EE 232 Lightwave Devices
Lecture 6: Electron-Photon Interaction, Optical Matrix Element, Absorption Coefficient

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Vector Potential

Maxwell's Equations

$$\begin{cases} \nabla\times\vec{E} = -\dfrac{\partial\vec{B}}{\partial t} \\ \nabla\times\vec{H} = \vec{J} + \dfrac{\partial\vec{D}}{\partial t} \\ \nabla\bullet\vec{D} = \rho \\ \nabla\bullet\vec{B} = 0 \end{cases}$$

$\vec{D} = \varepsilon\vec{E}$ and $\vec{B} = \mu\vec{H}$

Vector potential $\vec{A}$

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

$$\Rightarrow \nabla\bullet\vec{B} = \nabla\bullet\left(\nabla\times\vec{A}\right) = 0$$

Vector potential is not unique:

$$\vec{A}' = \vec{A} + \nabla\xi \rightarrow \nabla\times\vec{A}' = \vec{B}$$

$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t} = -\frac{\partial}{\partial t}\nabla\times\vec{A} = \nabla\times\left(-\frac{\partial\vec{A}}{\partial t}\right)$$

$$\vec{E} = -\frac{\partial\vec{A}}{\partial t} - \nabla\phi$$

Wave Equations:

$$\begin{cases} \left(\nabla^2\vec{A} - \mu\varepsilon\dfrac{\partial^2\vec{A}}{\partial t^2}\right) - \nabla\left(\nabla\bullet\vec{A} + \mu\varepsilon\dfrac{\partial\phi}{\partial t}\right) = -\mu\vec{J} \\ \nabla^2\phi + \dfrac{\partial}{\partial t}\left(\nabla\bullet\vec{A}\right) = -\dfrac{\rho}{\varepsilon} \end{cases}$$

Wave Equations are invariant under "Gauge Transformation"

$$\begin{cases} \vec{A}' = \vec{A} + \nabla\xi \\ \phi' = \phi - \dfrac{\partial\xi}{\partial t} \end{cases} \Rightarrow \text{One can choose the value of } \nabla\bullet\vec{A}$$

Lorenz and Coulomb Gauges

Lorenz Gauge:

Set $\nabla \bullet \vec{A} + \mu\varepsilon \frac{\partial \phi}{\partial t} = 0$

$$\begin{cases} \nabla^2 \vec{A} - \mu\varepsilon \frac{\partial^2 \vec{A}}{\partial t^2} = -\mu \vec{J} \\ \nabla^2 \phi - \mu\varepsilon \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\varepsilon} \end{cases}$$

Coulomb Gauge

Set $\nabla \bullet \vec{A} = 0$

$$\begin{cases} \left(\nabla^2 \vec{A} - \mu\varepsilon \frac{\partial^2 \vec{A}}{\partial t^2} \right) - \nabla \left(\mu\varepsilon \frac{\partial \phi}{\partial t} \right) = -\mu \vec{J} \\ \nabla^2 \phi = -\frac{\rho}{\varepsilon} \end{cases}$$

For optical field, $\rho = 0, \quad \phi = 0$

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t}$$

Electron-Photon Interaction

Hamiltonian in the absence of light

$$H_0 = \frac{P^2}{2m_0} + V(\vec{r})$$

Generalized momentum of a charged particle in an electromagnetic field

$$\vec{P} \rightarrow \left(\vec{P} - e\vec{A}\right)$$

Note: $\frac{\partial \vec{P}}{\partial t} = Force \rightarrow \left(\frac{\partial \vec{P}}{\partial t} - e\frac{\partial \vec{A}}{\partial t}\right) = \left(\frac{\partial \vec{P}}{\partial t} - e\vec{E}\right)$

(modification represents EM fields' ability to accelerate or decelerate electrons)

$$H = \frac{1}{2m_0}\left(\vec{P} - e\vec{A}\right)^2 + V(\vec{r})$$

$$= \frac{P^2}{2m_0} - \frac{e}{2m_0}\left(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P}\right) + \frac{e^2A^2}{2m_0} + V(\vec{r})$$

$$H' = -\frac{e}{2m_0}\left(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P}\right) + \frac{e^2A^2}{2m_0}$$

$$H' \approx -\frac{e}{2m_0}\left(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P}\right)$$

$$\left(\vec{P}\cdot\vec{A}\right)\phi = -i\hbar\nabla\cdot\vec{A}\phi$$

$$= -i\hbar\left[\left(\nabla\cdot\vec{A}\right)\phi + \vec{A}\cdot\nabla\phi\right]$$

$$= -i\hbar\vec{A}\cdot\nabla\phi \quad \text{under Coulomb Gauge}$$

$$= \left(\vec{A}\cdot\vec{P}\right)\phi$$

$$H' = -\frac{e}{m_0}\vec{A}\cdot\vec{P}$$

- For a brief review of Hamiltonian classical mechanics, see http://en.wikipedia.org/wiki/Hamiltonian_mechanics#Using_Hamilton.27s_equations

Optical Matrix Element

$$H' = -\frac{e}{m_0}\vec{A}\cdot\vec{P}$$

$$\vec{A} = \hat{e}A_0\cos\left(\vec{k}_{op}\cdot\vec{r}-\omega t\right) = \hat{e}\frac{A_0}{2}e^{i\vec{k}_{op}\cdot\vec{r}-i\omega t} + \hat{e}\frac{A_0}{2}e^{-i\vec{k}_{op}\cdot\vec{r}+i\omega t} \quad ;\ \hat{e} \text{ is optical polarization}$$

$$H' = -\frac{eA_0}{2m_0}e^{i\vec{k}_{op}\cdot\vec{r}-i\omega t}\hat{e}\cdot\vec{P} \approx -\frac{eA_0}{2m_0}e^{-i\omega t}\hat{e}\cdot\vec{P} \;;\ \text{(Dipole or long-wavelength approx)}$$

$$\boxed{H'_{ba}} = \left\langle b\left|\left(-\frac{eA_0}{2m_0}\hat{e}\cdot\vec{P}\right)\right|a\right\rangle = -\frac{eA_0}{2m_0}\hat{e}\cdot\left\langle b\left|\vec{P}\right|a\right\rangle = \boxed{-\frac{eA_0}{2m_0}\hat{e}\cdot\vec{P}_{ba}}$$

Alternative form:

$$\vec{P} = m_0\frac{d}{dt}\vec{r} = m_0\frac{1}{i\hbar}\left[\vec{r},H_0\right] = \frac{m_0}{i\hbar}\left(\vec{r}H_0 - H_0\vec{r}\right)$$

$$\left\langle b\left|\vec{P}\right|a\right\rangle = \frac{m_0}{i\hbar}\left\langle b\left|\left(\vec{r}H_0 - H_0\vec{r}\right)\right|a\right\rangle = \frac{m_0}{i\hbar}\left(E_a - E_b\right)\left\langle b\left|\vec{r}\right|a\right\rangle = \frac{m_0}{i\hbar}\hbar\omega\left\langle b\left|\vec{r}\right|a\right\rangle$$

$$\boxed{H'_{ba}} = \left(-\frac{e}{m_0}\vec{A}\right)\cdot\left(-i\omega m_0\right)\left\langle b\left|\vec{r}\right|a\right\rangle = \boxed{-e\vec{E}\cdot\vec{r}_{ba}}$$

Typical Values of Optical Matrix Element

$$H'_{ba} = -\frac{eA_0}{2m_0}\hat{e}\cdot\vec{P}_{cv} = -e\vec{E}\cdot\vec{r}_{ba} = -ei\omega\frac{A_0}{2}\hat{e}\cdot\vec{r}_{ba} \Rightarrow \left|\vec{r}_{ba}\right| = \frac{\left|\vec{P}_{cv}\right|}{m_0\omega}$$

The optical matrix element is often expressed in E_p :

$$\left|\hat{e}\cdot\vec{P}_{cv}\right|^2 = \frac{m_0}{6}E_p$$

Typical values of E_p (Table K.2 on p.709 of Chuang textbook)

GaAs: $E_p = 25.7$ eV

The corresponding $\left|\vec{r}_{ba}\right| \sim 0.4$ nm

AlAs: $E_p = 21.1$ eV

InAs: $E_p = 22.2$ eV

InP: $E_p = 20.7$ eV

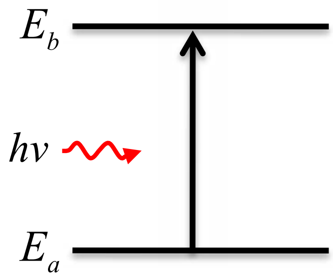
GaP: $E_p = 22.2$ eV

Fermi's Golden Rule

Two-level system, monochromatic light:

$$W_{ba} = \frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)$$

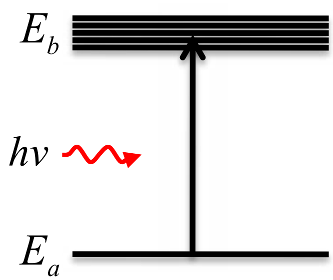
Unit: $[\frac{1}{\text{J-s}}\text{J}^2\frac{1}{\text{J}} = \frac{1}{s}]$



Final state with density of states ρ_b, monochromatic light:

$$W_{ba} = \int \frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)\rho_b(E_b)dE_b$$

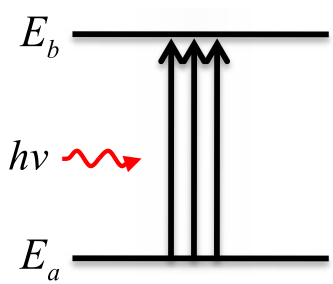
Unit: $[\frac{1}{\text{J-s}}\text{J}^2\frac{1}{\text{J}}\frac{1}{\text{cm}^3\text{-J}}\text{J} = \frac{1}{\text{s-cm}^3}]$



Two-level system, non-monochromatic light:

$$W_{ba} = \int \frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)\cdot P(\hbar\omega)d(\hbar\omega)$$

Unit: $[\frac{1}{\text{J-s}}\text{J}^2\frac{1}{\text{J}}\frac{1}{\text{cm}^3\text{-J}}\text{J} = \frac{1}{\text{s-cm}^3}]$



where $P(\hbar\omega)$: number of photons per unit volume per energy interval

Two-Level System in Non-Monochromatic EM Field

$$W_{ba} = \frac{1}{V}\sum_{k_{op}} \frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)\cdot 2n_{ph} = \boxed{\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 n_{ph} N(E_{ba})}$$

$$\boxed{n_{ph} = \frac{1}{e^{\hbar\omega_k/k_B T} - 1}}$$ Average number of photons per state (Bose-Einstein distribution)

To calculate density of states for photons: $e^{i\vec{k}\cdot\vec{r}}$ satisfies periodic boundary condition

$$\omega_k = \frac{kc}{n_r}$$ dispersion relation (~ E-k relation for electrons)

Number of states with photon energy E_{ba} per unit volume, per energy interval

$$N\left(E_{ba}\right) = \frac{2}{V}\int \frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3}\cdot\delta(E_b - E_a - \hbar\omega_k) = \frac{8\pi}{\left(2\pi\right)^3}\int\left(\frac{n_r\omega_k}{c}\right)^2 \frac{n_r}{c} d\omega_k$$

$$\boxed{N\left(E_{ba}\right) = \frac{8\pi n_r^{\,3} E_{ba}^2}{h^3 c^3}}$$

Joint Density of States for Semiconductor

The electron states associated with optical transition are related by conservation of mementum: $\vec{k}_b \approx \vec{k}_a \approx \vec{k}$

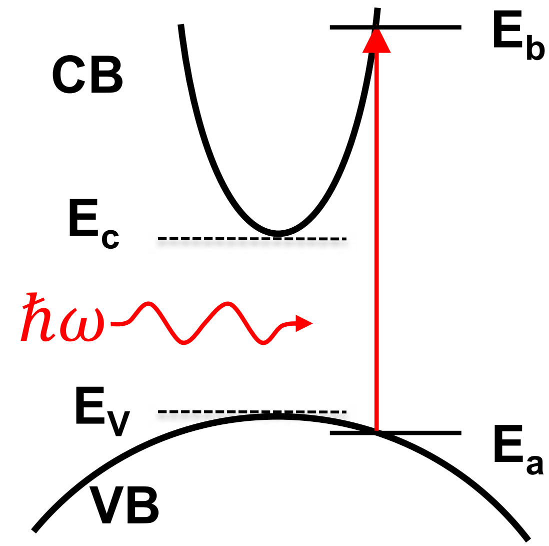
$$E_b = E_C + \frac{\hbar^2 k^2}{2m_e^*} \qquad E_a = E_V - \frac{\hbar^2 k^2}{2m_h^*}$$

$$E_b - E_a = (E_C - E_V) + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$$

$$\hbar\omega = E_g + \frac{\hbar^2 k^2}{2m_r^*}$$

Joint density of states for the pair of electron states:

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



Absorption Coefficient

CB completely full, VB completely empty, total upward transition at $\hbar\omega$:

$$R_0(\hbar\omega) = \frac{2}{V}\sum_k \left[\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)\right] = \frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \int \frac{2d\vec{k}}{(2\pi)^3}\delta(E_g + \frac{\hbar^2 k^2}{2m_r^*} - \hbar\omega)$$

$$\boxed{R_0(\hbar\omega) = \frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \rho_r(\hbar\omega - E_g)} \quad \text{unit: } [\frac{1}{m^3 s}]$$

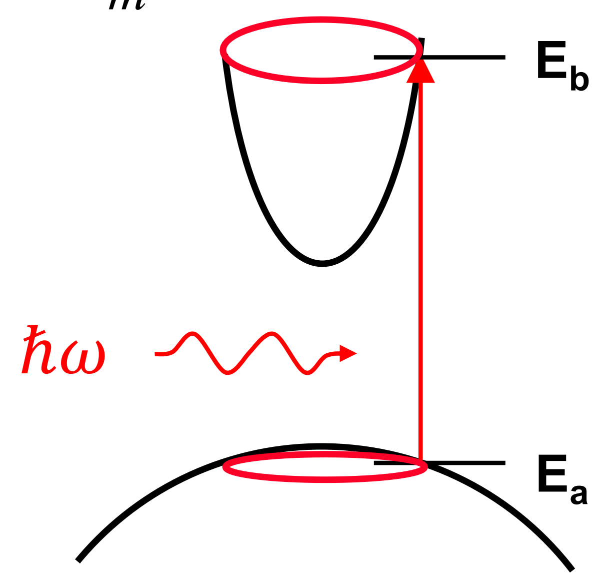
Absorption coefficient

$$\alpha_0(\hbar\omega) = \frac{R(\hbar\omega)}{\text{photon flux}} = \frac{R(\hbar\omega)}{\frac{\varepsilon_0\varepsilon_r E_0^2}{2}\frac{c}{n_r}\frac{1}{\hbar\omega}} = \frac{R(\hbar\omega)}{\frac{\varepsilon_0 n_r \omega^2 A_0^2 c}{2\hbar\omega}} \quad \text{unit: } [\frac{1}{m}]$$

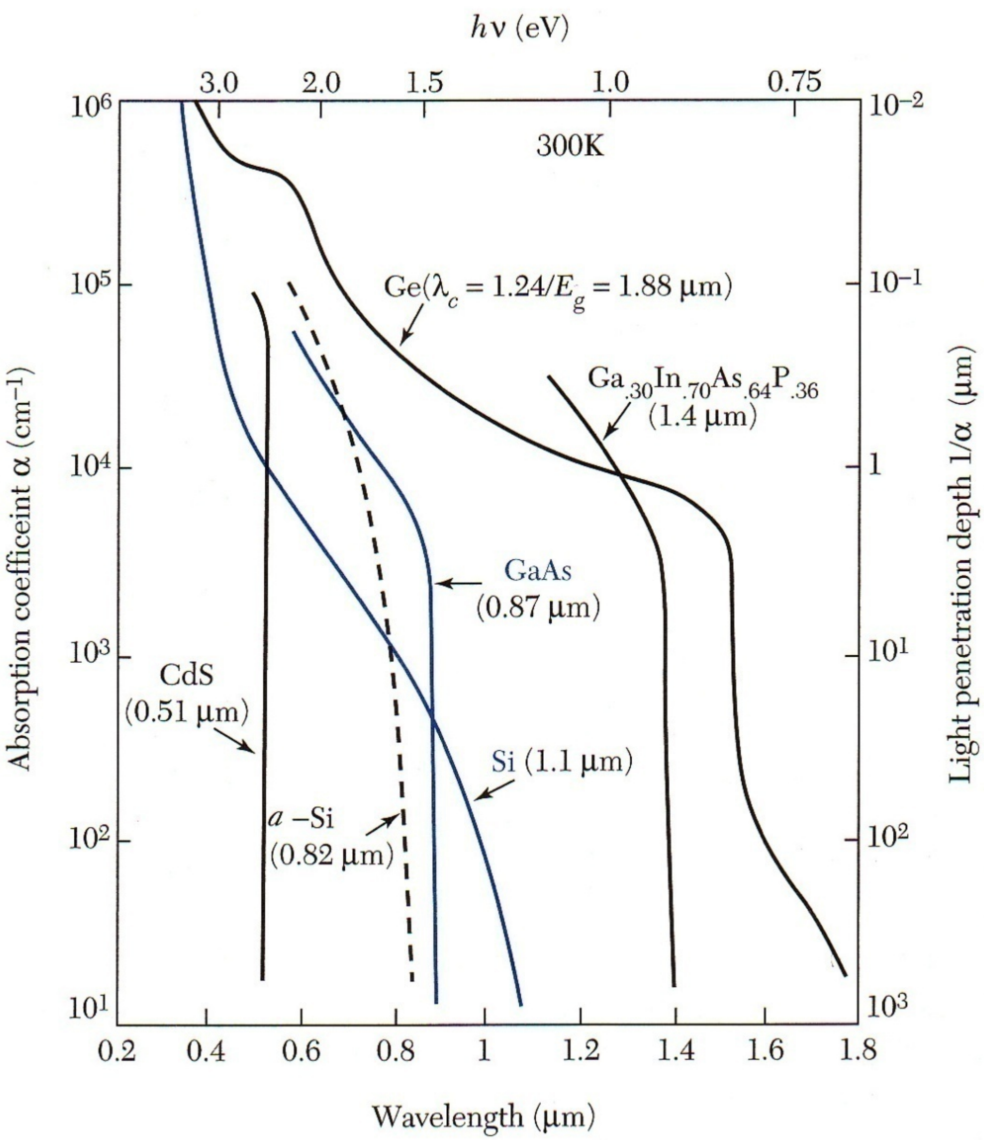
$$H'_{ba} = -\frac{eA_0}{2m_0}\hat{e}\cdot\vec{P}_{cv}$$

$$\boxed{\alpha_0(\hbar\omega) = C_0\left|\hat{e}\cdot\vec{P}_{cv}\right|^2 \rho_r(\hbar\omega - E_g)}$$

$$C_0 = \frac{\pi e^2}{n_r c \varepsilon_0 m_0^2 \omega} \approx 7\times 10^9 \quad \text{unit: } \left[\frac{m^2}{kg}\right]$$



Absorption Coefficient



- Light intensity decays exponentially in semiconductor:

$$I(x) = I_0 e^{-\alpha x}$$

- Direct bandgap semiconductor has a sharp absorption edge
- Si absorbs photons with hv > E_g = 1.1 eV, but the absorption coefficient is small
  - Sufficient for CCD
- At higher energy (~ 3 eV), absorption coefficient of Si becomes large again, due to direct bandgap transition to higher CB

Absorption Coefficient for GaAs

$$\alpha_0(\hbar\omega) = C_0 \left|\hat{e}\cdot\vec{P}_{cv}\right|^2 \rho_r(\hbar\omega - E_g)$$

$nr := 3.5$ $\quad \varepsilon 0 := 8.854\cdot 10^{-12}\,\frac{F}{m}$ $\quad h\_bar = 1.055\times 10^{-34}\,\frac{m^2\cdot kg}{s}$ $\quad 1eV = 1.6\times 10^{-19}\,J$

$Eg := 1.42eV$ $\quad \omega := \frac{Eg}{h\_bar}$ $\quad \omega = 2.154\times 10^{15}\,\frac{1}{s}$

$C0 := \frac{\pi\cdot q^2}{m0^2\cdot\omega\cdot\varepsilon 0\cdot c\cdot nr}$ $\quad C0 = 4.842\times 10^{9}\,\frac{m^2}{kg}$

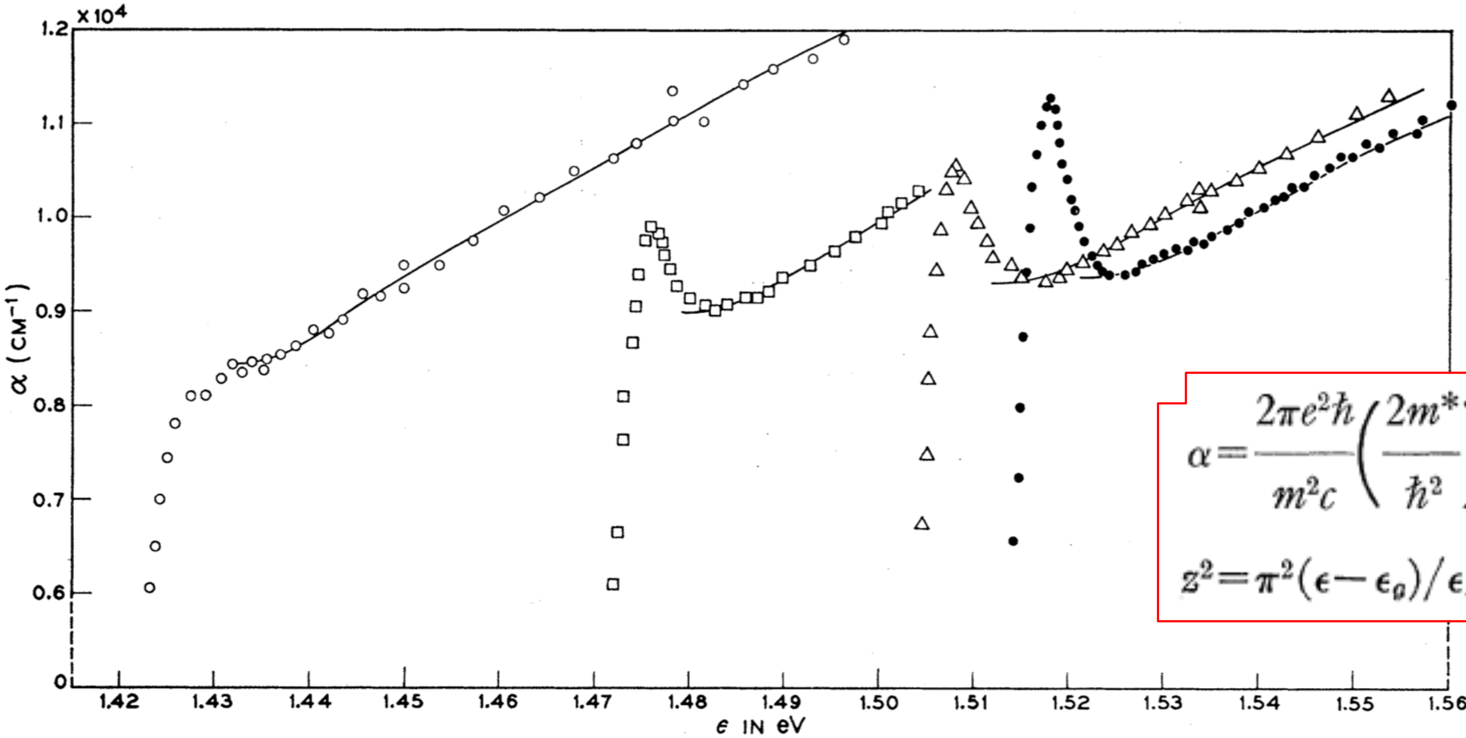
$Ep := 25.7eV$ $\quad \frac{m0}{6}\cdot Ep = 6.243\times 10^{-49}\,kg\cdot J$

$m\_r := \frac{0.067\cdot 0.5}{0.067 + 0.5}\cdot m0$

$\rho r(hv) := \frac{1}{2\pi^2}\cdot\left(\frac{2\cdot m\_r}{h\_bar^2}\right)^{\frac{3}{2}}\cdot\sqrt{hv - Eg}$ $\quad \rho r(1.43eV) = 6.102\times 10^{43}\,\frac{1}{m^3\cdot J}$

$\alpha 0(hv) := C0\cdot\frac{m0}{6}\cdot Ep\cdot\rho r(hv)$ $\quad \alpha 0(1.43eV) = 1.845\times 10^{5}\,\frac{1}{m}$ $\quad \alpha 0(1.43eV) = 1.845\times 10^{3}\,\frac{1}{cm}$

Comparison with Experimental Absorption Coefficients



$$\alpha = \frac{2\pi e^2 \hbar}{m^2 c}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} |P_{cv}|^2 \frac{\epsilon_x^{\frac{1}{2}}}{n\epsilon} \frac{\exp z}{\sinh z}, \quad \epsilon > \epsilon_g$$

$$z^2 = \pi^2(\epsilon - \epsilon_g)/\epsilon_x.$$

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

- M. D. Sturge, "Optical Absorption of Gallium Arsenide between 0.6 and 2.75 eV," Phys. Rev., vol. 127, no. 3, pp. 768–773, Aug. 1962.
- Absorption edge is more "square" than the square root function predicted by simple density of states theory
- Modified theory considers Coulomb interactions between electron and hole, and consequent formation of excitons (additional fitting needed to account for complex shape of hole bands).

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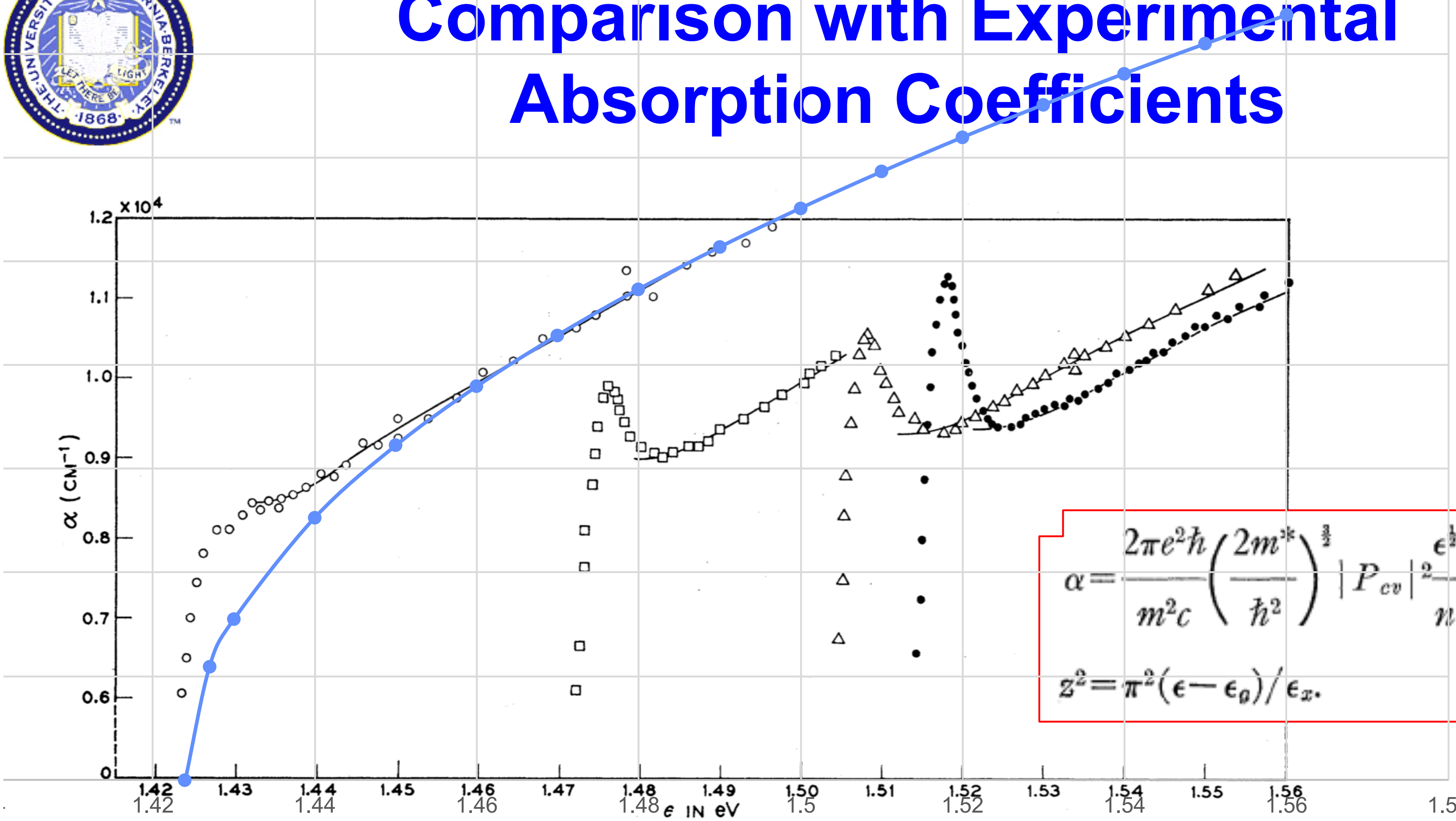

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