ECE 536 – Integrated Optics and Optoelectronics
Lecture 8 – February 10, 2022

Spring 2022

Tu-Th 11:00am-12:20pm

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Lecture 8 Outline

- Electron-Photon interaction
- Optical transitions using Fermi Golden Rule
- Optical Absorption
- Optical Gain

The Electron-Photon Interaction Hamiltonian

Representative crystal momentum for electron in a crystal

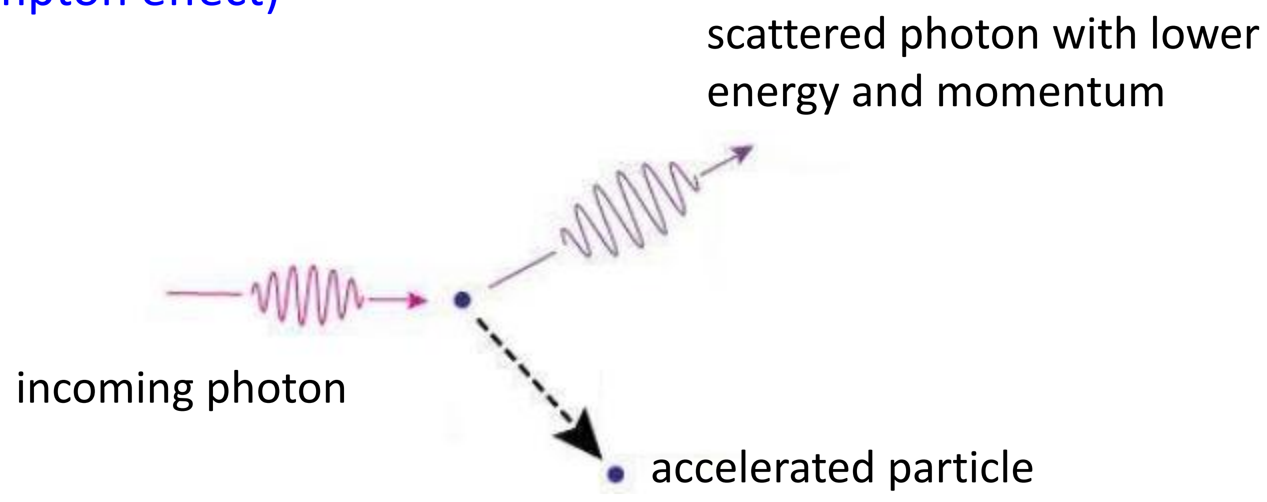
$$\mathbf{p} = \hbar k \approx \frac{\hbar \pi}{a}. \quad \text{With } a_o \approx 5.5\ \text{Å},$$

$$\mathbf{p} \approx \frac{\pi \times 1.054 \times 10^{-34}}{5.5 \times 10^{-10}} = 6.02 \times 10^{-25} \quad \mathrm{J \cdot s/m}$$

Momentum of a photon at 1μm wavelength

$$\hbar k_{opt} \approx \frac{\hbar 2\pi}{\lambda} \approx \frac{2\pi \times 1.054 \times 10^{-34}}{10^{-6}} = 6.6 \times 10^{-28} \quad \mathrm{J \cdot s/m}$$

In free space (Compton effect)



Energy in light wave

$$\mathbf{U_{wave}} = \varepsilon E^2$$

There is no obvious dependence on frequency

$$\mathbf{U_{photons}} = N \cdot \hbar\omega$$

Number of photons/m^3

There is an obvious dependence on frequency

Since we must have

$$\mathbf{U_{wave}} = \mathbf{U_{photons}}$$

the number of photons per unit volume N must be proportional to E^2 with constant of proportionality which depends on the wave frequency

Optical Transitions Using Fermi Golden Rule

Hamiltonian describing the electron-photon interaction in a semiconductor

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

periodic crystal potential

EM vector potential

electron charge

momentum variable

Expansion of the Hamiltonian

Hamiltonian for interaction with light: $H = \frac{1}{2m_0}(\mathbf{p} - e\mathbf{A})^2 + V(\mathbf{r})$

Expand the squared term

$$H = \underbrace{\frac{p^2}{2m_o} + V(\mathbf{r})}_{H_0} \underbrace{- \frac{e}{2m_o}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) + \frac{e^2A^2}{2m_o}}_{H'}$$

Unperturbed Hamiltonian

Perturbed Hamiltonian

Simplifications:

- In practical cases $|eA| \ll |\mathbf{p}|$ so the term $\frac{e^2A^2}{2m_0}$ is neglected
- Choice of Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ such that $\mathbf{p} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{p}$

⇨

$$H' \simeq -\frac{e}{m_o}\mathbf{A}\cdot\mathbf{p}$$

Expansion of the Hamiltonian

Hamiltonian for interaction with light: $H = \frac{1}{2m_0}(\mathbf{p} - e\mathbf{A})^2 + V(\mathbf{r})$

Expand the squared term

$$H = \underbrace{\frac{p^2}{2m_o} + V(\mathbf{r})}_{H_0} \underbrace{- \frac{e}{2m_o}(\mathbf{p}\bullet\mathbf{A} + \mathbf{A}\bullet\mathbf{p}) + \frac{e^2A^2}{2m_o}}_{H'}$$

H_0 Unperturbed Hamiltonian

H' Perturbed Hamiltonian

$$\left(\hat{\vec{p}}\cdot\vec{A} - \vec{A}\cdot\hat{\vec{p}}\right) f(\vec{r}) = \frac{\hbar}{i}\left(\vec{A}\cdot\nabla f + f\,\nabla\cdot\vec{A} - \vec{A}\cdot\nabla f\right) = \frac{\hbar}{i} f\,\nabla\cdot\vec{A}$$

- Choice of Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ such that $\mathbf{p} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{p}$

⇨ $$H' \simeq -\frac{e}{m_o}\mathbf{A}\bullet\mathbf{p}$$

$\mathbf{A}$ is the vector potential

ϕ is the scalar potential

Coulomb Gauge $\nabla \bullet \mathbf{A} = 0$

Lorenz Gauge $\nabla \bullet \mathbf{A} = -\mu\varepsilon \frac{\partial \phi}{\partial t}$

The number of possible gauges is infinite. We are free to some extent to choose the gauge which simplifies solution of a problem, as long as the underlining physics is not affected.

Coulomb gauge is often used when no sources are present.

The Lorenz gauge is necessary when the action of "retarded potentials" has to be considered.

Optical Fields

We define the perturbing field through the magnetic vector potential

$$\mathbf{A} = \hat{e} A_o \cos\left(\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r} - \omega t\right) = \hat{e}\frac{A_o}{2} e^{i\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r}} e^{-i\omega t} + \hat{e}\frac{A_o}{2} e^{-i\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r}} e^{+i\omega t}$$

unit vector (direction of Electric Field with assumption below)

Electric Field (V/m)

$$\mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{A}}{\partial t} \boxed{-\nabla \phi}$$

vanishes for optical field

$$= -\frac{\partial \mathbf{A}}{\partial t} = -\hat{e}\omega A_o \sin\left(\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r} - \omega t\right)$$

Magnetic Field (A/m)

$$\mathbf{H}(\mathbf{r},t) = \frac{1}{\mu}\nabla \times \mathbf{A} = -\frac{1}{\mu}\mathbf{k}_{\mathbf{op}} \times \hat{e} A_o \sin\left(\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r} - \omega t\right)$$

Assumption

$$\mu = \mu_o$$

Poynting Vector

$$\mathbf{P}(\mathbf{r},t)=\mathbf{E}(\mathbf{r},t)\times\mathbf{H}(\mathbf{r},t)=\ \hat{k}\ k_{op}\frac{\omega A_o^2}{\mu}\sin^2\left(\mathbf{k_{op}}\bullet\mathbf{r}-\omega t\right)$$

direction of power flow

Time Average Poynting Flux

$$\left|\left\langle\mathbf{P}(\mathbf{r},t)\right\rangle\right|=\frac{\omega A_o^2}{2\mu}k_{op}$$

We have used $\left|\left\langle\sin^2(x)\right\rangle\right|=\frac{1}{2}$

$$k_{op}=\frac{2\pi}{\lambda}=\frac{2\pi f}{\mathrm{v}_{ph}}=\frac{\omega\sqrt{\mu_r\varepsilon_r}}{c}=\frac{\omega\sqrt{\varepsilon_r}}{c}=\frac{\omega n_r}{c}$$

$$c=\frac{1}{\sqrt{\mu_0\varepsilon_0}}\quad\Rightarrow\quad\mu_0=\frac{1}{c^2\varepsilon_0}$$

$$\mu=\mu_o$$

$$\left|\left\langle\mathbf{P}(\mathbf{r},t)\right\rangle\right|=\frac{n_r c\varepsilon_o\omega^2 A_o^2}{2}$$

Interaction Hamiltonian

Substitute the assumed magnetic vector potential into the expanded Hamiltonian

$$\mathbf{A} = \hat{e} A_o \cos\left(\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r} - \omega t\right) = \hat{e} \frac{A_o}{2} e^{i\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r}} e^{-i\omega t} + \hat{e} \frac{A_o}{2} e^{-i\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r}} e^{+i\omega t}$$

$$H' \simeq -\frac{e}{m_o} \mathbf{A} \bullet \mathbf{p}$$

$$H'(\mathbf{r}, t) = -\frac{e A_o e^{i\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r}}}{2 m_o} (\hat{e} \bullet \mathbf{p}) e^{-i\omega t} - \frac{e A_o e^{-i\mathbf{k}_{\mathbf{op}} \bullet \mathbf{r}}}{2 m_o} (\hat{e} \bullet \mathbf{p}) e^{+i\omega t}$$

Interaction Hamiltonian

$$H'(\mathbf{r},t) = -\underbrace{\frac{eA_o e^{i\mathbf{k_{op}}\cdot\mathbf{r}}}{2m_o}(\hat{e}\cdot\mathbf{p})}_{H'(\mathbf{r})}e^{-i\omega t} - \underbrace{\frac{eA_o e^{-i\mathbf{k_{op}}\cdot\mathbf{r}}}{2m_o}(\hat{e}\cdot\mathbf{p})}_{H'^{+}(\mathbf{r})}e^{+i\omega t}$$

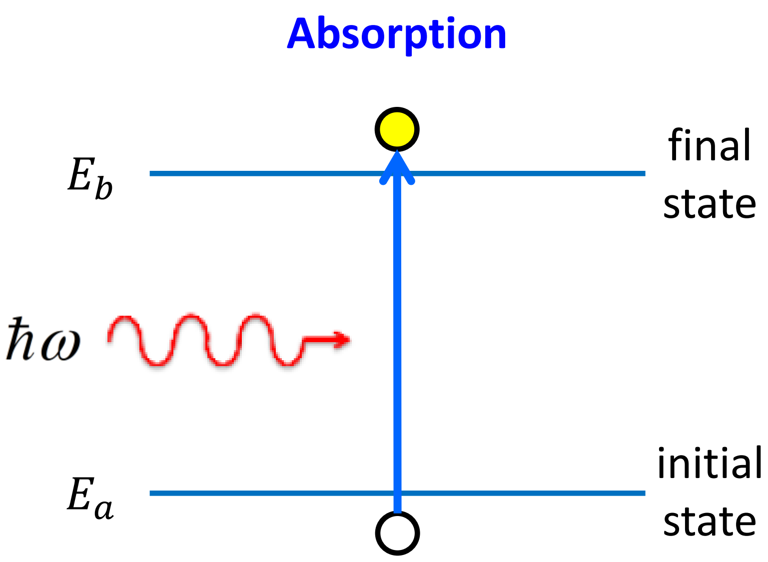
$$\boxed{H'(\mathbf{r},t) = H'(\mathbf{r})e^{-i\omega t} + H'^{+}(\mathbf{r})e^{+i\omega t}}$$

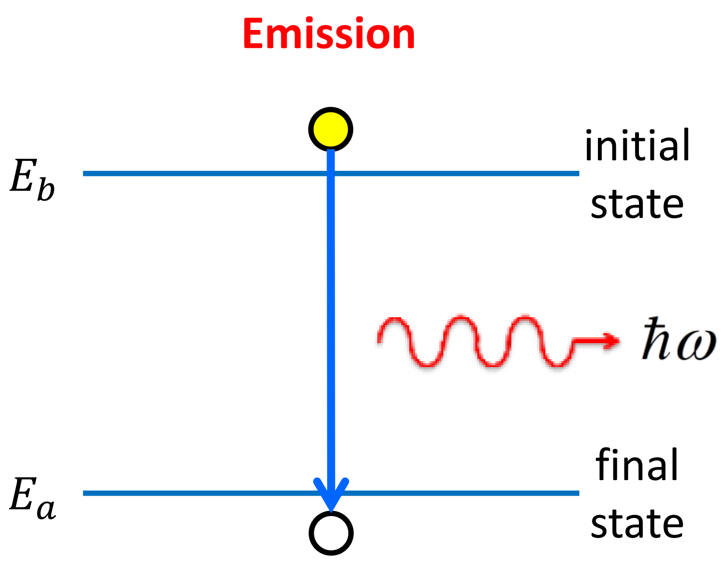
$$\begin{cases} H'(\mathbf{r}) = -\dfrac{eA_o e^{i\mathbf{k_{op}}\cdot\mathbf{r}}}{2m_o}(\hat{e}\cdot\mathbf{p}) \\ H'^{+}(\mathbf{r}) = -\dfrac{eA_o e^{-i\mathbf{k_{op}}\cdot\mathbf{r}}}{2m_o}(\hat{e}\cdot\mathbf{p}) \end{cases}$$

Hermitian adjoint (conjugate) of $H'(\mathbf{r})$

Hermitian Conjugate Operator: $\langle H^{+}\varphi|\psi\rangle = \langle\varphi|H\psi\rangle$

Transition Rate due to Electron-Photon Interaction





Transition Rate: Absorption

Transition Rate for Photon Absorption (single electron)

$$W_{abs} = \frac{2\pi}{\hbar} \left| \langle b | H'(\mathbf{r}) | a \rangle \right|^2 \delta\left(E_b - E_a - \hbar\omega\right)$$

Total Upward Transition Rate per unit volume (s^{-1} cm^{-3})

$$R_{a\to b} = \frac{2}{V} \sum_{k_a} \sum_{k_b} W_{abs} f_a \left(1 - f_b\right) = \frac{2}{V} \sum_{k_a} \sum_{k_b} \frac{2\pi}{\hbar} \left| H'_{ba} \right|^2 \delta\left(E_b - E_a - \hbar\omega\right) f_a \left(1 - f_b\right)$$

probability of occupation

$$H'_{ba} \equiv \langle b | H'(\mathbf{r}) | a \rangle = \int \Psi_b^*(\mathbf{r}) H'(\mathbf{r}) \Psi_a(\mathbf{r}) d^3\mathbf{r}$$

Transition Rate: Emission

Transition Rate for Photon Emission (single electron)

$$W_{ems} = \frac{2\pi}{\hbar} \left| \langle a | H'^{+}(\mathbf{r}) | b \rangle \right|^2 \delta\left(E_a - E_b + \hbar\omega\right)$$

Total Downward Transition Rate per unit volume (s^{-1} cm^{-3})

$$R_{b\to a} = \frac{2}{V}\sum_{k_a}\sum_{k_b} W_{ems} f_b\left(1 - f_a\right) = \frac{2}{V}\sum_{k_a}\sum_{k_b} \frac{2\pi}{\hbar}\left|H'^{+}_{ab}\right|^2 \delta\left(E_a - E_b + \hbar\omega\right) f_b\left(1 - f_a\right)$$

probability of occupation

$$H'^{+}_{ab} \equiv \langle a | H'^{+}(\mathbf{r}) | b \rangle = \int \Psi_a^*(\mathbf{r}) H'(\mathbf{r}) \Psi_b(\mathbf{r}) d^3\mathbf{r}$$

Net Absorption Rate

Net Upward Transition

$$R = R_{a\to b} - R_{b\to a}$$

$$= \frac{2}{V}\sum_{k_a}\sum_{k_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right) f_a\left(1 - f_b\right)$$

$$- \frac{2}{V}\sum_{k_a}\sum_{k_b}\frac{2\pi}{\hbar}\left|H'^{+}_{ab}\right|^2 \delta\left(E_a - E_b + \hbar\omega\right) f_b\left(1 - f_a\right)$$

Using

$$\delta(-x) = \delta(x) \longrightarrow \delta\left(E_b - E_a - \hbar\omega\right) = \delta\left(-E_b + E_a + \hbar\omega\right)$$

$$\left|H'_{ba}\right| = \left|H'^{+}_{ab}\right|$$

$$R = \frac{2}{V}\sum_{k_a}\sum_{k_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right)\left[\left(f_a - f_a f_b\right) - \left(f_b - f_b f_a\right)\right]$$

$$\boxed{R = \frac{2}{V}\sum_{k_a}\sum_{k_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right)\left(f_a - f_b\right)}$$

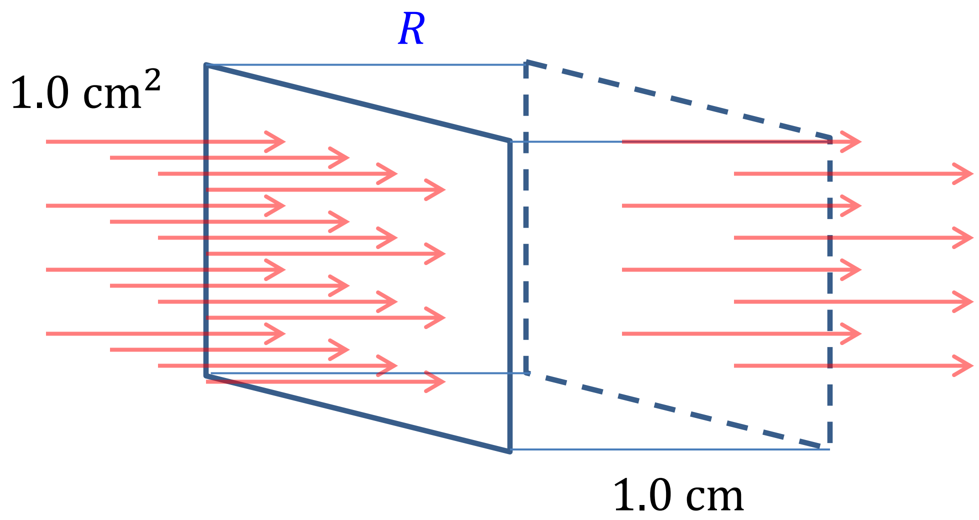
Optical Absorption Coefficient

Absorption Coefficient

Absorption Coefficient [cm^{-1}] = fraction of photons absorbed per unit distance

$$\alpha = \frac{\text{Number of photons absorbed per second per unit volume}}{\text{Number of photons injected per second per unit area}}$$

$$\frac{\text{optical intensity}}{\text{energy per photon}} = \frac{|\langle P \rangle|}{\hbar\omega}$$



We have already derived what we need for the absorption coefficient.

Absorption Coefficient

$$\frac{\text{optical intensity}}{\text{energy per photon}} = \frac{|\langle P\rangle|}{\hbar\omega} = \frac{n_r c\varepsilon_0\omega^2 A_0^2}{2\ \hbar\omega}$$

$$\alpha = \frac{R}{(P/\hbar\omega)} = \frac{\hbar\omega}{\left(\frac{n_r c\varepsilon_o\omega^2 A_o^2}{2}\right)}\frac{2}{V}\sum_{k_a}\sum_{k_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2\delta\left(E_b - E_a - \hbar\omega\right)\left(f_a - f_b\right)$$

We found earlier

$$H'(\mathbf{r}) = -\frac{eA_o e^{i\mathbf{k}_{\mathrm{op}}\bullet\mathbf{r}}}{2m_o}(\hat{e}\bullet\mathbf{p})$$

Long wavelength (dipole) approximation: wavelength of light is large compared to the spatial distance between energy levels involved on the transition

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}e^{i\mathbf{k}_{\mathrm{op}}\bullet\mathbf{r}} \simeq \mathbf{A}$$

$$H'_{ba} \simeq -\frac{e}{m_o}\mathbf{A}\bullet\langle b|\mathbf{p}|a\rangle = -\frac{eA_o}{2m_o}\hat{e}\bullet\mathbf{p}_{ba}$$

substitute into α →

Absorption Coefficient

$$\alpha = \frac{\hbar\omega}{\left(\frac{n_r c\varepsilon_o \omega^2 A_o^2}{2}\right)} \frac{2}{V} \sum_{k_a}\sum_{k_b} \frac{2\pi}{\hbar}\left(\frac{eA_o}{2m_o}\right)^2 \left|\hat{e}\bullet\mathbf{p}_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right)\left(f_a - f_b\right)$$

$$= C_o \frac{2}{V}\sum_{k_a}\sum_{k_b}\left|\hat{e}\bullet\mathbf{p}_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right)\left(f_a - f_b\right)$$

with $$C_o = \frac{\pi e^2}{n_r c\varepsilon_0 m_0^2 \omega}$$

The intensity factors A_0^2 cancel out. The absorption coefficient is independent of optical intensity in linear regime.

Recall also: $$\boldsymbol{p}_{ba} = \left\langle b\left|\frac{\hbar}{i}\nabla\right|a\right\rangle = \int \Psi_b^*(\boldsymbol{r})\frac{\hbar}{i}\nabla\Psi_a(\boldsymbol{r})$$

The Hamiltonian can also be written in terms of the electric dipole moment which has form $\boldsymbol{\mu} = -e\mathbf{r}$

We had $$H'_{ba} \simeq -\frac{e}{m_o}\mathbf{A} \bullet \langle b|\mathbf{p}|a\rangle$$

$$p_{ba} = \langle b|\mathbf{p}|a\rangle = \langle b|\frac{\hbar}{i}\nabla|a\rangle = \int \Psi_b^*(r)\frac{\hbar}{i}\nabla\Psi_a(r)$$

Using the property $$\mathbf{p} = m_o\frac{d}{dt}\mathbf{r} = \frac{m_o}{i\hbar}(\mathbf{r}H_o - H_o\mathbf{r})$$

H_0 = unperturbed Hamiltonian

$$H'_{ba} \simeq \frac{-e}{i\hbar}\mathbf{A} \bullet \langle b|\mathbf{r}H_o - H_o\mathbf{r}|a\rangle$$

$$= -\frac{e(E_a - E_b)}{i\hbar}\mathbf{A} \bullet \langle b|\mathbf{r}|a\rangle \simeq -\boldsymbol{\mu}_{ba} \bullet \mathbf{E}$$

$$\mathbf{E} = i\omega\mathbf{A} \qquad H_o|a\rangle = E_a|a\rangle \qquad \boldsymbol{\mu}_{ba} = e\langle b|\mathbf{r}|a\rangle = e\mathbf{r}_{ba}$$

$$E_b - E_a = \hbar\omega \qquad \langle b|H_o = \langle b|E_b$$

With

$$H'_{ba} \simeq \frac{-e}{i\hbar}\mathbf{A} \bullet \langle b|\mathbf{r}H_o - H_o\mathbf{r}|a\rangle$$
$$= -\frac{e(E_a - E_b)}{i\hbar}\mathbf{A} \bullet \langle b|\mathbf{r}|a\rangle \simeq -\boldsymbol{\mu}_{ba} \bullet \mathbf{E}$$

The absorption coefficient becomes

$$\alpha(\hbar\omega) = \frac{\pi\omega}{n_r c \varepsilon_0}\frac{2}{V}\sum_{k_a}\sum_{k_b}\left|\hat{e} \bullet \boldsymbol{\mu}_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)(f_a - f_b)$$

In practice, scattering causes linewidth broadening. The delta function can be replaced by a Lorentzian function

Real and Imaginary Parts of the Permittivity Function

Power decay

The absorption coefficient comes from the wave vector in the expression for power

$$\hat{\gamma} = \mathbf{Re}(\hat{\gamma}) + i\ \mathbf{Im}\{\hat{\gamma}\}$$

$$\hat{\gamma} = \frac{2\pi}{\hat{\lambda}} = \frac{2\pi f}{v_{ph}} = \omega\sqrt{\mu(\varepsilon_1 + i\varepsilon_2)}$$

$$P(z) = P_0\ e^{2\ i\hat{\gamma}z}$$

$$= P_0 e^{2i\mathbf{Re}\{\hat{\gamma}\}z + 2i[i\ \mathbf{Im}\{\hat{\gamma}\}]z}$$

$$= P_0 e^{[2i\mathbf{Re}\{\hat{\gamma}\}z - 2\mathbf{Im}\{\hat{\gamma}\}z]}$$

$$\Rightarrow \quad |P(z)| = |P_0| e^{-\alpha z}$$

Absorption Coefficient and Permittivity

The absorption coefficient and the permittivity are related by

$$\alpha = 2\,\mathrm{Im}\,\omega\sqrt{\mu(\varepsilon_1 + i\varepsilon_2)} \simeq 2\,\mathrm{Im}\left[\frac{\omega}{c} n_r \left(1 + i\frac{\varepsilon_2}{2\varepsilon_1}\right)\right] = \frac{\omega}{n_r c}\frac{\varepsilon_2}{\varepsilon_0}$$

$$|\varepsilon_2| \ll \varepsilon_1$$

(Factor of 2 because α refers to absorption of optical intensity)

Rearranging:

$$\varepsilon_2(\omega) = \frac{n_r c \varepsilon_0}{\omega}\alpha(\hbar\omega)$$

$$= \frac{\pi e^2}{m_0^2 \omega^2}\frac{2}{V}\sum_{k_a}\sum_{k_b}\left|\hat{e}\cdot\mathbf{p}_{ba}\right|^2 \delta(E_b - E_a - \hbar\omega)(f_a - f_b)$$

Absorption Coefficient and Permittivity

The real part of the permittivity can be obtained from the imaginary part using Kramers-Kronig relation (in Appendix 5A)

$$\varepsilon_1(\omega) = \varepsilon_0 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$

P denotes the Principal Value of the integral

$$\varepsilon_1(\omega) = \varepsilon_0 + \frac{2e\hbar^2}{m_0^2} \frac{2}{V} \sum_{k_a} \sum_{k_b} \left| \hat{e} \cdot \mathbf{p}_{ba} \right|^2 \frac{(f_a - f_b)}{(E_b - E_a)\left[(E_b - E_a)^2 - (\hbar\omega)^2\right]}$$

Note: for a semiconductor, E_a and E_b are obtained from the band structure

$$E_a = E(k_a) \text{ and } E_b = E(k_b)$$

Interband Absorption and Gain of Bulk Semiconductors

We found the Net Upward Transition

$$R = R_{a\to b} - R_{b\to a} = \frac{2}{V}\sum_{k_a}\sum_{k_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2\delta\left(E_b - E_a - \hbar\omega\right)\left(f_a - f_b\right)$$

$$H'_{ba} = \left\langle b\left|\frac{-eA(\mathbf{r})}{m_0}\cdot\mathbf{p}\right|a\right\rangle$$

How do we calculate the interband optical matrix element?

Evaluation of the Interband Optical Matrix Element

Vector Potential of the optical field

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}e^{i\mathbf{k}_{op}\cdot\mathbf{r}} = \frac{\hat{e}A_0}{2}e^{i\mathbf{k}_{op}\cdot\mathbf{r}}$$

Interband absorption involves two states in the band structure

$$\psi_a = \frac{u_v(\mathbf{r})e^{i\mathbf{k}_v\cdot\mathbf{r}}}{\sqrt{Vol}} \Rightarrow \psi_b = \frac{u_c(\mathbf{r})e^{i\mathbf{k}_c\cdot\mathbf{r}}}{\sqrt{Vol}}$$

valence band E_a | conduction band E_b

$u_v(\mathbf{r})$ and $u_c(\mathbf{r})$ are the periodic parts of the Bloch functions

Evaluation of the Interband Optical Matrix Element

In general from $H'_{ba} = \left\langle b \left| \frac{-eA(\mathbf{r})}{m_0} \bullet \mathbf{p} \right| a \right\rangle$ and $\mathbf{A}(\mathbf{r}) = \mathbf{A} e^{i\mathbf{k}_{op} \bullet \mathbf{r}} = \frac{\hat{e} A_0}{2} e^{i\mathbf{k}_{op} \bullet \mathbf{r}}$

$$H'_{ba} = \left\langle b \left| -\frac{eA_o e^{i\mathbf{k}_{op} \bullet \mathbf{r}}}{2m_o} (\hat{e} \bullet \mathbf{p}) \right| a \right\rangle = -\frac{eA_o}{2m_o} \hat{e} \bullet \left\langle b \left| e^{i\mathbf{k}_{op} \bullet \mathbf{r}} \mathbf{p} \right| a \right\rangle$$

ψ_a^* $\quad$ ψ_b

$$H'_{ba} = -\frac{eA_o}{2m_o} \hat{e} \bullet \int \frac{u_c^*(\mathbf{r}) e^{-i\mathbf{k}_c \bullet \mathbf{r}}}{\sqrt{Vol}} \, e^{i\mathbf{k}_{op} \bullet \mathbf{r}} \left(-i\hbar\nabla\right) \frac{u_v(\mathbf{r}) e^{i\mathbf{k}_v \bullet \mathbf{r}}}{\sqrt{Vol}} \, d^3\mathbf{r}$$

Evaluation of the Interband Optical Matrix Element

$$H'_{ba} = -\frac{eA_o}{2m_o}\hat{e}\bullet\int \frac{u_c^*(\mathbf{r})e^{-i\mathbf{k}_c\bullet\mathbf{r}}}{\sqrt{Vol}}\, e^{i\mathbf{k}_{\mathbf{op}}\bullet\mathbf{r}}\,(-i\hbar\nabla)\frac{u_v(\mathbf{r})e^{i\mathbf{k}_v\bullet\mathbf{r}}}{\sqrt{Vol}}\, d^3\mathbf{r}$$

$$\Downarrow$$

$$H'_{ba} = -\frac{eA_0}{2m_0}\hat{e}\cdot\int u_c^*(\mathrm{r})\, e^{-i\mathrm{k}_c\cdot\mathrm{r}}\, e^{i\mathrm{k}_{op}\cdot\mathrm{r}}\left[\left(-i\hbar\,\nabla u_v(r)\right)e^{i\mathrm{k}_v\cdot\mathrm{r}} + \hbar\mathrm{k}_v\, u_v(r)e^{i\mathrm{k}_v\cdot\mathrm{r}}\right]\frac{d^3\mathrm{r}}{V}$$

$$\left.\begin{array}{c} u_c^*(\mathrm{r})\,\left(-i\hbar\,\nabla u_v(r)\right) \\ u_c^*(\mathrm{r})\, u_v(r) \end{array}\right\}$$ periodic and fast varying over a unit cell

$$\left.\begin{array}{c} e^{-i\mathrm{k}_c\cdot\mathrm{r}} \\ e^{i\mathrm{k}_v\cdot\mathrm{r}} \end{array}\right\}$$ slowly varying over a unit cell

The integral can be separated into the product of two integrals, one over the unit cell for the fast varying part and one over the volume for the slowly varying part

Evaluation of the Interband Optical Matrix Element

$$H'_{ba} = -\frac{eA_0}{2m_0}\,\hat{e}\cdot\int u_c^*(\mathrm{r})\, e^{-i\mathrm{k}_c\cdot\mathrm{r}}\, e^{i\mathrm{k}_{op}\cdot\mathrm{r}}\left[\left(-i\hbar\,\nabla u_v(r)\right)e^{i\mathrm{k}_v\cdot\mathrm{r}} + \hbar\mathrm{k}_v\, u_v(r)e^{i\mathrm{k}_v\cdot\mathrm{r}}\right]\frac{d^3\mathrm{r}}{V}$$

⇩

$$\simeq -\frac{eA_0}{2m_0}\,\hat{e}\cdot\int_\Omega u_c^*(\mathrm{r})\left(-i\hbar\,\nabla u_v(r)\right)\frac{d^3\mathrm{r}}{\Omega}\int_V e^{i(-\mathrm{k}_c+\mathrm{k}_v+\mathrm{k}_{op})\cdot\mathrm{r}}\frac{d^3\mathrm{r}}{V} + 0$$

over unit cell Ω

orthogonality of wave functions

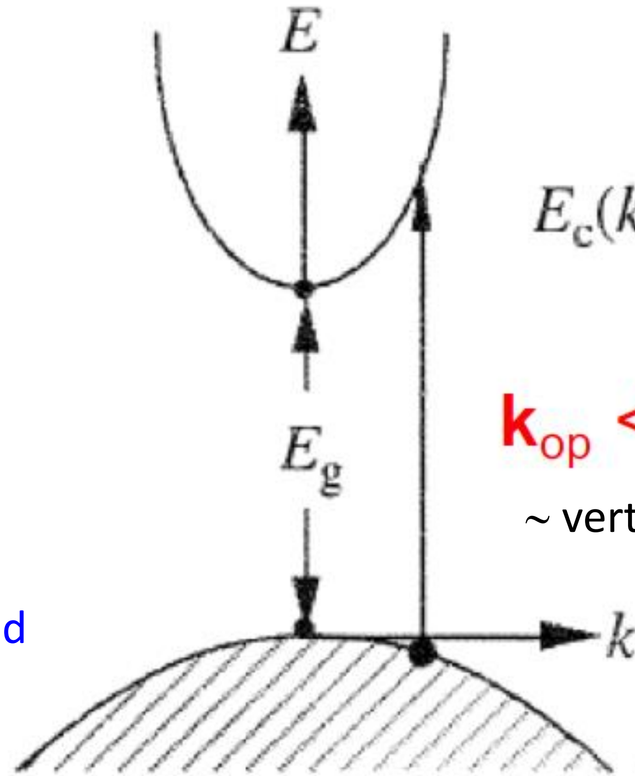
$$= -\frac{eA_0}{2m_0}\,\hat{e}\cdot\mathrm{p}_{cv}\,\delta(k_c, k_v + k_{op})$$

momentum conservation

with $$\mathrm{p}_{cv} = \int_\Omega u_c^*(\mathrm{r})\left(-i\hbar\,\nabla u_v(r)\right)\frac{d^3\mathrm{r}}{\Omega}$$

k-selection Rule

$$H'_{ba} \simeq -\frac{eA_o}{2m_o}\hat{e}\bullet\mathbf{p}_{cv}\delta_{\mathbf{k}_c,\mathbf{k}_v}$$



$$E_c(k) = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

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

$\mathbf{k}_{op} \ll \mathbf{k}_c, \mathbf{k}_v$

~ vertical transition

energies are measured
from top of valence band

$$E_c - E_v = E_g + \frac{\hbar^2 k^2}{2m_e^*} + \frac{\hbar^2 k^2}{2m_h^*} = E_g + \frac{\hbar^2 k^2}{2m_r^*}$$

with $\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$

Optical Absorption Spectrum

$$\alpha(\hbar\omega) = \frac{\hbar\omega}{\left(\frac{n_r c \varepsilon_o \omega^2 A_o^2}{2}\right)} \frac{2}{V} \sum_{k_a} \sum_{k_b} \frac{2\pi}{\hbar} \left|H'_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right)\left(f_a - f_b\right)$$

$$= \frac{\hbar\omega}{\left(\frac{n_r c \varepsilon_o \omega^2 A_o^2}{2}\right)} \frac{2}{V} \sum_{k_v} \sum_{k_c} \frac{2\pi}{\hbar} \left|\frac{-eA_o}{2m_o} \hat{e} \bullet \mathbf{p}_{cv} \delta_{\mathbf{k}_c,\mathbf{k}_v}\right|^2 \delta\left(E_c - E_v - \hbar\omega\right)\left(f_v - f_c\right)$$

$$= \frac{\pi e^2}{n_r c \varepsilon_o m_o^2 \omega} \frac{2}{V} \sum_{k_v} \sum_{k_c} \left|\hat{e} \bullet \mathbf{p}_{cv}\right|^2 \delta_{\mathbf{k}_c,\mathbf{k}_v} \delta\left(E_c - E_v - \hbar\omega\right)\left(f_v - f_c\right)$$

$$= C_o \frac{2}{V} \sum_{k} \left|\hat{e} \bullet \mathbf{p}_{cv}\right|^2 \delta\left(E_c - E_v - \hbar\omega\right)\left(f_v(\mathbf{k}) - f_c(\mathbf{k})\right)$$

k represents both $\mathbf{k}_c$ and $\mathbf{k}_v$
They are equal by the k-selection rule

Optical Absorption Spectrum

Starting with the general expression

$$\alpha(\hbar\omega) = C_o \frac{2}{V} \sum_{\mathbf{k}} \left|\hat{e} \bullet \mathbf{p}_{cv}\right|^2 \delta\left(E_c - E_v - \hbar\omega\right)\left(f_v - f_c\right)$$

we assume an **undoped bulk** material in **thermal equilibrium**, with valence band fully occupied and conduction band completely empty

$$F_c = F_v = E_F \qquad f_v = 1 \qquad f_c = 0$$

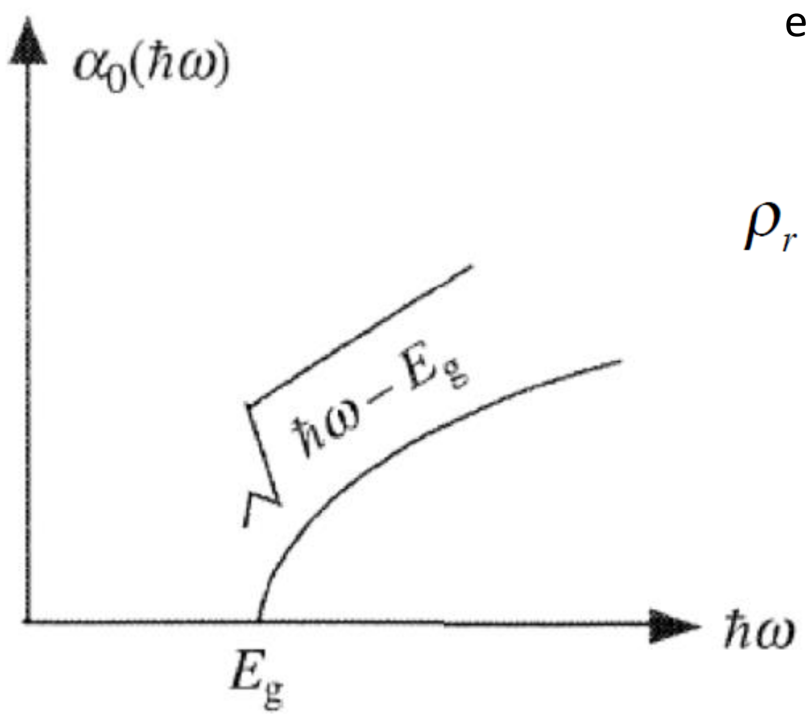
$$\alpha_0(\hbar\omega) = C_0 \left|\hat{e} \cdot \mathrm{p}_{cv}\right|^2 \int \frac{2d^2k}{(2\pi)^3} \delta\left(E_g + \frac{\hbar^2 k^2}{2m_r} - \hbar\omega \right)$$

$$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Optical Absorption Spectrum

The integral can solved analytically arriving at the **bulk absorption coefficient**

$$\alpha_o(\hbar\omega) = C_o \underbrace{\left|\hat{e}\bullet\mathbf{p}_{cv}\right|^2}_{\text{momentum matrix element}} \underbrace{\rho_r\left(\hbar\omega - E_g\right)}_{\text{joint (reduced) density of states}}$$



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

$$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Optical Gain Spectra (with carriers)

Under current injection or optical pumping, we have quasi-Fermi levels F_c and F_v

$$\alpha(\hbar\omega) = C_o \frac{2}{V} \sum_k \left| \hat{e} \bullet \mathbf{p}_{cv} \right|^2 \delta\left(E_c - E_v - \hbar\omega\right)\left(f_v(\mathbf{k}) - f_c(\mathbf{k})\right)$$

$$f_v(\mathbf{k}) = \frac{1}{1 + e^{(E_v(\mathbf{k}) - F_v)/\mathrm{kT}}} \qquad f_c(\mathbf{k}) = \frac{1}{1 + e^{(E_c(\mathbf{k}) - F_c)/\mathrm{kT}}}$$

We carry out the integral as before

$$\alpha(\hbar\omega) = C_0 \left|\hat{e} \cdot \mathrm{p}_{cv}\right|^2 \int \frac{2d^2k}{(2\pi)^3} \delta\left(E_g + \frac{\hbar^2 k^2}{2m_r} - \hbar\omega\right) \left[f_v(k) - f_c(k)\right]$$

Optical Gain Spectra (with carriers)

$$\alpha(\hbar\omega) = C_0 |\hat{e}\cdot \mathrm{p}_{cv}|^2 \int \frac{2d^2k}{(2\pi)^3}\,\delta\left(E_g + \frac{\hbar^2 k^2}{2m_r} - \hbar\omega\right)\,[f_v(k) - f_c(k)]$$

$$\Downarrow$$

$$\alpha(\hbar\omega) = \alpha_0(\hbar\omega)\big(f_v(\mathrm{k}_0) - f_c(\mathrm{k}_0)\big)$$

$$|\mathbf{k}| = \sqrt{\frac{2m_r^*}{\hbar^2}(\hbar\omega - E_g)} \equiv \mathrm{k}_0$$

Optical Gain Spectra (with carriers)

$$\alpha(\hbar\omega) = \alpha_0(\hbar\omega)\left(f_v(\mathrm{k}_0) - f_c(\mathrm{k}_0)\right)$$

We have **Gain** (negative absorption) when

$$f_v(\mathrm{k}_0) < f_c(\mathrm{k}_0)$$

$$\Downarrow$$

$$E_g < \hbar\omega < F_c - F_v$$

$$F_c - F_v > E_c - E_v = \hbar\omega$$

population inversion condition
(Bernard-Duraffourg condition)

Optical Gain Spectra (with carriers)

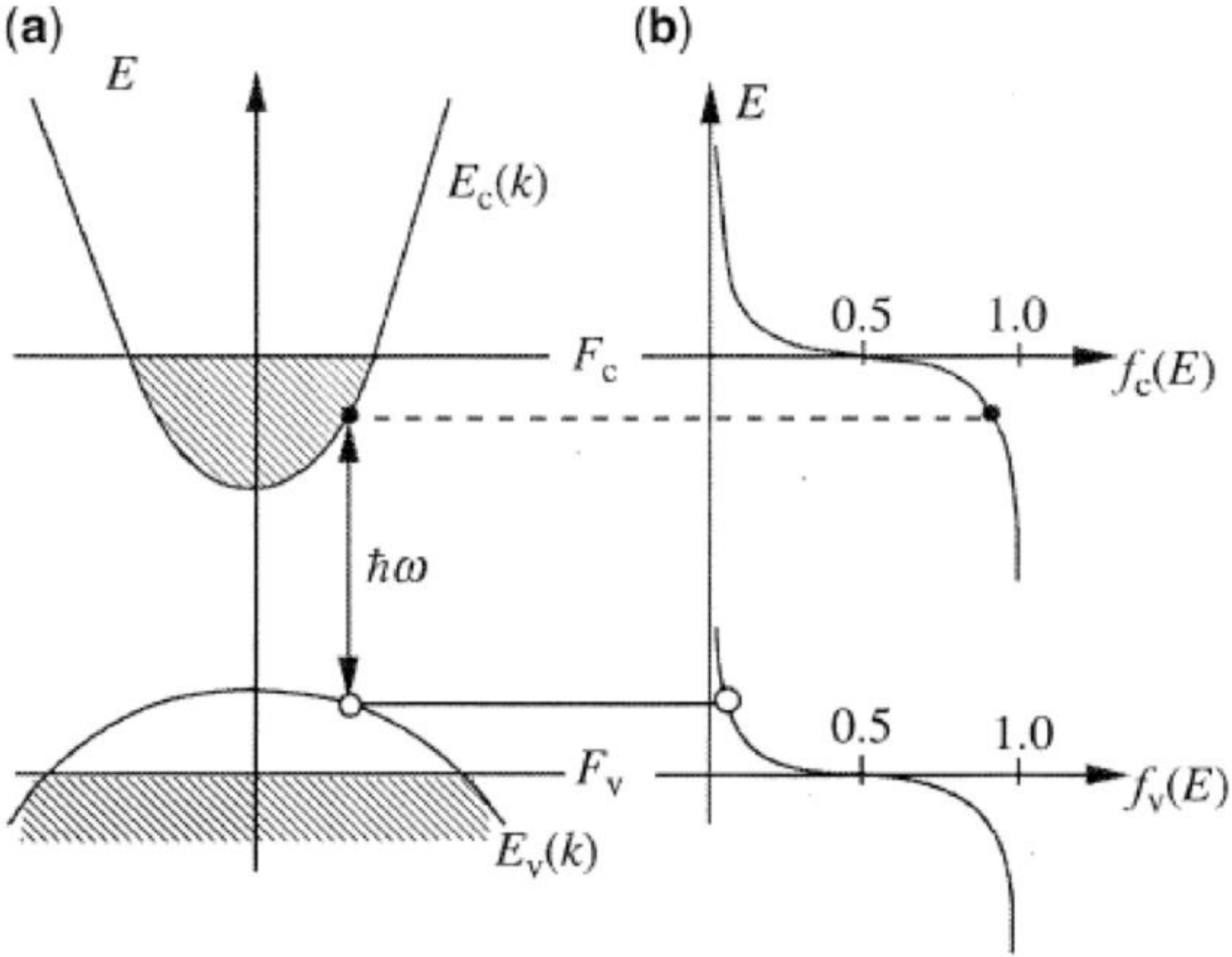
The magnitude of the loss (or gain) depends on wavelength. **If the separation of the quasi-Fermi levels is greater than the band gap, there is gain**.

- Photons with energies greater than the bandgap but less than the energy separation of the quasi-Fermi levels will experience gain
- Photons with energies greater than the separation of the quasi-Fermi levels will experience loss

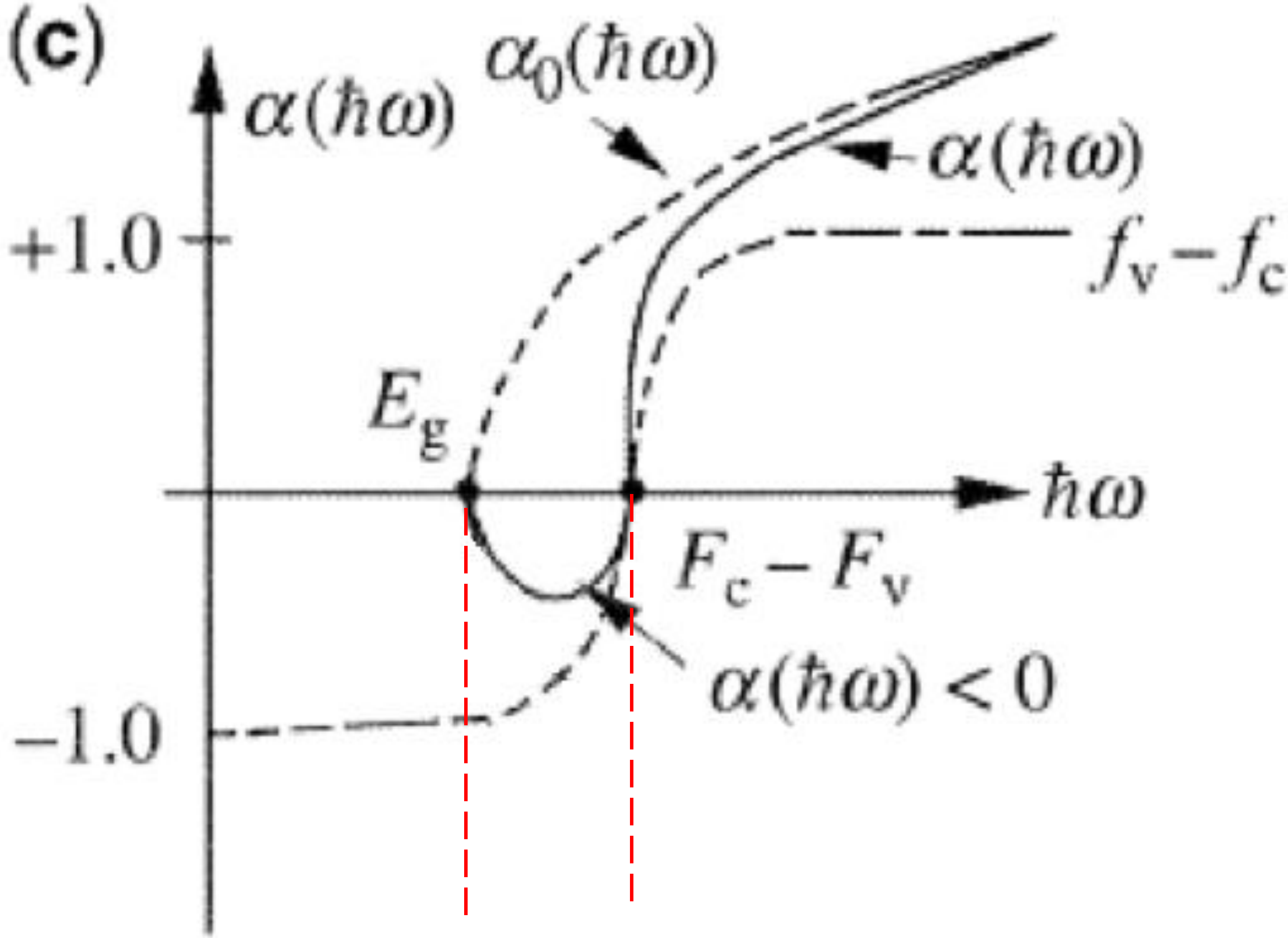
Gain condition $$F_C - F_V > \hbar\omega > E_C - E_V$$

$$E_g$$

Optical Gain Spectra (with carriers)



Optical Gain Spectra (with carriers)



Reading Assignments:

Section 9.3 of Chuang's book