# Optical Matrix Element

In bulk semiconductor

$$g(\hbar\omega) = C_0 \cdot |\hat{e}\cdot\vec{P}_{cv}|^2 \cdot \rho_r(\hbar\omega)\cdot [f_c - f_v]$$

$$C_0 = \frac{\pi e^2}{n_r c \epsilon_0 m_0^2 \omega}$$

$$\rho_r(\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{2m_r^*}{\hbar^2}\right)^{3/2}(\hbar\omega - E_g)^{1/2}$$

In quantum wells

$$g(\hbar\omega) = C_0 \sum_{n,m} |I_{hm}^{en}|^2 \, |\hat{e}\cdot\vec{P}_{cv}|^2 \cdot \underbrace{\rho_r^{2D} \cdot H(\hbar\omega - E_{hm}^{en})}_{\text{2D reduced density of states}} \, [f_c - f_v]$$

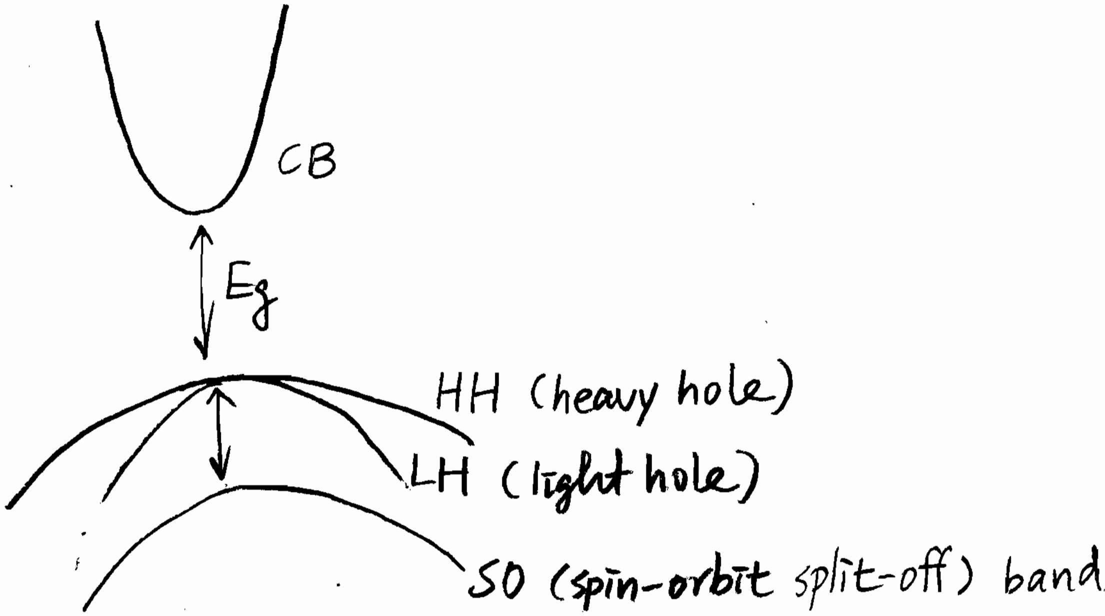
$$\rho_r^{2D} = \frac{m_r^*}{\pi\hbar^2 L_z}$$

Optical matrix element

$|\hat{e}\cdot\vec{P}_{cv}|^2$ – usually isotropic in bulk semiconductor

– polarization-dependent in QW

# Detailed band structure (E-k)




$$\psi_{nk}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \cdot u_{nk}(\vec{r})$$

At band edges ($\vec{k}=0$), $u_{n0}(\vec{r})$ are

CB: conduction band: $|S\uparrow\rangle, |S\downarrow\rangle$

VB: Valance band: $|X\uparrow\rangle, |Y\uparrow\rangle, |Z\uparrow\rangle, |X\downarrow\rangle, |Y\downarrow\rangle, |Z\downarrow\rangle$

$|S\rangle$ : similar to S atomic orbital, symmetric in $x, y, z$

$|X\rangle$ ~ p. atomic orbital

$\begin{cases} \text{odd symmetry in } x. \\ \text{even} \quad " \quad \text{in } y, z. \end{cases}$

Similarly for $|Y\rangle$, $|Z\rangle$

$$\langle S|X\rangle = \langle S|Y\rangle = \langle S|Z\rangle = 0$$

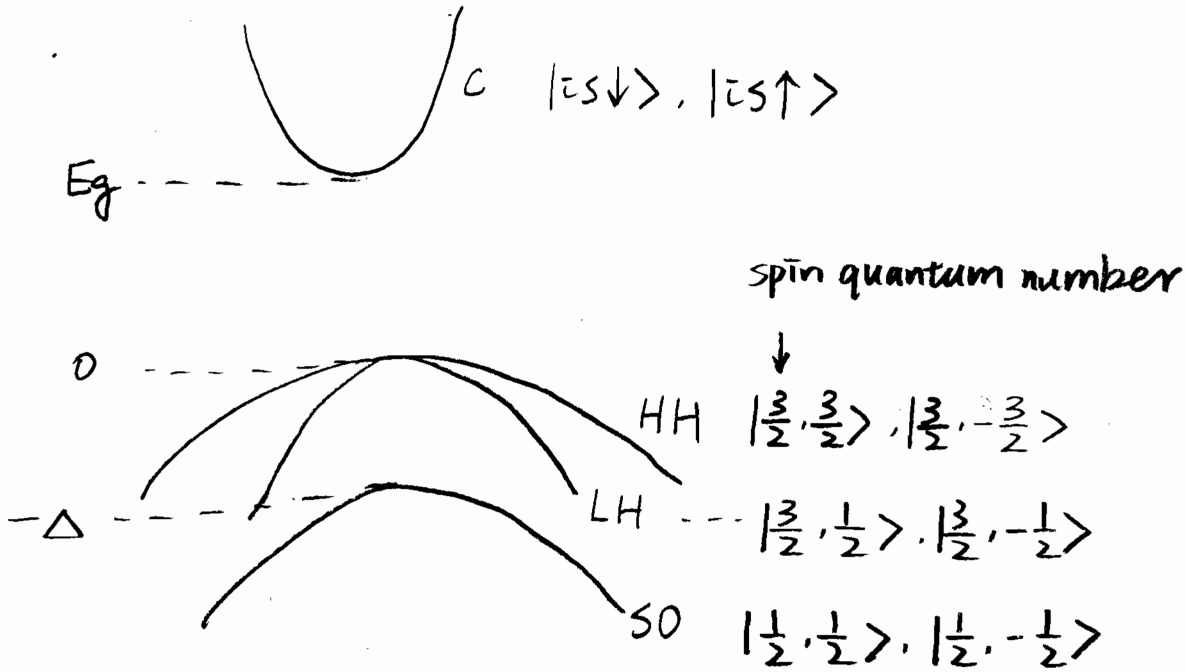
$$\langle S|P_z|X\rangle = \langle S|P_z|Y\rangle = 0$$

$$\langle S|P_z|Z\rangle \neq 0$$

Kane's P parameter (p. 132 in Chuang)

$$P = -i\frac{\hbar}{m_0}\langle S|p_z|Z\rangle$$

Using a second-order pertubation technique known as $\vec{k}\cdot\vec{p}$ method, we can find eigenvalues (energies) and eigenfunctions around $\vec{k}=0$




CB: $$E_c(k) = E_g + \frac{\hbar^2 k^2}{2m_0} + \frac{k^2P^2}{3}\cdot\frac{3E_g+2\Delta}{E_g(E_g+\Delta)} \equiv E_g + \frac{\hbar^2k^2}{2m_e^*}$$

$|iS\downarrow\rangle$

$|iS\uparrow\rangle$

VB: Heavy Holes (HH)

$$E_{hh}(k) = \frac{\hbar^2k^2}{2m_0}$$ (incorrect in this approximation)

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

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

Light Holes (LH)

$$E_{lh} = \frac{\hbar^2 k^2}{2m_0} - \frac{2k^2 P^2}{3E_g} \equiv -\frac{\hbar^2 k^2}{2m_{lh}^*}$$

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

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

Spin-orbit split-off band (SO)

$$E_{SO} = -\Delta + \frac{\hbar^2 k^2}{2m_0} - \frac{k^2 P^2}{3(E_g + \Delta)} \equiv -\Delta - \frac{\hbar^2 k^2}{2m_{SO}^*}$$

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

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

Kane's P parameter is related to $m_e^*$

$$\frac{\hbar^2 k^2}{2m_0} + \frac{k^2 P^2}{3} \cdot \frac{(3E_g + 2\Delta)}{E_g(E_g + \Delta)} = \frac{\hbar^2 k^2}{2m_e^*}$$

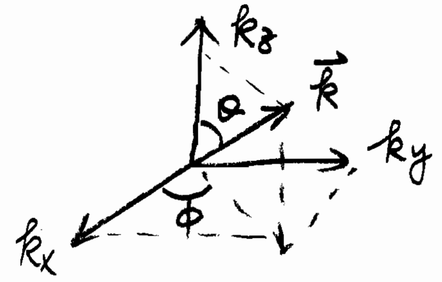
$$\Rightarrow P^2 = \underbrace{\left(1 - \frac{m_e^*}{m_0}\right)}_{\approx 1} \frac{\hbar^2 E_g (E_g + \Delta)}{2m_e^* \left(E_g + \frac{2}{3}\Delta\right)}$$

$$P = -i\frac{\hbar}{m_0}\langle S|p_z|Z\rangle = \frac{\hbar}{m_0}\langle iS|p_z|Z\rangle = \frac{\hbar}{m_0} P_X$$

$$P_X = \langle iS|p_x|X\rangle = \langle iS|p_y|Y\rangle = \langle iS|p_z|Z\rangle$$

Previous derivation. $\vec{k} = k\cdot\hat{z}$ : electron wavevector

Generally




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

$u_c$ and $u_v$ are modified also:

$$\left|\tfrac{3}{2},\tfrac{3}{2}\right\rangle' = \frac{-1}{\sqrt{2}}\left|(X'+iY')\uparrow'\right\rangle \qquad \text{(p.137)}$$

$$= \frac{-1}{\sqrt{2}}\Big|(\cos\theta\cos\phi - i\sin\phi)X + (\cos\theta\sin\phi + i\cos\phi)Y - \sin\theta\, Z\Big\rangle\left|\uparrow'\right\rangle$$

$$\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle' = \frac{1}{\sqrt{2}}\Big|(\cos\theta\cos\phi + i\sin\phi)X + (\cos\theta\sin\phi - i\cos\phi)Y - \sin\theta\, Z\Big\rangle\left|\downarrow'\right\rangle$$

$$\langle iS\uparrow'|\vec{p}\,|\tfrac{3}{2},\tfrac{3}{2}\rangle' = \frac{-1}{\sqrt{2}}\Big[\underset{\shortparallel}{\underbrace{\langle iS|P_x|X\rangle}}\cdot(\cos\theta\cos\phi - i\sin\phi)\cdot\hat{x} + \underset{\shortparallel}{\langle iS|P_y|Y\rangle}(\cos\theta\sin\phi + i\cos\phi)\cdot\hat{y} + \underset{\underset{P_x}{\shortparallel}}{\langle iS|P_z|Z\rangle}\cdot(-\sin\theta)\,\hat{z}\Big]$$

$$= \frac{-P_x}{\sqrt{2}}\Big[(\cos\theta\cos\phi - i\sin\phi)\hat{x} + (\cos\theta\sin\phi + i\cos\phi)\hat{y} + (-\sin\theta)\hat{z}\Big]$$

$$\langle iS\uparrow' | \vec{P} | \tfrac{3}{2}, -\tfrac{3}{2} \rangle' = 0 \qquad \because \langle \uparrow' | \downarrow' \rangle = 0$$

$$\langle iS\downarrow' | \vec{P} | \tfrac{3}{2}, \tfrac{3}{2} \rangle' = 0$$

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

## Optical Matrix Element

$$\vec{M} = \langle u_c | \vec{P} | u_v \rangle = \vec{P}_{cv}$$

$$= \hat{x} \langle u_c | \underset{\substack{\| \\ \frac{\hbar}{i}\frac{\partial}{\partial x}}}{P_x} | u_v \rangle + \hat{y} \langle u_c | P_y | u_v \rangle + \hat{z} \langle u_c | P_z | u_v \rangle$$

$u_c = |iS\uparrow'\rangle$ or $|iS\downarrow'\rangle$

$u_v = u_{hh}$ or $u_{lh}$

$u_{hh} = |\tfrac{3}{2}, \tfrac{3}{2}\rangle'$ or $|\tfrac{3}{2}, -\tfrac{3}{2}\rangle'$

$u_{lh} = |\tfrac{3}{2}, \tfrac{1}{2}\rangle'$ or $|\tfrac{3}{2}, -\tfrac{1}{2}\rangle'$

$\hat{e} \cdot \vec{M}$

$\hat{e}$: Polarization of optical wave

$$\begin{cases} \hat{e} = \hat{x} \text{ or } \hat{y} & \text{for TE polarization} \\ \hat{e} = \hat{z} & \text{for TM} \end{cases}$$

For bulk semiconductor, C$-$HH, consider $\begin{cases} |u_c\rangle = |iS\uparrow'\rangle \\ \hat{e} = \hat{x} \end{cases}$

$$|\hat{e}\cdot\vec{P}_{cv}|^2 = |\langle iS\uparrow'|P_x|\tfrac{3}{2},\tfrac{3}{2}\rangle'|^2$$

$$= \frac{P_x^2}{2}\cdot\langle \cos^2\theta\cos^2\phi + \sin^2\theta\rangle$$

Integrate over $4\pi$ solid angle

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

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

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

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

roughly $\propto \dfrac{E_g}{m_e^*}$

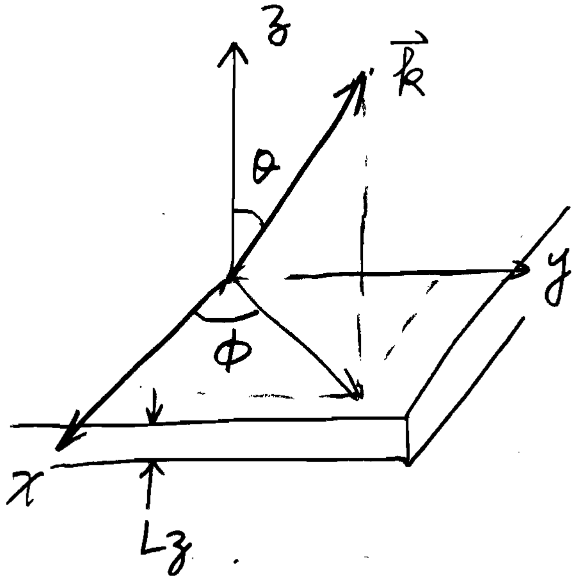
Similarly $|\hat{y}\cdot\vec{P}_{cv}| = M_b^2$

$|\hat{z}\cdot\vec{P}_{cv}| = M_b^2$

C$-$LH has the same matrix element!

$\Rightarrow$ Bulk semiconductor is polarization independent

# Matrix Element for QW




The optical matrix elements have similar expressions, but are averaged only over $\phi$, i.e. the in-plane components of $\vec{k}$

For TE, $\hat{e} = \hat{x}$, C–HH transition, consider $\langle u_c| = \langle iS\uparrow'|$

$$|\hat{e}\cdot\vec{P}_{cv}|^2 = \langle |\hat{x}\cdot\vec{M}_{c-hh}|^2\rangle$$

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

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

TE, $\hat{e} = \hat{x}$ C–LH, consider $\langle u_c| = \langle iS\downarrow'|$

$$|\hat{e}\cdot\vec{P}_{cv}|^2 = \langle |\hat{x}\cdot\vec{M}_{c-lh}|^2\rangle$$

$$= \frac{1}{2\pi}\int_0^{2\pi} d\phi\,\left(|\langle iS\downarrow'|P_x|\tfrac{3}{2},\tfrac{1}{2}\rangle'|^2 + \langle iS\downarrow'|P_x|\tfrac{3}{2},-\tfrac{1}{2}\rangle|^2\right)$$

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

Sum Rule:

$$\langle|\hat{x}\cdot\vec{M}_{c-hh}|^2\rangle + \langle|\hat{x}\cdot\vec{M}_{c-lh}|^2\rangle = 2M_b^2 \quad \text{(same as bulk)}$$

Summary of optical matrix element (Table 9.1)
(Based on Parabolic Band model)

* Bulk semiconductor: Isotropic

$$|\hat{x}\cdot\vec{P}_{cv}|^2 = |\hat{y}\cdot\vec{P}_{cv}|^2 = |\hat{z}\cdot\vec{P}_{cv}|^2 = M_b^2 = \frac{m_0}{6}E_P$$

( $E_p$ Tabulated in Table K.2 (p. 709)
$E_p = 25.7$ eV for GaAs
20.7 eV " InP
22.2 eV " InAs )

* QW

| | TE ($\hat{e}=\hat{x}$ or $\hat{y}$) | TM ($\hat{e}=\hat{z}$) | $\langle\lvert\hat{x}\cdot\vec{M}\rvert^2\rangle+\langle\lvert\hat{y}\cdot\vec{M}\rvert^2\rangle+\langle\lvert\hat{z}\cdot\vec{M}\rvert^2\rangle$ All Polarizations |
|---|---|---|---|
| HH: $\langle\lvert\hat{e}\cdot\vec{M}_{c-hh}\rvert^2\rangle$ | $(\frac{3}{4}+\frac{3}{4}\cos^2\theta)M_b^2$ | $(\frac{3}{2}\sin^2\theta)\cdot M_b^2$ | $3M_b^2$ |
| LH: $\langle\lvert\hat{e}\cdot\vec{M}_{c-lh}\rvert^2\rangle$ | $(\frac{5}{4}-\frac{3}{4}\cos^2\theta)M_b^2$ | $(\frac{1}{2}+\frac{3}{2}\cos^2\theta)M_b^2$ | $3M_b^2$ |
| Sum Rule HH+LH | $2M_b^2$ | $2M_b^2$ | |

* Angular Factor

$$\cos^2\theta = \frac{k_z^2}{k_z^2+k_x^2+k_y^2} = \frac{\frac{\hbar^2k_z^2}{2m_e^*}}{\frac{\hbar^2}{2m_e^*}(k_z^2+k_x^2+k_y^2)} = \frac{E_{en}}{E_{en}+\frac{\hbar^2}{2m_e^*}k_t^2}$$

$k_t^2 = k_x^2 + k_y^2$
can be estimated from $\hbar\omega - E_g - E_{en} - |E_{hm}|$