In This Lecture:

- **Interband Transitions in Bulk Se/c**
  - **Momentum Matrix Element**
  - **Polarization dependence**

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)

For parabolic bands:

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

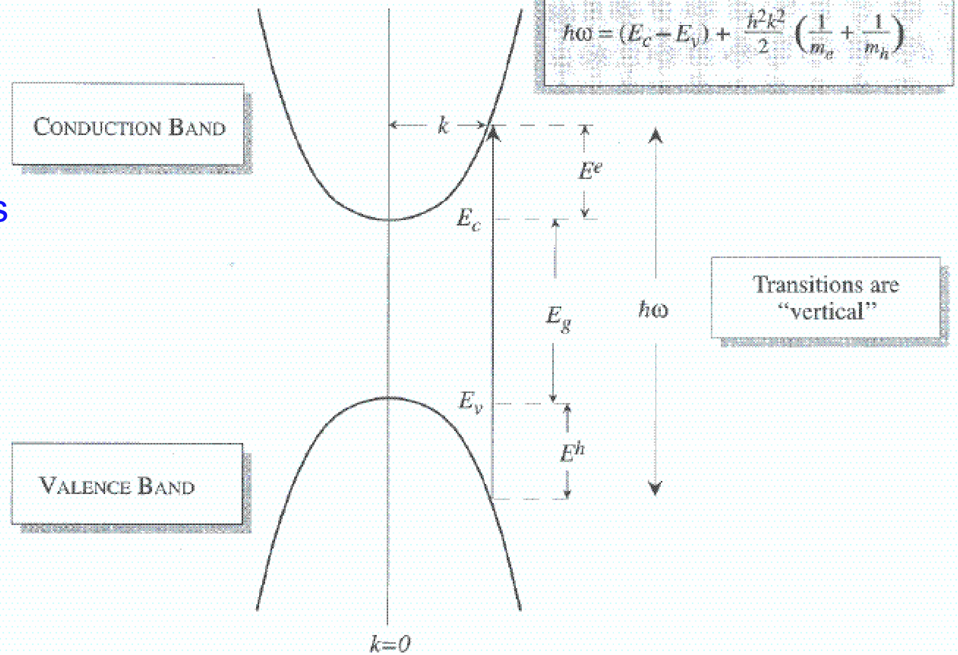


Figure 9.5: The positions of the electron and hole energies at vertical k-values. The electron and hole energies are determined by the photon energy and the carrier masses. Since the photon momentum is negligible the transitions are vertical.

Ref: Singh

Momentum Matrix Elements

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

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

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:

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

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:

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

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

$$\begin{cases} P = \dfrac{\hbar^2\gamma_1}{2m_0}\left(k_x^2 + k_y^2 + k_z^2\right) \\ Q = \dfrac{\hbar^2\gamma_2}{2m_0}\left(k_x^2 + k_y^2 - 2k_z^2\right) \\ R = \dfrac{\hbar^2}{2m_0}\left[-\sqrt{3}\,\gamma_2\left(k_x^2 - k_y^2\right) + i2\sqrt{3}\,\gamma_3 k_x k_y\right] \\ S = \dfrac{\hbar^2\gamma_3}{m_0}\sqrt{3}\,(k_x - ik_y)k_z \end{cases}$$

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: $|iS\downarrow'\rangle$ and $|iS\uparrow'\rangle$

HH:

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

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

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

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

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

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

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

Ref: Chuang

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

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

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

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

Consider, for instance optical transition from the CB of one spin, say $< \mathrm{i}S\uparrow'|$ 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

What about the other 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),

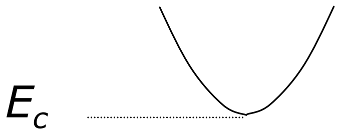
$$\left| \left\langle iS \downarrow' \left| ex \right| \frac{3}{2}, \frac{1}{2} \right\rangle' \right|^2 + \left| \left\langle iS \downarrow' \left| ex \right| \frac{3}{2}, -\frac{1}{2} \right\rangle' \right|^2$$

Joint Density of States (also called reduced DOS)

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

Single Parabolic Band DOS:

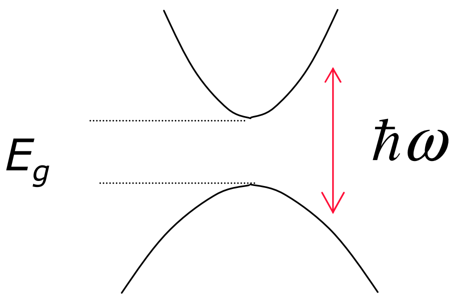
$$N_m(E) = \sum_{\vec{k}\in 1^{\text{st}}\ \text{BZ}} \sum_{\sigma} \delta\left(E - E_m(\vec{k})\right)$$



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

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

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:

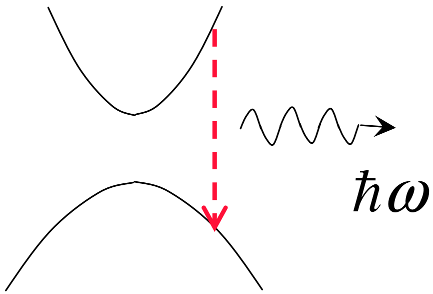
$$W_{abs} = \frac{\pi e^2 \hbar n_{ph}}{m_0^2 \hbar \omega \varepsilon} \left(2M_b^2\right) N_{cv}(\hbar\omega)$$

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



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

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

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

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