EE 232: Lightwave Devices
Lecture #7 – Absorption in bulk semiconductors

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Vector potential form of Hamiltonian

$$\hat{H} = \frac{1}{2m_0}(\mathbf{p} - q\mathbf{A})^2 + V(\mathbf{r})$$

↑ light

$$\nabla \cdot \mathbf{B} = 0$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} = -\frac{\partial \mathbf{A}}{\partial t} \quad \text{for } \rho = 0$$

$$\nabla \cdot \mathbf{A} = 0 \quad \text{(Coulomb gauge)}$$

We won't show it here but this
Hamiltonian can be derived from the Lorentz force equation:

$$\frac{d}{dt}\mathbf{p} = \mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

Expanding the momentum term

$$(\mathbf{p} - q\mathbf{A})^2 = (-i\hbar\nabla - q\mathbf{A})^2$$

$$= q\frac{i\hbar}{2m_0}\left[\mathbf{A}\cdot\nabla + \nabla\cdot\mathbf{A}\right] - \frac{\hbar^2}{2m_0}\nabla^2 + \frac{q^2}{2m_0}A^2 + V(\mathbf{r})$$

$$= -\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r}) - \frac{q}{m_0}\mathbf{A}\cdot\mathbf{p} + \frac{q^2}{2m_0}A^2$$

Vector potential form of Hamiltonian

$$(\mathbf{p}-q\mathbf{A})^2 = -\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r}) - \frac{q}{m_0}\mathbf{A}\cdot\mathbf{p} + \frac{q^2}{2m_0}A^2$$

$$\cong -\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r}) - \frac{q}{m_0}\mathbf{A}\cdot\mathbf{p}$$ for small amplitudes of $\mathbf{A}$

$$= \hat{H}_0 + \hat{H}'(\mathbf{r},t) \quad \text{where} \quad \boxed{\hat{H}'(\mathbf{r},t) = -\frac{q}{m_0}\mathbf{A}\cdot\mathbf{p}}$$

$$\mathbf{A} = \hat{e}A_0\cos(\mathbf{k}_{op}\cdot\mathbf{r}-\omega t)$$

$$\mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t} = -\hat{e}\omega A_0\sin(\mathbf{k}_{op}\cdot\mathbf{r}-\omega t)$$

$$\text{Intensity} = \text{Energy density} \times \text{group velocity}$$

$$= \left(\frac{1}{2}\epsilon_0 n^2|\mathbf{E}|^2\right)\left(\frac{c}{n}\right)$$

$$= \frac{1}{2}\epsilon_0 n^2(\omega A_0)^2\frac{c}{n}$$

$$\boxed{= \frac{1}{2}nc\epsilon_0\omega^2A_0^2}$$

Transition matrix element

$$\hat{H}'(\mathbf{r},t) = -\frac{q}{m_0}\mathbf{A}\cdot\mathbf{p}$$

$$= -\frac{qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0}\hat{e}\cdot\mathbf{p}\left(e^{i\omega t} + e^{-i\omega t}\right)$$

$$= H'(\mathbf{r})\left(e^{i\omega t} + e^{-i\omega t}\right)$$

$$w_{fi} = \frac{2\pi}{\hbar^2}\left|\hat{H}_{fi}\right|^2 \delta(\omega_{fi} - \omega) = \frac{2\pi}{\hbar^2}\left|\left\langle \psi_f \middle| \hat{H}'(\mathbf{r}) \middle| \psi_i \right\rangle\right|^2 \delta(\omega_{fi} - \omega)$$

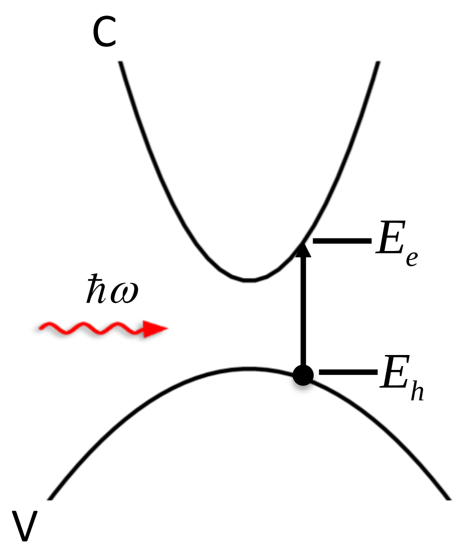
$$= \frac{2\pi}{\hbar^2}\left|\left\langle \psi_f \middle| \frac{-qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0}\hat{e}\cdot\mathbf{p} \middle| \psi_i \right\rangle\right|^2 \delta(\omega_{fi} - \omega)$$

$$\boxed{\left|\hat{H}_{fi}\right|^2 = \left|\left\langle \psi_f \middle| \frac{-qA_0 e^{i\mathbf{k}_{op}\cdot\mathbf{r}}}{2m_0}\hat{e}\cdot\mathbf{p} \middle| \psi_i \right\rangle\right|^2}$$

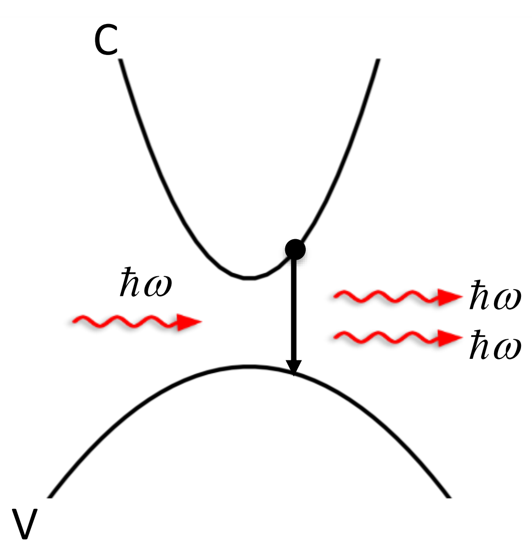
Absorption coefficient

Consider transition rate for between valence and conduction bands

$$w_{abs} = \frac{2\pi}{\hbar^2}\left|\hat{H}_{fi}\right|^2 \delta(\omega_{fi} - \omega)$$
$$= \frac{2\pi}{\hbar}\left|\hat{H}_{cv}\right|^2 \delta(E_e - E_h - \hbar\omega)$$



$$w_{ems} = \frac{2\pi}{\hbar^2}\left|\hat{H}_{if}\right|^2 \delta(\omega_{if} - \omega)$$
$$= \frac{2\pi}{\hbar}\left|\hat{H}_{cv}\right|^2 \delta(E_e - E_h - \hbar\omega)$$



Absorption coefficient

Now, for a semiconductor we have a continuum of final and initial states. Upward transition rate considering the probability that the valence band state is filled and the conduction band state is empty is given by

$$R_{v\to c} = \frac{2}{V}\sum_{k_v}\sum_{k_c}\frac{2\pi}{\hbar}\left|\hat{H}_{cv}\right|^2 \delta(E_e - E_h - \hbar\omega) f_v(1 - f_c) \quad \left(\mathrm{s^{-1}cm^{-3}}\right)$$

Similarly, the downward transition rate,

$$R_{c\to v} = \frac{2}{V}\sum_{k_v}\sum_{k_c}\frac{2\pi}{\hbar}\left|\hat{H}_{cv}\right|^2 \delta(E_e - E_h - \hbar\omega) f_c(1 - f_v) \quad \left(\mathrm{s^{-1}cm^{-3}}\right)$$

The total net upward rate is then,

$$R = R_{v\to c} - R_{c\to v} = \frac{2}{V}\sum_{k_v}\sum_{k_c}\frac{2\pi}{\hbar}\left|\hat{H}_{cv}\right|^2 \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right) \quad \left(\mathrm{s^{-1}cm^{-3}}\right)$$

Spin degeneracy

Absorption coefficient

$$\text{Absorption coefficient } (\alpha) = \frac{\text{\# photons absorbed per second per unit volume}}{\text{\# injected photons per second per unit area}}$$

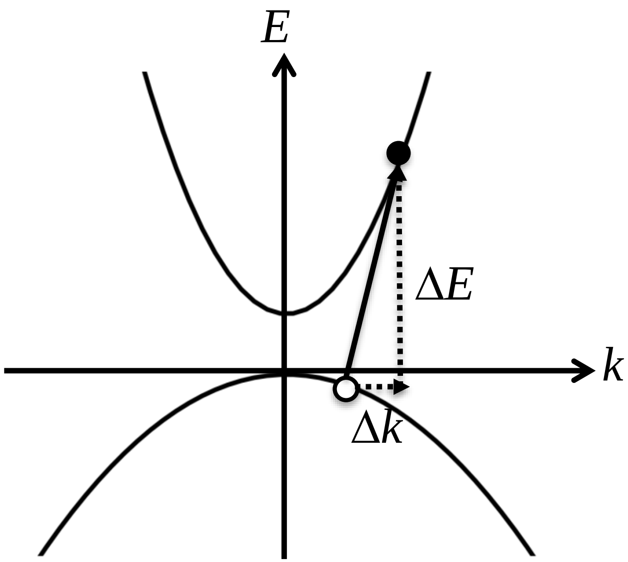
$$\alpha = \frac{R}{I/\hbar\omega} = \frac{\hbar\omega}{nc\epsilon_0\omega^2 A_0^2/2} R$$

$$= \frac{\hbar\omega}{nc\epsilon_0\omega^2 A_0^2/2} \frac{2}{V} \sum_{k_v}\sum_{k_c} \frac{2\pi}{\hbar} \left|\hat{H}_{cv}\right|^2 \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right)$$

$$= \frac{\pi q^2}{nc\epsilon_0\omega m_0^2} \frac{2}{V} \sum_{k_v}\sum_{k_c} |\hat{e}\cdot\mathbf{p}_{cv}|^2 \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right)$$

$$\boxed{\alpha = C_0 \frac{2}{V} \sum_{k_v}\sum_{k_c} |\hat{e}\cdot\mathbf{p}_{cv}|^2 \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right)}$$

Momentum conservation



- **Energy conservation:**

$$E_e - E_h = \hbar\omega$$

- **Momentum conservation:**

$$k_e - k_h = k_p$$

k_e: electron momentum

k_h: hole momentum

k_p: photon momentum

$$k_e, k_h \approx \frac{\pi}{a}$$ a: lattice constant

$$k_p = \frac{2\pi}{\lambda}$$

$$\lambda \gg a \rightarrow \boxed{\Delta k \approx 0}$$

Optical transitions
are vertical transitions in k-space

Reduced density of states

$$2\sum_{k_v}\sum_{k_c} \rightarrow 2\sum_{k} \rightarrow \int \frac{2d^3k}{(2\pi)^3} = \int \frac{2(4\pi k^2)d^3k}{(2\pi)^3} = \int \frac{1}{2\pi^2}\left(\frac{2m_r^*}{\hbar^2}\right)^{3/2} E^{\frac{1}{2}}dE = \int \rho_r(E)dE$$

(k-selection rule)

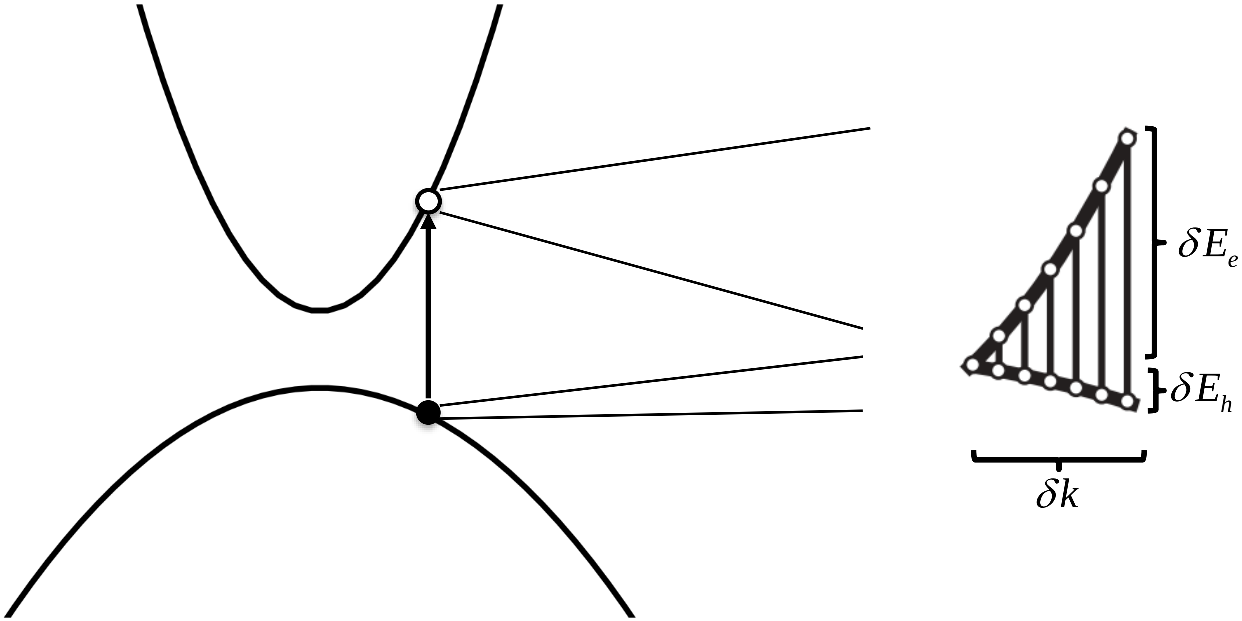
$$E_e = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

$$E_h = -\frac{\hbar^2 k^2}{2m_h^*}$$

$$E_e - E_h = E_g + \frac{\hbar^2 k^2}{2m_r^*} \quad \text{where } \frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

$$\text{Let } E = \frac{h^2 k^2}{2m_r^*}$$

Reduced density of states



$$\delta E = \delta E_e + \delta E_h$$

$$\delta N = \rho_r \delta E = \rho_c \delta E_e = \rho_v \delta E_h$$

$\delta N =$ differential # states available for transition in δE

$$\rho_r (\delta E_e + \delta E_h) = \rho_c \delta E_e$$

$$\rho_r \left(\delta E_e + \frac{\rho_c}{\rho_v} \delta E_e \right) = \rho_c \delta E_e$$

$$\boxed{\frac{1}{\rho_r} = \frac{1}{\rho_c} + \frac{1}{\rho_v}}$$

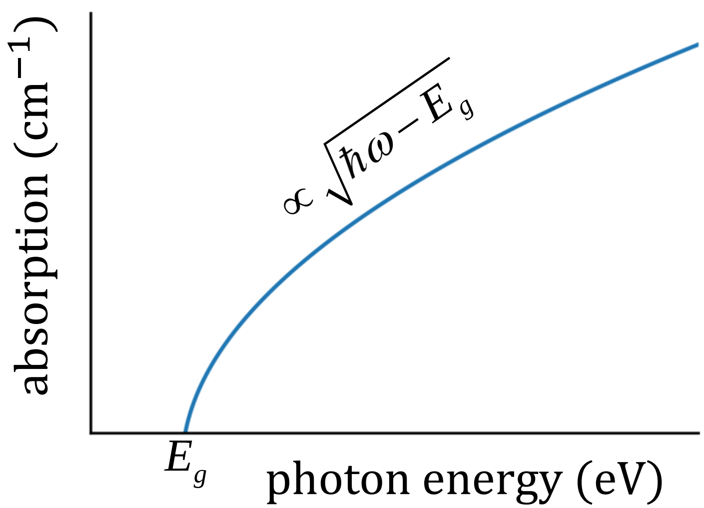
Absorption coefficient

$$\alpha = C_0 \frac{2}{V} \sum_{k_v} \sum_{k_c} |\hat{e} \cdot \mathbf{p}_{cv}|^2 \; \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right)$$

$$= C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \int \rho_r(E) \delta(E_e - E_h - \hbar\omega)\left(f_v - f_c\right) dE$$

$$= C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \int \rho_r(E) \delta(E + E_g - \hbar\omega)\left(f_v - f_c\right) dE$$

$$\boxed{\alpha(\hbar\omega) = C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \; \rho_r(\hbar\omega - E_g)(f_v - f_c)}$$



Fermi factor

$$f_c(E_e) = \frac{1}{1+\exp[(E_e - F_c)/kT]} \qquad f_v(E_h) = \frac{1}{1+\exp[(E_h - F_v)/kT]}$$

We need a change of variables from $E_e, E_h \rightarrow E = \frac{\hbar^2 k^2}{2m_r^*}$

$$E = \hbar\omega - E_g = \frac{\hbar^2 k^2}{2m_r^*} \rightarrow k = \sqrt{\frac{2m_r^*}{\hbar^2}(\hbar\omega - E_g)}$$

$$E_e = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

$$= E_g + (\hbar\omega - E_g)\left(\frac{m_r^*}{m_e^*}\right)$$

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

$$E_h = -\frac{\hbar^2 k^2}{2m_h^*}$$

$$= -(\hbar\omega - E_g)\left(\frac{m_r^*}{m_h^*}\right)$$

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

Summary

$$\boxed{\alpha(\hbar\omega) = C_0\, |\hat{e}\cdot\mathbf{p}_{cv}|^2\, \rho_r(\hbar\omega - E_g)(f_v - f_c)}$$

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

$$\mathbf{p}_{cv} = \langle \psi_c | \mathbf{p} | \psi_v \rangle$$

ψ_c and ψ_v are bloch states

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

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

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

Comparison with measured data

M.D. Sturge. Phys. Rev. 127, 768 (1963).

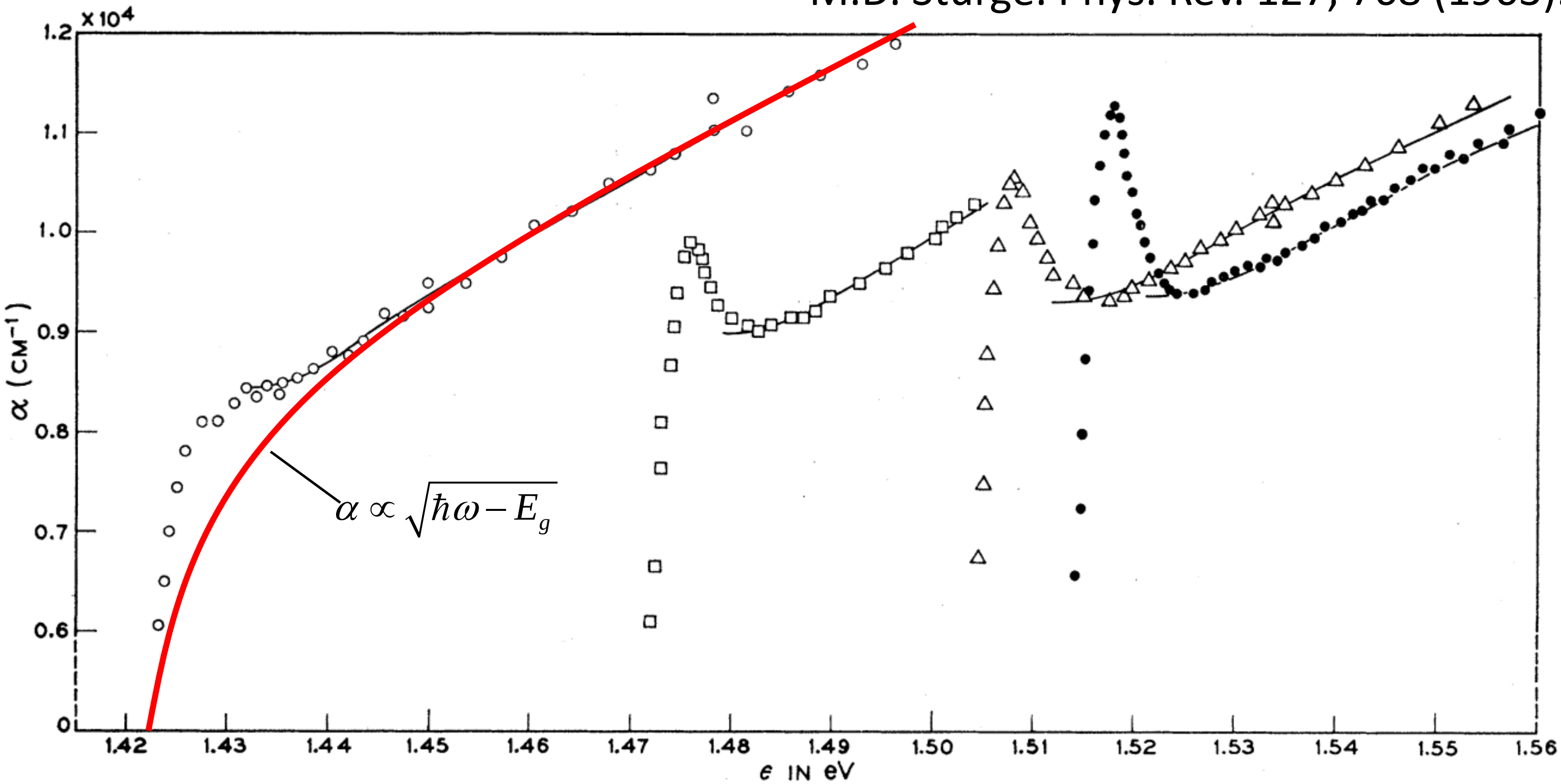


FIG 3 Exciton absorption in GaAs; ○ 294°K, □ 186°K, Δ90°K, ● 21°K.

Absorption follows square root dependence fairly well at room temperature. Our simple model did not include Coulombic interaction between electron and hole which leads to excitonic effect and enhancement of absorption particularly near the bandedge.