is almost like a direct gap semiconductor, since *k*-selection is not applicable.

Note the contrast in $W_{\rm abs}$

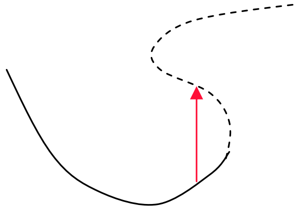
Direct Bandgap: $(\hbar\omega - E_g)^{1/2}$

Indirect Bandgap: $(\hbar\omega - E_{\rm th})^2$

In **amorphous** se/c, *k*-conservation requirement
is relaxed (no periodicity, xtal momentum not a good quantum label)
This results in higher absorption coefficient

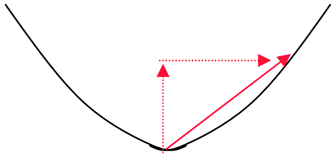
Intraband Transitions in Bulk Se/c

- As each band at a *k*-state is single-valued 1st order vertical intraband transitions are not possible



- Intraband transitions must involve some second mechanism (phonon, ionized imp, defects...) to ensure momentum conservation

- Intraband transitions are also known as **free carrier absorption** and are effective in the cladding layers of lasers



Drude Model (to explain free carrier absorption)

$$m^*\ddot{x} + \boxed{m^*\gamma\dot{x}} + m^*\omega_0^2 = eE_0\cos(\omega t)$$

w/o scattering no net energy xfer; *e*'s oscillate back and forth within the band

By introducing a scattering mechanism, energy gained by the *e* in one cycle will be partially lost in the form of, say phonon emission by the electron.

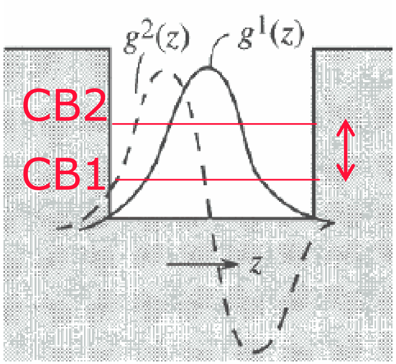
$$\alpha(\hbar\omega) \propto \frac{1}{\omega^2}$$

$$\propto \frac{1}{\mu}$$

mobility

If the mobility is large (weak scattering) absorption coefficient becomes small

Intraband Transitions in Quantum Wells



- ➢Since a number of subbands may originate from the same bulk band, certain inter-subband transitions (CB1-CB2) may be termed as intraband transitions in QWs

- ➢Such inter-subband transitions have great importance in for far infrared detectors and forms the basis of **Quantum Cascade Lasers**

$$\begin{aligned}\psi^1(\boldsymbol{k},z) &= g^1(z)\, e^{ik\cdot\rho}\, u^1_{n\mathbf{k}}(\boldsymbol{r})\\ \psi^2(\boldsymbol{k},z) &= g^2(z)\, e^{ik\cdot\rho}\, u^2_{n\mathbf{k}}(\boldsymbol{r})\end{aligned}$$

orthogonal