In This Lecture:

- Interband Transitions in Bulk Se/c
  - Momentum Matrix Element
  - Polarization dependence
- Interband Transitions in Quantum Wells
- Intraband Transitions in Bulk & QWs

Interband Transitions in Bulk Se/c

As the photon momentum is negligible compared to electronic crystal momenta, the transitions are (almost) vertical (k_{op}=0)
[See, next page]

For parabolic bands:

$$\hbar\omega = (E_c - E_v) + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_e} + \frac{1}{m_h}\right)$$

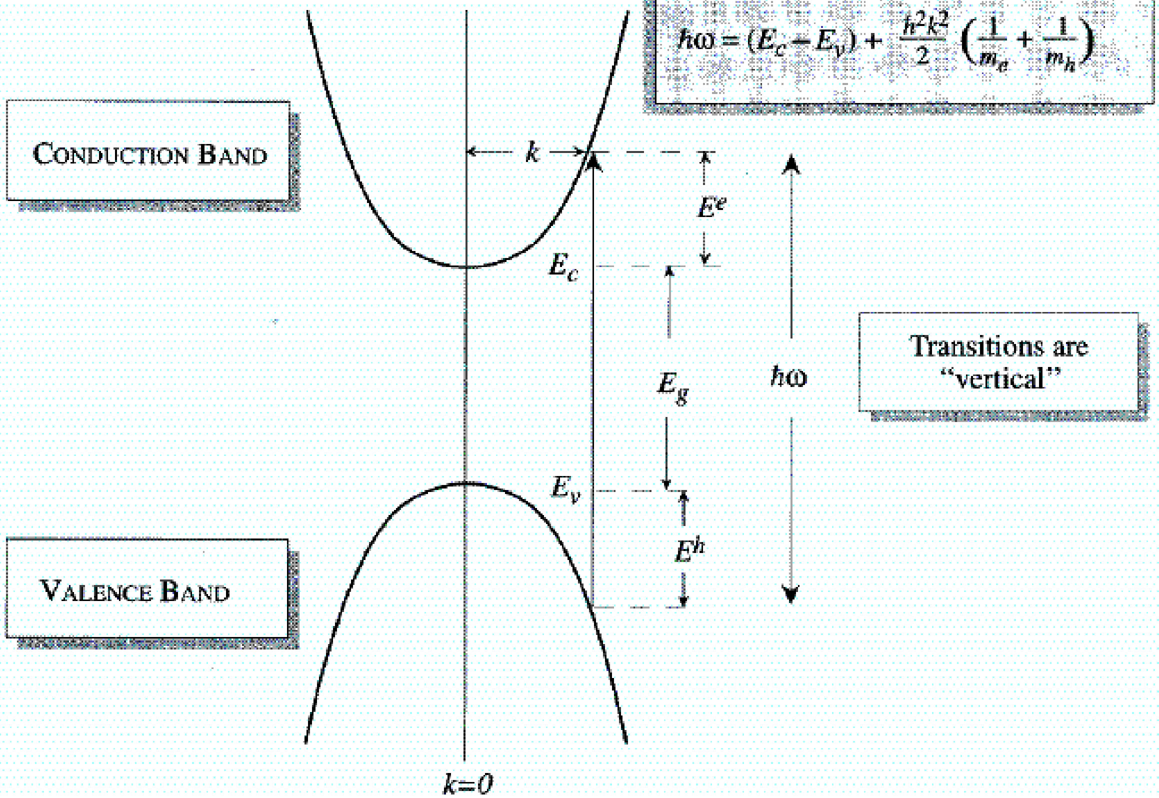


Figure 9.5: The positions of the electron and hole energies at vertical k-values. The electron and hole energies are determined by the photon energy and the carrier masses. Since the photon momentum is negligible the transitions are vertical.

Ref: Singh

Momentum Matrix Elements

Predominantly we are interested in transitions between CB and VB so that $i \rightarrow \upsilon$, $f \rightarrow c$

$$\hat{e}\cdot\vec{p} = \hat{e}\cdot\int \psi^{*}_{c,\vec{k}_c}\; e^{i\vec{k}_{op}\cdot\vec{r}}\,\vec{p}\;\psi_{\upsilon,\vec{k}_\upsilon}\, d^3r$$

where

$$\psi_{c,\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}_c\cdot\vec{r}} u_{c,\vec{k}_c}(\vec{r}); \quad \text{similarly for } \psi_{\upsilon,\vec{k}_\upsilon}(\vec{r})$$

vanishes when k_{op}=0 due to Bloch fn orthogonality

$$\vec{p}_{c\upsilon} = \boxed{\int u^{*}_{c,\vec{k}_c}(\vec{r})\; e^{-i\vec{k}_c\cdot\vec{r}} e^{i\vec{k}_{op}\cdot\vec{r}}\hbar k_\upsilon e^{i\vec{k}_\upsilon\cdot\vec{r}} u_{\upsilon,\vec{k}_\upsilon}(\vec{r})\;\frac{d^3r}{V}}$$

$$+\int u^{*}_{c,\vec{k}_c}(\vec{r})\; e^{-i\vec{k}_c\cdot\vec{r}} e^{i\vec{k}_{op}\cdot\vec{r}}\left(\frac{\hbar}{i}\vec{\nabla}u_{\upsilon,\vec{k}_\upsilon}(\vec{r})\right) e^{i\vec{k}_\upsilon\cdot\vec{r}}\;\frac{d^3r}{V}$$

Treat slowly-varying (envelopes) and the cell-periodic parts separately

$$\vec{p}_{c\upsilon} = \int_\Omega u^{*}_{c,\vec{k}_c}(\vec{r})\left(\frac{\hbar}{i}\vec{\nabla}u_{\upsilon,\vec{k}_\upsilon}(\vec{r})\right)\frac{d^3r}{\Omega}\;\underbrace{\int_V e^{i(-\vec{k}_c+\vec{k}_\upsilon+\vec{k}_{op})\cdot\vec{r}}\,\frac{d^3r}{V}}_{\delta_{\vec{k}_c,\vec{k}_\upsilon+\vec{k}_{op}}}$$

unit cell volume

xtal volume

$$\vec{p}_{c\upsilon} = \delta_{\vec{k}_c,\vec{k}_\upsilon+\vec{k}_{op}}\int_\Omega u^{*}_{c,\vec{k}_c}(\vec{r})\left(\frac{\hbar}{i}\vec{\nabla}u_{\upsilon,\vec{k}_\upsilon}(\vec{r})\right)\frac{d^3r}{\Omega}$$

Electric dipole forbidden transitions

When certain $\boldsymbol{p}_{cv}$ transition matrix element vanishes (due to some symmetry reason etc.) this is termed as a electric dipole-forbidden-transition.
In this case higher-order contributions such as electric quadrupole and magnetic dipole transitions become important. Compared to the electric dipole transitions they are reduced in strength by a factor of (lattice constant/wavelength of light)^2, that requires very high frequencies (UV to X-rays)...

Polarization Dependence

Recall se/c band edge states:

Conduction Band:

$$|iS\uparrow\rangle,\ |iS\downarrow\rangle$$

Valence Bands (only HH, LH):

$$\left|\frac{3}{2},\frac{3}{2}\right\rangle = \frac{-1}{\sqrt{2}}\left|(X+iY)\uparrow\right\rangle,$$

$$\left|\frac{3}{2},-\frac{3}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|(X-iY)\downarrow\right\rangle,$$

$$\left|\frac{3}{2},\frac{1}{2}\right\rangle = \frac{-1}{\sqrt{6}}\left|(X+iY)\downarrow\right\rangle + \sqrt{\frac{2}{3}}\left|Z\uparrow\right\rangle,$$

$$\left|\frac{3}{2},-\frac{1}{2}\right\rangle = \frac{1}{\sqrt{6}}\left|(X-iY)\uparrow\right\rangle + \sqrt{\frac{2}{3}}\left|Z\downarrow\right\rangle$$

Momentum-matrix parameter:

$$P_x = \langle iS|p_x|X\rangle = \langle iS|p_y|Y\rangle = \langle iS|p_z|Z\rangle = \frac{m_0}{\hbar}P$$

CB to HH Transitions:

$$\left.\begin{aligned}
&\left\langle iS\uparrow\middle|\vec{p}\middle|\frac{3}{2},\frac{3}{2}\right\rangle = -\frac{P_x}{\sqrt{2}}(\hat{x}+i\hat{y}),\\
&\left\langle iS\downarrow\middle|\vec{p}\middle|\frac{3}{2},\frac{3}{2}\right\rangle = 0,\\
&\left\langle iS\downarrow\middle|\vec{p}\middle|\frac{3}{2},-\frac{3}{2}\right\rangle = \frac{P_x}{\sqrt{2}}(\hat{x}-i\hat{y}),\\
&\left\langle iS\uparrow\middle|\vec{p}\middle|\frac{3}{2},-\frac{3}{2}\right\rangle = 0,
\end{aligned}\right\}$$

WATCH OUT:
No coupling of the *z*-polarized light between CB & HH

CB to LH Transitions:

$$\left\langle iS\uparrow\middle|\vec{p}\middle|\frac{3}{2},\frac{1}{2}\right\rangle = P_x\sqrt{\frac{2}{3}}\,\hat{z},$$

$$\left\langle iS\downarrow\middle|\vec{p}\middle|\frac{3}{2},\frac{1}{2}\right\rangle = -\frac{P_x}{\sqrt{6}}(\hat{x}+i\hat{y}),$$

$$\left\langle iS\downarrow\middle|\vec{p}\middle|\frac{3}{2},-\frac{1}{2}\right\rangle = P_x\sqrt{\frac{2}{3}}\,\hat{z},$$

$$\left\langle iS\uparrow\middle|\vec{p}\middle|\frac{3}{2},-\frac{1}{2}\right\rangle = \frac{P_x}{\sqrt{6}}(\hat{x}-i\hat{y}),$$

Reflections on the polarization dependence

- For a cubic xtal what differentiates *z* from *x* or *y*?
- Recall that in defining the expansion basis vectors we assumed electron wavevector to be along *z* direction
- For that reason we are also using the *z*-projection of the spin

- Does that give enough support for singling out z from x or y direction?
- After all that's just for the sake of formulation, say a convention
- Away from **k**=0 HH & LH become mixed
- So only at **k**=0 we could talk about such a selectivity
- But at **k**=0 we lose any sense of direction of the k-vector!

To Remind you the LK Hamiltonian

$$\overline{\overline{\mathbf{H}}}^{\mathrm{LK}} = -\begin{bmatrix} P+Q & -S & R & 0 & -S/\sqrt{2} & \sqrt{2}R \\ -S^{+} & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{3/2}S \\ R^{+} & 0 & P-Q & S & \sqrt{3/2}S^{+} & \sqrt{2}Q \\ 0 & R^{+} & S^{+} & P+Q & -\sqrt{2}R^{+} & -S^{+}/\sqrt{2} \\ -S^{+}/\sqrt{2} & -\sqrt{2}Q^{+} & \sqrt{3/2}S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^{+} & \sqrt{3/2}S^{+} & \sqrt{2}Q^{+} & -S/\sqrt{2} & 0 & P+\Delta \end{bmatrix}$$

complex conjugate

where

$$P = \frac{\hbar^2\gamma_1}{2m_0}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$Q = \frac{\hbar^2\gamma_2}{2m_0}\left(k_x^2 + k_y^2 - 2k_z^2\right)$$

$$R = \frac{\hbar^2}{2m_0}\left[-\sqrt{3}\,\gamma_2\left(k_x^2 - k_y^2\right) + i2\sqrt{3}\,\gamma_3 k_x k_y\right]$$

$$S = \frac{\hbar^2\gamma_3}{m_0}\sqrt{3}\,(k_x - ik_y)k_z$$

Ref: Chuang

Averaging over the polarization for bulk

- These considerations suggest us to consider unpolarized light
- Equivalently we shall consider electron wavevector to point along a general direction and average the matrix element over the solid angle

Let the electron wavevector to be along a direction (θ,Φ):

$$\mathbf{k} = k \sin\theta \cos\phi \, \hat{x} + k \sin\theta \sin\phi \, \hat{y} + k \cos\theta \, \hat{z}$$

For illustration consider CB-HH transition:

$$|\hat{e} \cdot \mathbf{p}_{cv}|^2 \equiv \left\langle |\hat{e} \cdot \mathbf{M}_{c-hh}|^2 \right\rangle = \underbrace{\frac{1}{4\pi} \int |\hat{x} \cdot \mathbf{M}_{c-hh}|^2 \sin\theta \, d\theta \, d\phi}_{\text{averaging over the solid angle}}$$

CB: $|\mathrm{i}S\downarrow'\rangle$ and $|\mathrm{i}S\uparrow'\rangle$

HH:

$$\left|\frac{3}{2},\frac{3}{2}\right\rangle' = \frac{-1}{\sqrt{2}}|(X' + \mathrm{i}Y')\uparrow'\rangle$$

$$= \frac{-1}{\sqrt{2}}|(\cos\theta\cos\phi - \mathrm{i}\sin\phi)X$$

$$+ (\cos\theta\sin\phi + \mathrm{i}\cos\phi)Y - \sin\theta Z\rangle\,|\uparrow'\rangle$$

$$\left|\frac{3}{2},-\frac{3}{2}\right\rangle' = \frac{1}{\sqrt{2}}|(X' - \mathrm{i}Y')\downarrow'\rangle$$

$$= \frac{1}{\sqrt{2}}|(\cos\theta\cos\phi + \mathrm{i}\sin\phi)X$$

$$+ (\cos\theta\sin\phi - \mathrm{i}\cos\phi)Y - \sin\theta Z\rangle\,|\downarrow'\rangle$$

Note that for ease of calculation we keep the spin parts in the new (rotated) coordinate system…

Ref: Chuang

$$\left\langle iS\uparrow'|\mathbf{p}|\frac{3}{2},\frac{3}{2}\right\rangle' = -\Big[(\cos\theta\cos\phi - i\sin\phi)\hat{x} + (\cos\theta\sin\phi + i\cos\phi)\hat{y} - \sin\theta\hat{z}\Big]\frac{P_x}{\sqrt{2}}$$

$$\left\langle iS\downarrow'|\mathbf{p}|\frac{3}{2},-\frac{3}{2}\right\rangle' = \Big[(\cos\theta\cos\phi + i\sin\phi)\hat{x} + (\cos\theta\sin\phi - i\cos\phi)\hat{y} - \sin\theta\hat{z}\Big]\frac{P_x}{\sqrt{2}}$$

$$\left\langle iS\uparrow'|\mathbf{p}|\frac{3}{2},-\frac{3}{2}\right\rangle' = 0$$

$$\left\langle iS\downarrow'|\mathbf{p}|\frac{3}{2},\frac{3}{2}\right\rangle' = 0$$

Consider, for instance optical transition from the CB of one spin, say $< iS\uparrow'|$ to either of the HH bands $\left|\frac{3}{2},\frac{3}{2}\right\rangle'$ $\left|\frac{3}{2},-\frac{3}{2}\right\rangle'$; one of them is already zero

Ref: Chuang

Bulk Momentum Matrix Element for Unpolarized Light

$$|\hat{e}\cdot\mathbf{p}_{cv}|^2 \equiv \langle |\hat{e}\cdot\mathbf{M}_{c-hh}|^2 \rangle = \frac{1}{4\pi}\int |\hat{x}\cdot\mathbf{M}_{c-hh}|^2 \sin\theta \, d\theta \, d\phi$$

$$= \frac{1}{4\pi}\int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \left(\cos^2\theta\cos^2\phi + \sin^2\phi\right)\frac{P_x^2}{2}$$

$$= \frac{1}{3}P_x^2 \equiv M_b^2$$

where

$$M_b^2 = \frac{1}{3}P_x^2 = \frac{m_0^2}{3\hbar^2}P^2$$

Kane's parameter, (not a surprise)

$$= \left(\frac{m_0}{m_e^*} - 1\right)\frac{m_0 E_g(E_g + \Delta)}{6\left(E_g + \frac{2}{3}\Delta\right)}$$

Alternatively, an energy parameter E_p can be defined as:

$$E_p = \frac{2m_0}{\hbar^2}P^2, \quad \text{so that} \quad M_b = \frac{m_0}{6}E_p$$

Ref: Chuang

The other polarizations, spin, and LH band

Same result M_b^2 is obtained for

* For $\hat{e}=\hat{y}$ or $\hat{e}=\hat{z}$ (cubic symmetry)

* For the other spin component of the CB, $\langle iS\downarrow'|$

* For the transition between the LH band (per spin),

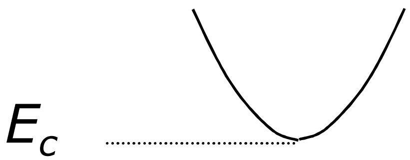
$$\left|\left\langle iS\downarrow'\left|ex\right|\frac{3}{2},\frac{1}{2}\right\rangle'\right|^2+\left|\left\langle iS\downarrow'\left|ex\right|\frac{3}{2},-\frac{1}{2}\right\rangle'\right|^2$$

Joint Density of States (also called reduced DOS)

This is an important piece that appears inside total transition rate expressions

Single Parabolic Band DOS:

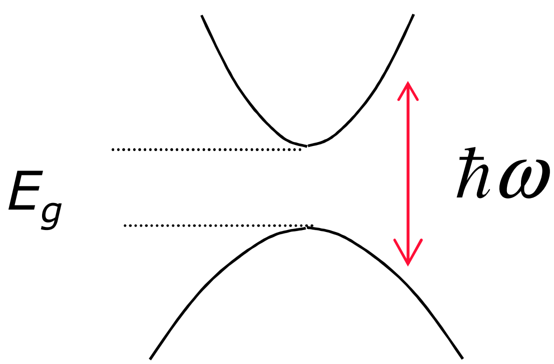
$$N_m(E) = \sum_{\vec{k}\in 1^{\text{st}}\ \text{BZ}} \sum_{\sigma} \delta\left(E - E_m(\vec{k})\right)$$



For a parabolic band: $E - E_c = \dfrac{\hbar^2 k^2}{2m^*_{dos}}$

$$N_m(E) = \sqrt{2}\,\frac{(m^*_{dos})^{3/2}\sqrt{E - E_c}}{\pi^2\hbar^3},$$

Joint DOS of CB-VB:



Between two parabolic CB and VB: $\hbar\omega - E_g = \dfrac{\hbar^2 k^2}{2}\underbrace{\left(\dfrac{1}{m^*_e} + \dfrac{1}{m^*_h}\right)}_{\frac{1}{m^*_r}}$

$$N_{cv}(\hbar\omega) = \sum_{\vec{k}\in 1^{\text{st}}\ \text{BZ}} \sum_{\sigma} \delta\left(E_v(\vec{k}) - E_c(\vec{k}) + \hbar\omega\right)$$

$$N_{cv}(\hbar\omega) = \sqrt{2}\,\frac{(m^*_r)^{3/2}\sqrt{\hbar\omega - E_g}}{\pi^2\hbar^3}$$

Absorption Rate (Final Expression)

With all these ingredients the bulk absorption rate for unpolarized light becomes:

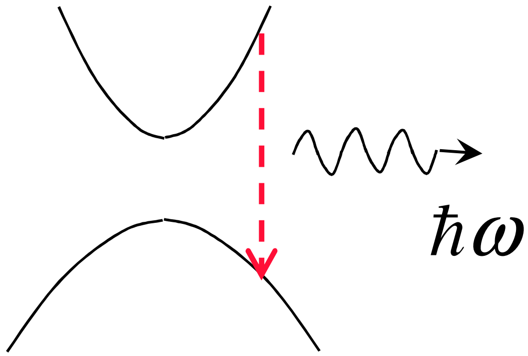
$$W_{abs} = \frac{\pi e^2 \hbar n_{ph}}{m_0^2 \hbar \omega \varepsilon} \left(2M_b^2 \right) N_{cv}(\hbar\omega)$$

JDOS

$$N_{cv}(\hbar\omega) = \sqrt{2}\,\frac{(m_r^*)^{3/2}\sqrt{\hbar\omega - E_g}}{\pi^2 \hbar^3}$$

Radiative e-h Recombination Time: Emission

In the case of interband recombination rate of an e with a hole at the same **k** state, we integrate over all possible photon states



$$W_{\mathrm{em}} = \frac{\pi e^2 \hbar}{m_o^2 \hbar\omega\epsilon} \left(n_{ph} + 1\right) \left|\boldsymbol{a} \cdot \boldsymbol{p}_{\mathrm{if}}\right|^2 \rho_a(\hbar\omega)$$

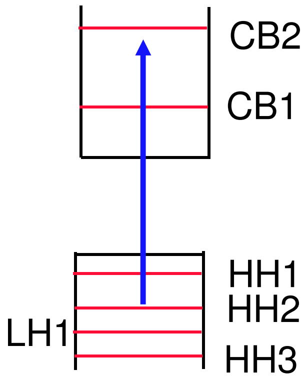
$$\rho(\hbar\omega) = \frac{2\omega^2}{2\pi^2 \hbar v^3}$$ 3D total photon DOS

For $n_{ph}=0, \quad W_{em} \rightarrow W_{spon}$

Associated e-h radiative recombination time is $\tau_0 = \dfrac{1}{W_{spon}}$

Interband Transitions in Quantum Wells

transitions between subbands derived from different bulk bands



Subband Wavefunctions

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

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

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

Ref: Singh

Momentum Matrix Element in QWs

In going from 3D to 2D:

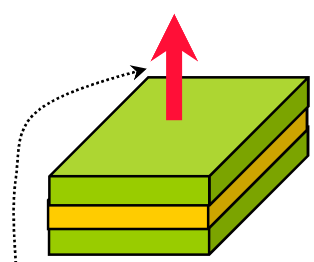
$$p_{\text{if}}^{3D} = \frac{1}{V}\int e^{i(\mathbf{k}_e-\mathbf{k}_h)\cdot\mathbf{r}}\langle u_v^{\nu}|p_a|u_c\rangle\, d^3r$$

Cartesian component

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

[Other term, p_a acting on $g_c^n(z)$ leaves $\left\langle u_v^{\nu m}\middle| u_c\right\rangle = 0$ 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 $\langle iS\uparrow'|$

$$|\hat{e}\cdot\mathbf{p}_{cv}|^2 \equiv \langle|\hat{e}\cdot\mathbf{M}_{c-hh}|^2\rangle = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\,|\hat{x}\cdot\mathbf{M}_{c-hh}|^2$$
$$= \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\left(\cos^2\theta\cos^2\phi+\sin^2\phi\right)\frac{P_x^2}{2}$$
$$= \frac{3}{4}(1+\cos^2\theta)M_b^2$$

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)

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

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

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

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

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

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:

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

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

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

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

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

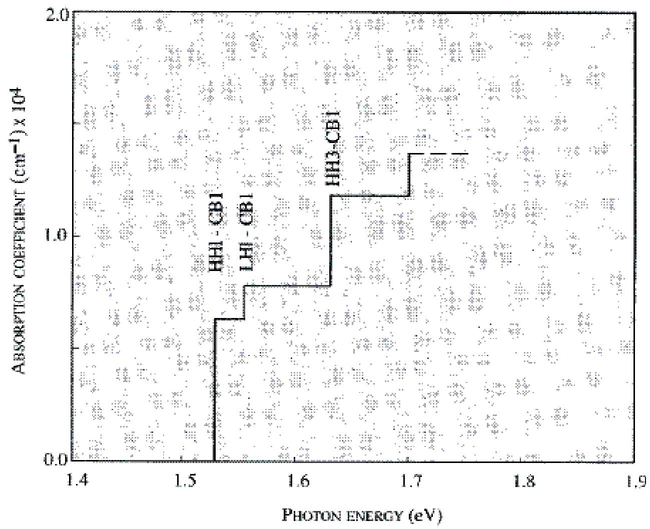


Figure 9.7: Calculated absorption coefficient in a 100 Å GaAs/Al$_{0.3}$Ga$_{0.7}$As quantum well structure for in-plane polarized light. The HH transition is about three times stronger than the LH transition in this polarization. In a real material excitonic transition dominate near the bandedges as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

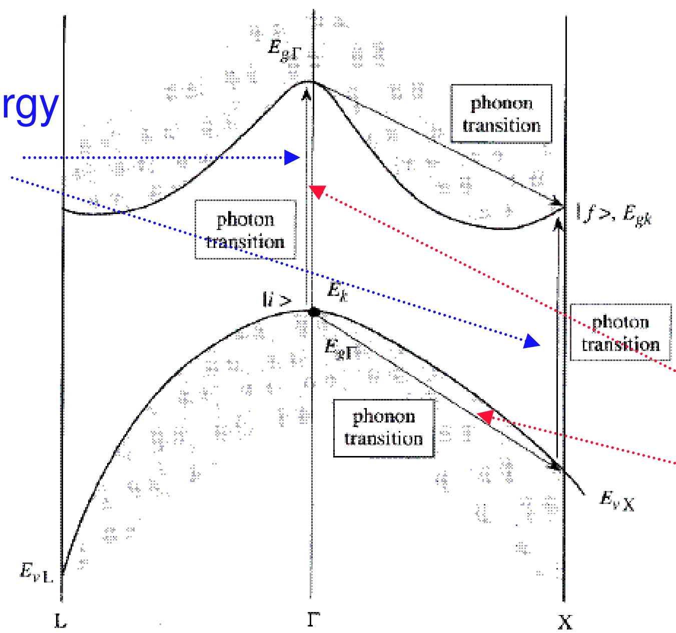


Figure 9.9: Two processes showing how a photon and a phonon can take an electron from state $|i\rangle$ to state $|f\rangle$. The photon energy need not be equal to the vertical energy, since the intermediate transitions are "virtual," i.e., the electron does not reside there for any length of time.

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

Ref: Singh

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

Pathways which require phonon emission/absorption

Form of the matrix elements:

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

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

direct optical transitions

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

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

D_{ij} : Deformation potential

ρ : Mass density

ω_{ij} : Intervalley phonon frequency

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

Ref: Singh

For parabolic bands, the absorption rate results in:

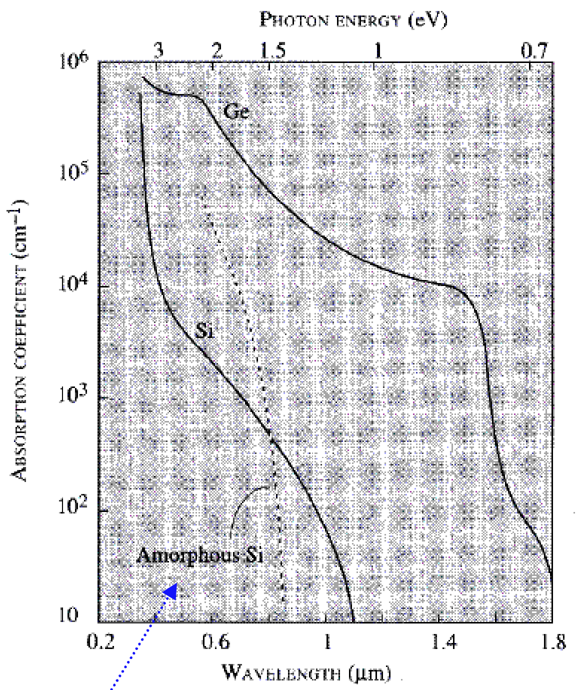


Figure 9.10: Absorption coefficient of Si and Ge. Also shown is absorption coefficient for amorphous silicon which is almost like a direct gap semiconductor, since k-selection is not applicable.

\# equivalent valleys

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

Photon-related matrix element

$$M_{\mathrm{ph}}^2 = \frac{e^2 \hbar n_{\mathrm{ph}} \left|\mathbf{a}\cdot\mathbf{p}_{\mathrm{if}}\right|^2}{2 m_o^2 \epsilon \omega}$$

Note the contrast in W_{abs}

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

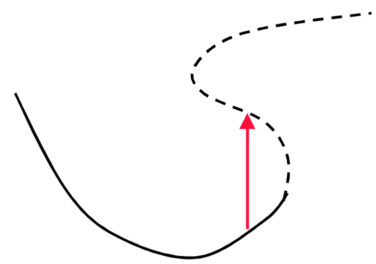
Indirect Bandgap: $(\hbar\omega - E_{\mathrm{th}})^2$

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

Ref: Singh

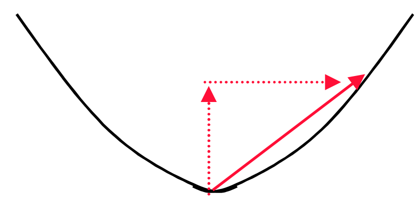
Intraband Transitions in Bulk Se/c

- 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.

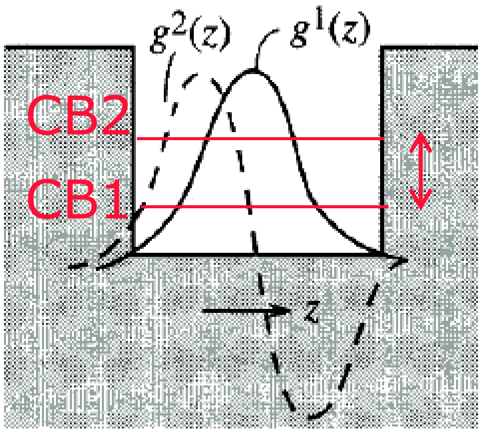
$$\alpha(\hbar\omega) \propto \frac{1}{\omega^2}$$

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

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 for far infrared detectors and forms the basis of **Quantum Cascade Lasers**

$$\psi^1(\boldsymbol{k},z) = \boxed{g^1(z)}\, e^{i\mathbf{k}\cdot\rho}\, \boxed{u^1_{n\mathbf{k}}(\boldsymbol{r})}$$
$$\psi^2(\boldsymbol{k},z) = \boxed{g^2(z)}\, e^{i\mathbf{k}\cdot\rho}\, \boxed{u^2_{n\mathbf{k}}(\boldsymbol{r})}$$

orthogonal

Approximately same for the CB

Ref: Singh

Momentum Matrix Element:

$$\boldsymbol{p}_{\mathrm{if}} = -\frac{i\hbar}{W}\int g^{2*}(z)\, e^{-i\mathbf{k}\cdot\rho}\, \boldsymbol{a}\cdot\nabla g^{1}(z)\, e^{i\mathbf{k}\cdot\rho}\, d^2\rho\, dz$$

If the polarization lies on the QW plane, then due to the orthogonality of the remaining envelope parts (g^1,g^2), p_{if}=0

- Thus for EM wave polarized in the plane of the QW, inter-subband transition rate is zero (This can be relaxed under strong mixing of the cell-periodic parts as in the VB.)

- For EM wave polarized along the QW growth axis (say z), we get

$$\boldsymbol{p}_{\mathrm{if}} = \frac{-i\hbar}{W}\int g^{2*}(z)\,\hat{z}\,\boxed{\frac{\partial}{\partial z}}g^{1}(z)\,dz \quad\Longrightarrow\quad |\boldsymbol{p}_{\mathrm{if}}| \approx \frac{\hbar}{W}$$

Brings g^1 to the same parity with g^2

Ref: Singh