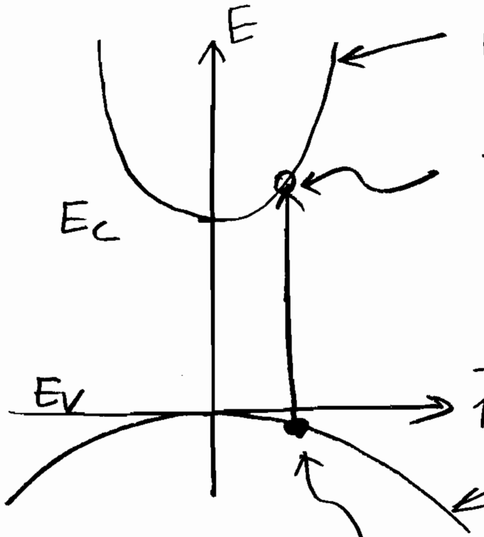
Interband Absorption and Gain



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

$$\psi_b(\vec{r}) = u_c(\vec{r})\cdot\frac{e^{i\vec{k}_c\cdot\vec{r}}}{\sqrt{V}}$$

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

$$\psi_a(\vec{r}) = u_v(\vec{r})\cdot\frac{e^{i\vec{k}_v\cdot\vec{r}}}{\sqrt{V}}$$

* Periodic Potential in crystals

$e^{i\vec{k}_c\cdot\vec{r}}$: Plane wave envelop function

$u_c(\vec{r})$: localized periodic wavefunction

$$u_c(\vec{r}+\vec{R}) = u_c(\vec{r})$$

$\vec{R}$ ↑ lattice vector

Matrix element

$$\vec{E} = \hat{e}\cdot E_0\cos(\vec{k}_{op}\cdot\vec{r} - \omega t) = \hat{e}\frac{E_0}{2}e^{i\vec{k}_{op}\cdot\vec{r} - i\omega t} + \hat{e}\frac{E_0}{2}e^{-i\vec{k}_{op}\cdot\vec{r} + i\omega t}$$

$$H'_{ba} = -\vec{E}\cdot\vec{\mu}_{ba} = -\langle b|\vec{E}\cdot(e\vec{r})|a\rangle$$

$$= -\frac{E_0}{2}\hat{e}\cdot\int\psi_b^*(\vec{r})\cdot e^{i\vec{k}_{op}\cdot\vec{r}}(e\vec{r})\,\psi_a(\vec{r})\,d\vec{r}$$

$$= -\frac{eE_0}{2}\hat{e}\cdot\int \underbrace{u_c^*(\vec{r})\, e^{-i\vec{k}_c\cdot\vec{r}} \cdot e^{i\vec{k}_{op}\cdot\vec{r}} \cdot \vec{r}\cdot u_v(\vec{r})\cdot e^{i\vec{k}_v\cdot\vec{r}}} \, d\vec{r}\,\frac{1}{V}$$

$$\underbrace{u_c^*(\vec{r})\,\vec{r}\,u_v(\vec{r})}_{\downarrow} \cdot \underbrace{e^{i(\vec{k}_{op}+\vec{k}_v-\vec{k}_c)\cdot\vec{r}}}_{\downarrow}$$

Fast varying function

Slowly varying envelop

In a unit cell, envelop ~ const

$$= -\frac{eE_0}{2}\,\hat{e}\underbrace{\int_\Omega}_{\substack{\uparrow \\ \text{unit cell}}} u_c^*(\vec{r})\,\vec{r}\,u_v(\vec{r})\frac{d\vec{r}}{\Omega}\cdot\underbrace{\int_V e^{i(\vec{k}_{op}+\vec{k}_v-\vec{k}_c)\cdot\vec{r}}\,d\vec{r}\cdot\frac{1}{V}}_{\delta_{\vec{k}_c,\,\vec{k}_v+\vec{k}_{op}}}$$

$$= -\frac{eE_0}{2}\,\hat{e}\cdot\vec{r}_{cv}\cdot\delta_{\vec{k}_c,\,\vec{k}_v+\vec{k}_{op}}$$

Fermi's Golden Rule:

$$W_{ab} = \frac{2\pi}{\hbar}|H'_{ba}|^2\cdot\delta(E_2-E_1-\hbar\omega)$$

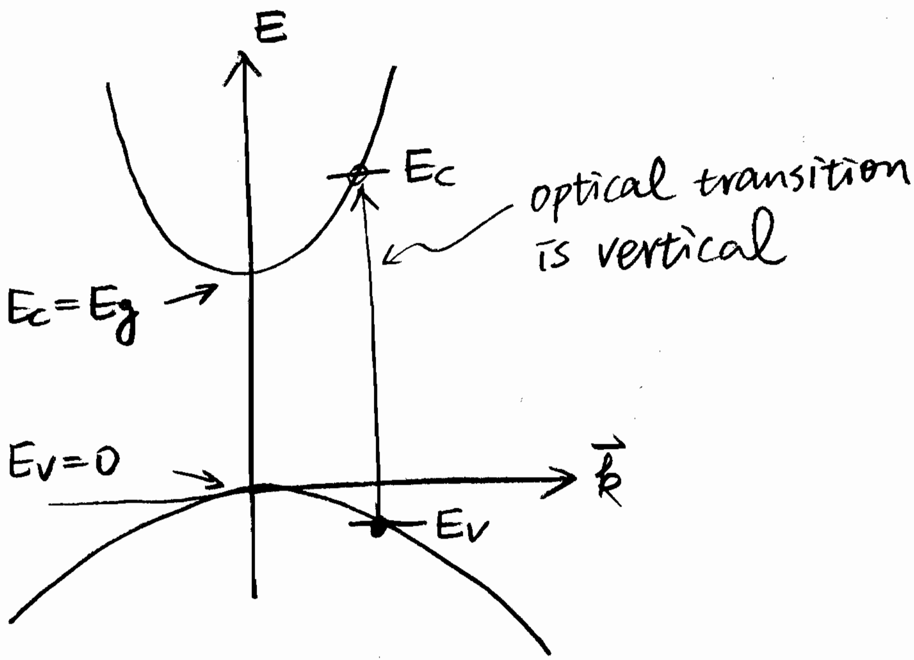
$$= \frac{2\pi}{\hbar}\cdot\frac{e^2E_0^2}{4}\,|\hat{e}\cdot\vec{r}_{cv}|^2\cdot\delta_{\vec{k}_c,\,\vec{k}_v+\vec{k}_{op}}\cdot\delta(E_2-E_1-\hbar\omega)$$

$\downarrow$ $\vec{k}_c = \vec{k}_v + \vec{k}_{op}$ conservation of momentum

$\downarrow$ $\hbar\omega = E_2 - E_1$ conservation of energy

$$k_{op} = \frac{2\pi}{\lambda} \ll \frac{2\pi}{a} \sim \vec{k}_{c,v}$$

$$\Rightarrow \vec{k}_c \cong \vec{k}_v$$



$$E_c = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$ (energy ref: valance band edge)

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

$$\hbar\omega = E_c - E_v = E_g + \frac{\hbar^2 k^2}{2m_e^*} + \frac{\hbar^2 k^2}{2m_h^*} = E_g + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$$

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

$$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$ m_r^*: reduced effective mass

Follow the same derivation for $\rho_e(E)$, electron DOS.

$$\frac{2}{(2\pi)^3}\int d\vec{k} = \frac{2}{(2\pi)^3}\int 4\pi k^2 dk = \int \rho_r(E)\,dE$$

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

Joint optical density of states (or "reduced" DOS)

Absorption Coefficient

$$\alpha(\hbar\omega) = \frac{\pi\omega}{n_r c \epsilon_0} \cdot \frac{2}{V} \underbrace{\sum_{k_a} \sum_{k_b}}_{\vec{k}_a = \vec{k}_b} \left| \hat{e} \cdot \vec{\mu}_{ab} \right|^2 \cdot \delta(E_b - E_a - \hbar\omega) \cdot (f_v - f_c)$$

$$\sum_{k} \longrightarrow \int \frac{d\vec{k}}{\left[\frac{(2\pi)^3}{V}\right]}$$

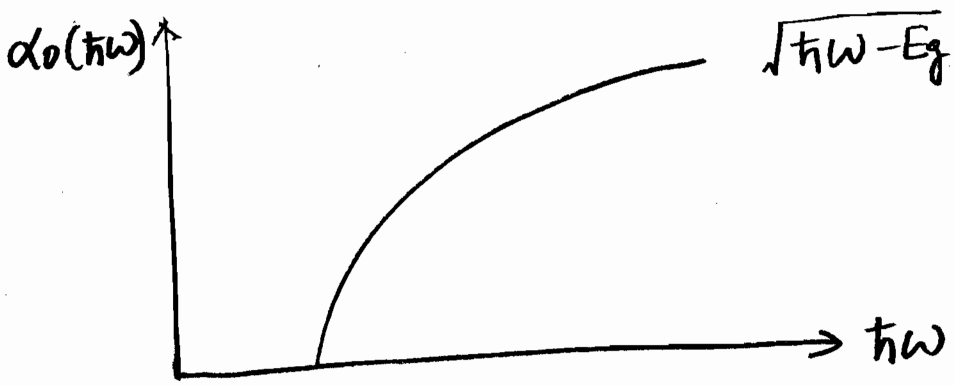
$\alpha(\hbar\omega) \rightarrow \alpha_0(\hbar\omega)$ when $f_v = 1$, $f_c = 0$

$$\alpha_0(\hbar\omega) = \frac{\pi\omega \left|\hat{e}\cdot\vec{\mu}_{cv}\right|^2}{n_r c \epsilon_0} \int \frac{2}{(2\pi)^3} d\vec{k} \cdot \delta\left(E_g + \frac{\hbar^2 k^2}{2m_r^*} - \hbar\omega\right)$$

$$= \frac{\pi\omega \left|\hat{e}\cdot\vec{\mu}_{cv}\right|^2}{n_r c \epsilon_0} \int \rho_r(E) \cdot \delta(E_g + E - \hbar\omega)\, dE$$

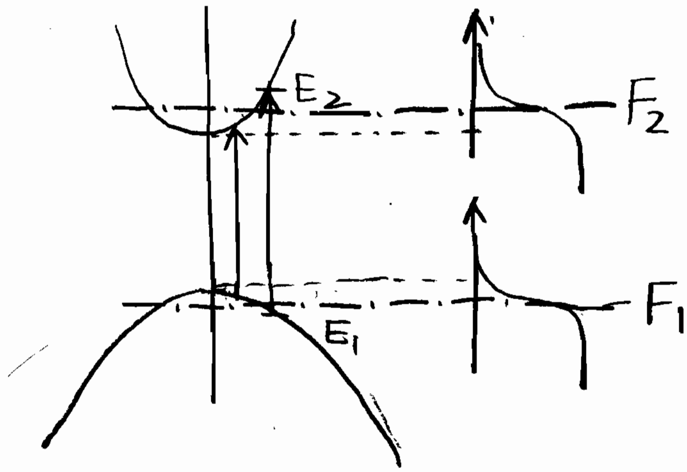
$$= \frac{\pi\omega \left|\hat{e}\cdot\vec{\mu}_{cv}\right|^2}{n_r c \epsilon_0} \cdot \rho_r(\hbar\omega)$$

$$\alpha_0(\hbar\omega) = \frac{\pi\omega}{n_r c \cdot \epsilon_0} \left|\hat{e}\cdot\vec{\mu}_{cv}\right|^2 \cdot \frac{1}{2\pi^2} \left(\frac{2m_r^*}{\hbar^2}\right)^{\frac{3}{2}} \cdot \sqrt{\hbar\omega - E_g}$$



spectral shape of $\alpha_0(\hbar\omega) \longrightarrow$ from joint optical DOS

$$\alpha(\hbar\omega) = \alpha_0(\hbar\omega)\left[f_v(E_1) - f_c(E_2)\right], \quad E_2 - E_1 = \hbar\omega$$



$$\begin{cases} E_2 - E_c \doteq \dfrac{\hbar^2 k^2}{2m_e^*} & \propto \dfrac{1}{m_e^*} \\ E_v - E_1 = \dfrac{\hbar^2 k^2}{2m_h^*} \end{cases}$$

$$E_2 - E_c = (\hbar\omega - E_g)\cdot \frac{\frac{1}{m_e^*}}{\frac{1}{m_e^*} + \frac{1}{m_h^*}} = (\hbar\omega - E_g)\cdot \frac{m_r^*}{m_e^*}$$

$$E_v - E_1 = (\hbar\omega - E_g)\cdot \frac{m_r^*}{m_h^*}$$

① If $E_1 > F_1$ $\Rightarrow$ $f_v(E_1) < \frac{1}{2}$ $\Rightarrow$ $f_v(E_1) - f_c(E_2) < 0$

$E_2 < F_2$ $\quad f_c(E_2) > \frac{1}{2}$

$\Rightarrow \underbrace{E_2 - E_1}_{\hbar\omega} < F_2 - F_1 = \Delta F$,

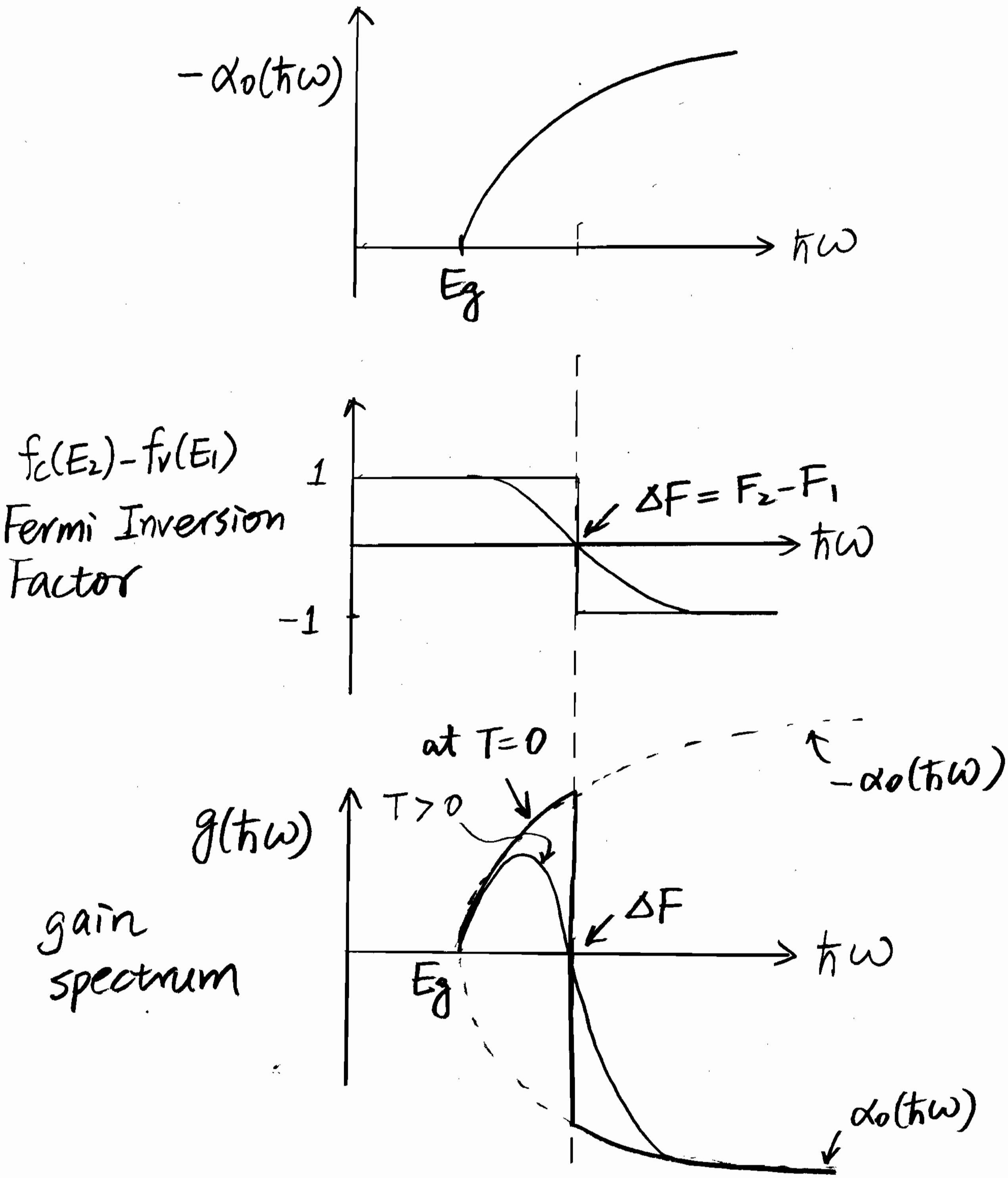
When $\hbar\omega < \Delta F \Rightarrow \alpha(\hbar\omega) < 0$, $g(\hbar\omega) = -\alpha(\hbar\omega) > 0$

$\Rightarrow$ gain!

② If $E_1 < F_1$ $\Rightarrow$ $f_c(E_1) > \frac{1}{2}$ $\Rightarrow$ $f_v(E_1) - f_c(E_2) > 0$

$E_2 > F_1$ $\quad f_v(E_2) < \frac{1}{2}$

When $\hbar\omega > \Delta F$, $\Rightarrow \alpha(\hbar\omega) > 0 \Rightarrow$ absorption.



Gain Bandwidth

$$\Delta F > \hbar\omega > E_g$$