EE 232: Lightwave Devices
Lecture #8 – Optical transition matrix element

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Optical transition matrix element

Optical transition matrix element

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

Bloch states

$$\psi_c = u_c(\mathbf{r}) \frac{e^{i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{V}} \qquad \psi_v = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{V}}$$

periodic with lattice

envelope function

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

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

Optical transition matrix element

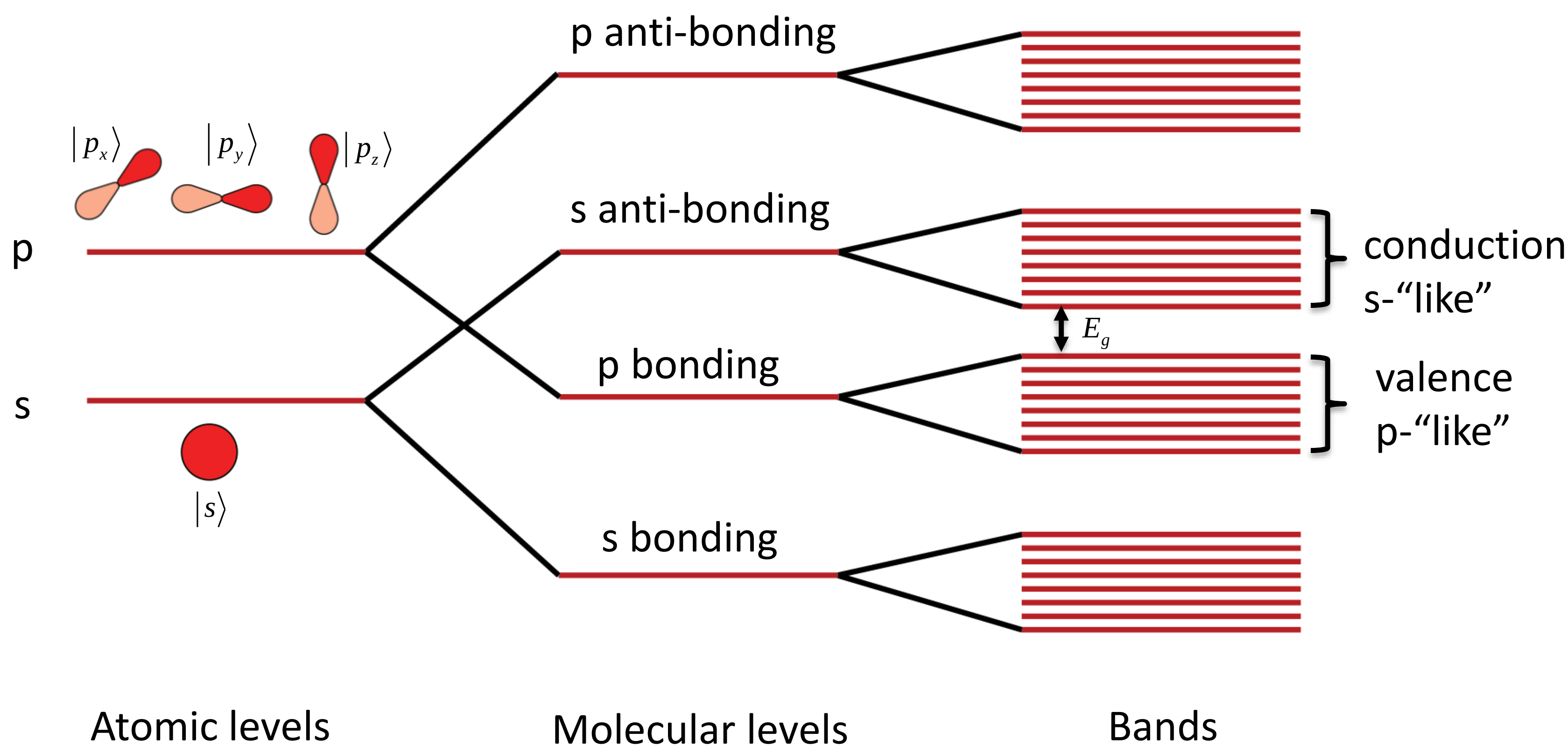
$$\hat{H}_{cv} = \frac{-qA_0}{2m_0}\int u_c^*(\mathbf{r})\frac{e^{-i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{V}}e^{i\mathbf{k}_{op}\cdot\mathbf{r}}\hat{e}\cdot\mathbf{p}u_v(\mathbf{r})\frac{e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{V}}d^3\mathbf{r}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\int u_c^*(\mathbf{r})e^{-i\mathbf{k}_c\cdot\mathbf{r}}e^{i\mathbf{k}_{op}\cdot\mathbf{r}}[-i\hbar\nabla]u_v(\mathbf{r})e^{i\mathbf{k}_v\cdot\mathbf{r}}\frac{d^3\mathbf{r}}{V}$$

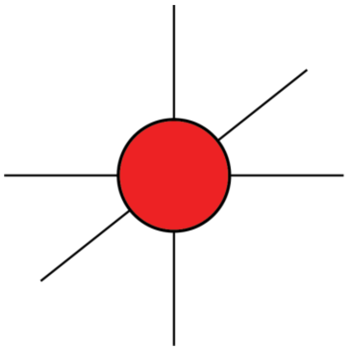
$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\int u_c^*(\mathbf{r})e^{-i\mathbf{k}_c\cdot\mathbf{r}}e^{i\mathbf{k}_{op}\cdot\mathbf{r}}\left[-i\hbar\nabla u_v(\mathbf{r})e^{i\mathbf{k}_v\cdot\mathbf{r}} - \hbar k_v u_v(\mathbf{r})e^{i\mathbf{k}_v\cdot\mathbf{r}}\right]\frac{d^3\mathbf{r}}{V}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\int e^{i(-\mathbf{k}_c+\mathbf{k}_v+\mathbf{k}_{op})\cdot\mathbf{r}}\left[u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r}) - \hbar k_v u_v(\mathbf{r})u_c^*(\mathbf{r})\right]\frac{d^3\mathbf{r}}{V}$$

Bloch functions u_c and u_v

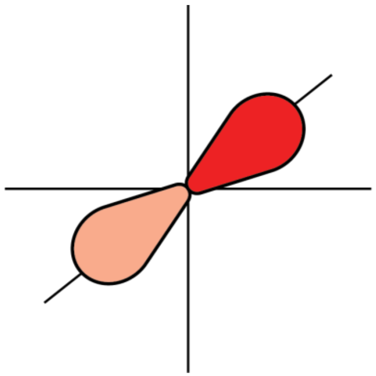


Bloch functions u_c and u_v

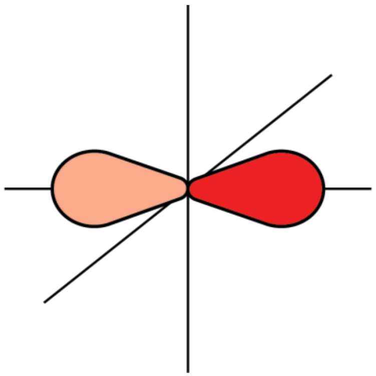


$|s\rangle$

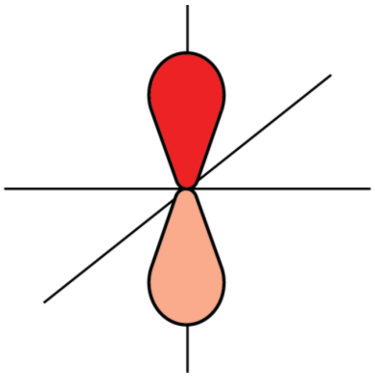
Conduction band $u_c \sim |s\rangle$



$|p_x\rangle$



$|p_y\rangle$



$|p_z\rangle$

Valence band $u_v \sim \alpha|p_x\rangle + \beta|p_y\rangle + \gamma|p_z\rangle$

Optical transition matrix element

$$u_c \sim |s\rangle \quad u_v \sim \alpha|p_x\rangle + \beta|p_y\rangle + \gamma|p_z\rangle$$

$$\langle s|p_x\rangle = \langle s|p_y\rangle = \langle s|p_z\rangle = 0$$

$$\rightarrow \langle u_c|u_v\rangle = 0$$

$$\hat{H}_{cv} = \frac{-qA_0}{2m_0}\hat{e}\cdot\int e^{i(-\mathbf{k}_c+\mathbf{k}_v+\mathbf{k}_{op})\cdot\mathbf{r}}\left[u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r}) - \underbrace{\cancel{\hbar k_v u_v(\mathbf{r})u_c^*(\mathbf{r})}}_{0}\right]\frac{d^3\mathbf{r}}{V}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\int e^{i(-\mathbf{k}_c+\mathbf{k}_v+\mathbf{k}_{op})\cdot\mathbf{r}}\left[u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})\right]\frac{d^3\mathbf{r}}{V}$$

$$= \frac{-qA_0}{2m_0}\hat{e}\cdot\int F(\mathbf{r})\underbrace{\left[u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})\right]}\frac{d^3\mathbf{r}}{V}$$

Envelope function
Varies slowly
over unit cell of the crystal

Varies rapidly
over unit cell of the crystal

Optical transition matrix element

$$\int F(\mathbf{r})\left[u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})\right]d^3\mathbf{r}$$

$$u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r}) = \sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot\mathbf{r}}$$

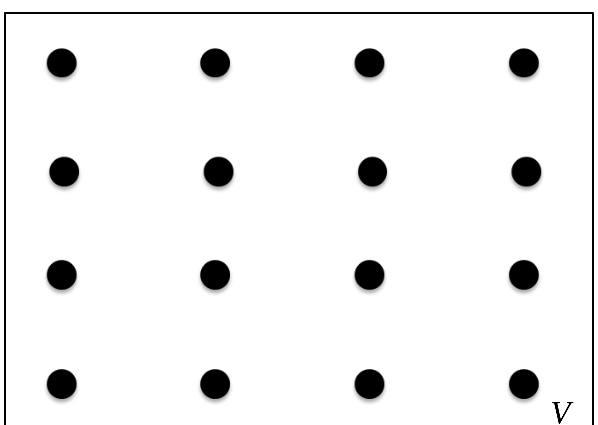
$u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})$ is periodic and can be represented by a Fourier series where $\boldsymbol{G}$ are the reciprocal lattice vectors

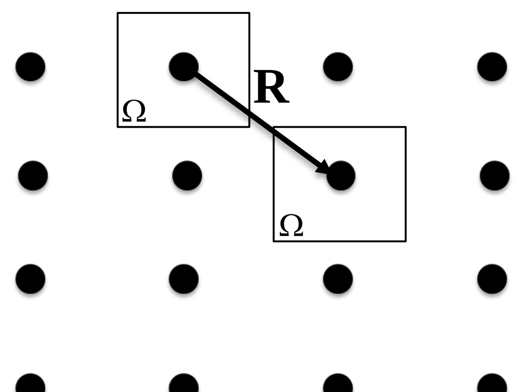
$$= \int F(\mathbf{r})\sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot\mathbf{r}} d^3\mathbf{r}$$

$$= \sum_{\mathbf{R}}\int_{\Omega} F(\mathbf{r}+\mathbf{R})\sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})} d^3\mathbf{r}$$

$$\simeq \sum_{\mathbf{R}} F(\mathbf{R})\int_{\Omega}\sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})} d^3\mathbf{r}$$

$$\int_V d^3\mathbf{r}$$





$$\sum_{\mathbf{R}}\int_{\Omega} d^3\mathbf{r}$$

Optical transition matrix element

$$\int F(\mathbf{r})\left[u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})\right]d^3\mathbf{r} = \sum_{\mathbf{R}} F(\mathbf{R})\int_{\Omega}\sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot\mathbf{r}} d^3\mathbf{r}$$

Note: $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$

$$= \int_V F(\mathbf{r})\frac{d^3\mathbf{r}}{\Omega}\int_{\Omega}\sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot\mathbf{r}} d^3\mathbf{r}$$

$$= \int_V F(\mathbf{r})d^3\mathbf{r}\int_{\Omega}\sum_{\mathbf{G}} C_G e^{i\mathbf{G}\cdot\mathbf{r}} \frac{d^3\mathbf{r}}{\Omega}$$

$$= \int_V F(\mathbf{r})d^3\mathbf{r}\int_{\Omega} u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})\frac{d^3\mathbf{r}}{\Omega}$$

Plug back into optical matrix element

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

Non-zero only if $\mathbf{k}_c = \mathbf{k}_{op} + \mathbf{k}_v \rightarrow \mathbf{k}_c \sim \mathbf{k}_v$

Optical transition matrix element

$$\hat{H}_{cv} = \frac{-qA_0}{2m_0}\hat{e}\cdot\int_{\Omega} u_c^*(\mathbf{r})(-i\hbar\nabla)u_v(\mathbf{r})\frac{d^3\mathbf{r}}{\Omega}\delta_{\mathbf{k}_c,\mathbf{k}_v} = \frac{-qA_0}{2m_0}\hat{e}\cdot\mathbf{p}_{cv}\delta_{\mathbf{k}_c,\mathbf{k}_v}$$

$$\longrightarrow \boxed{\left|\hat{H}_{cv}\right|^2 = \left(\frac{qA_0}{2m_0}\right)^2\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2\delta_{\mathbf{k}_c,\mathbf{k}_v}}$$

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

u_c and u_v are bloch functions

$\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2$ can be evaluated using the $\mathbf{k}\cdot\mathbf{p}$ method where it is shown that

$$\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2 = \boxed{M_b^2 = \left(\frac{m_0}{m_e^*}-1\right)\frac{m_0E_g(E_g+\Delta)}{6\left(E_g+\frac{2}{3}\Delta\right)}}$$

Δ is the spin-orbit split-off band separation

It is also common to see M_b^2 written as

$$\boxed{M_b^2 = \frac{m_0}{6}E_p}$$

where E_p can be experimentally measured

GaAs: E_p= 25.7 eV

InP: E_p= 20.7 eV

Absorption coefficient

$$\boxed{\alpha(\hbar\omega) = C_0 M_b^2 \rho_r (f_v - f_c)}$$

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

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

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

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

$$M_b^2 = \frac{m_0}{6} E_p$$

Simplified two-band $k \cdot p$ theory

$$\left[-\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r})\right]\psi_{nk}(\mathbf{r}) = E_n(\mathbf{k})\psi_{nk}(\mathbf{r})$$

General solution: $\psi_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$

n : band

Plug general solution in Schrodinger's eqn:

$$\left[-\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r}) + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}\right]u_{nk}(\mathbf{r}) = \left(E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m_0}\right)u_{nk}(\mathbf{r})$$

$$\left[\hat{H}_0 + \hat{H}'\right]u_{nk}(\mathbf{r}) = \left(E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m_0}\right)u_{nk}(\mathbf{r})$$

where: $\hat{H}' = \dfrac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}$

$$\hat{H}_0 u_{n0}(\mathbf{r}) = E_0(0)u_{n0}(\mathbf{r})$$

See Chuang Ch.4
Haug and Koch Ch. 3

Simplified two-band $k \cdot p$ theory

Second order time-independent perturbation theory:

$$E_n(\mathbf{k}) = E_n(0) + \hat{H}'_{nn} + \frac{\hbar^2 k^2}{2m_0} + \sum_{m\neq n} \frac{\hat{H}'_{nm}\hat{H}'_{mn}}{E_n(0) - E_m(0)}$$

$$= E_n(0) + \frac{\hbar}{m_0}\cancelto{0}{\mathbf{k}\cdot\mathbf{p}_{nn}} + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar^2}{2m_0}\sum_{m\neq n} \frac{2\left(\mathbf{k}\cdot\langle n|\mathbf{p}|m\rangle\right)\left(\mathbf{k}\cdot\langle m|\mathbf{p}|n\rangle\right)}{E_n(0) - E_m(0)}$$

Consider two states: $E_e(0) = E_g$ (bottom of conduction band)

$E_h(0) = 0$ (top of valence band)

$$E_e(\mathbf{k}) = E_e(0) + \frac{\hbar^2 k^2}{2}\left(1 + \frac{2|\mathbf{p}_{cv}|^2}{m_0 E_g}\right) m_0^{-1} = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

$$E_h(\mathbf{k}) = E_h(0) + \frac{\hbar^2 k^2}{2}\left(1 - \frac{2|\mathbf{p}_{cv}|^2}{m_0 E_g}\right) m_0^{-1} = \frac{\hbar^2 k^2}{2(-m_h^*)}$$

Assuming cubic symmetry
(Lots of math details skipped)

Simplified two-band $k \cdot p$ theory

$$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*} = m_0^{-1}\left(1 + \frac{2\left|\mathbf{p}_{cv}\right|^2}{m_0 E_g}\right) + m_0^{-1}\left(\frac{2\left|\mathbf{p}_{cv}\right|^2}{m_0 E_g} - 1\right)$$

$$\frac{1}{m_r^*} = \frac{4\left|\mathbf{p}_{cv}\right|^2}{m_0^2 E_g} \rightarrow \boxed{\left|\hat{e}\cdot\mathbf{p}_{cv}\right|^2 = M_b^2 = \frac{m_0^2 E_g}{12 m_r^*}}$$

Reduced mass and bandgap can be measured
from absorption coefficient. This allows for empirical determination
of the transition matrix element.

More rigorous treatment includes multiple valence bands (hh,lh, and so) and degeneracy at k = 0 (result given without proof on slide 9).
But, this simple approximation derived here gives surprisingly reasonable estimate (within about a factor of 2) of the true matrix element.