Handout 06

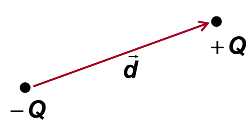
Dielectric Constant and Refractive Index of Semiconductors

In this lecture you will learn:

- Dielectric constant of solids
- Interband and Intraband contributions to the dielectric constant of solids
- Interband and Intraband contributions to the loss coefficient of solids
- Linear response functions
- Kramers-Kronig relations

Charge Dipole, Dipole Moment, and Polarization Density

A charge dipole consists of a negative and a positive charge separated by some distance:

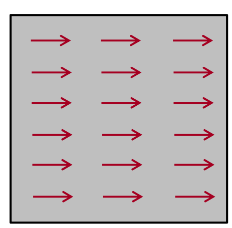


Dipole moment of a charge dipole is a vector $\vec{p}$ such that:

$$\vec{p} = |Q|\,\vec{d}$$

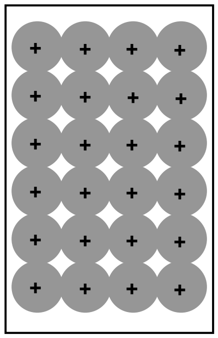
Polarization density vector $\vec{P}$ of a medium consisting of charge dipoles is the product of the number N of dipoles per unit volume (i.e. dipole density) and the strength of each dipole given by $\vec{p}$:

$$\vec{P} = N\vec{p} = N|Q|\vec{d}$$



Dielectric Constant of Materials

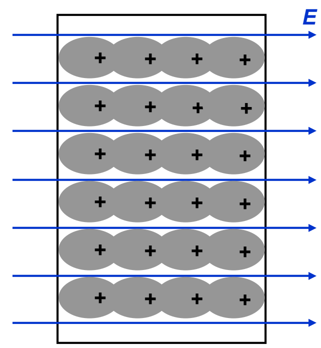
Dielectric Material (Insulator or Intrinsic Semiconductor)



+ +ve nucleus

-ve electron cloud (valence band and core electrons)

Dielectric in an E-field



Material gets polarized when placed in an electric field (i.e. develops charge dipoles) because the electron cloud shifts relative to the nuclei

$\vec{P} =$ Polarization density (# of dipoles per unit volume times the strength of one dipole)

$$\vec{P} = \varepsilon_o \chi_e \vec{E}$$

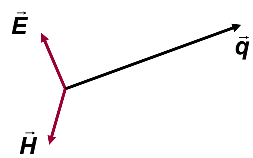
$$\vec{D} = \varepsilon_o \vec{E} + \vec{P} = \varepsilon \vec{E}$$

$$\varepsilon = \varepsilon_o (1 + \chi_e)$$

High Frequency Dielectric Constant of Solids

Consider a sinusoidal E&M wave of frequency ω propagating in a solid:

$$\vec{E}(\vec{r},t) = \hat{n}\, E_o \cos(\vec{q}\,.\,\vec{r} - \omega\, t) = \mathrm{Re}\left\{ \vec{E}(\vec{r},\omega)\, e^{-i\,\omega\, t} \right\}$$



Where the electric field "phasor" is:

$$\vec{E}(\vec{r},\omega) = \hat{n}\, E_o\, e^{i\,\vec{q}\,.\,\vec{r}}$$

Similarly, the magnetic field phasor is:

$$\vec{H}(\vec{r},\omega) = (\hat{q} \times \hat{n})\, H_o\, e^{i\,\vec{q}\,.\,\vec{r}}$$

And the two field are related by the two Maxwell equations:

$$\nabla \times \vec{E}(\vec{r},\omega) = i\omega\, \mu_o \vec{H}(\vec{r},\omega) \qquad \text{Faraday's Law}$$

$$\nabla \times \vec{H}(\vec{r},\omega) = -i\omega\, \varepsilon(\omega)\, \vec{E}(\vec{r},\omega) \qquad \text{Ampere's Law}$$

These two equations together give the dispersion relation of the E&M wave:

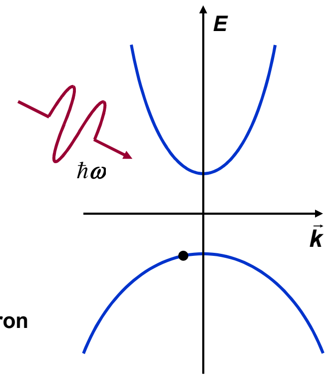
$$\omega = \frac{|\vec{q}|}{\sqrt{\varepsilon(\omega)\, \mu_o}} = q \frac{c}{\sqrt{\varepsilon(\omega)/\varepsilon_o}} = q \frac{c}{n(\omega)}$$

Strategy to Calculate the Dielectric Constant of Materials

1) Start with the Hamiltonian describing the interaction of the electrons with the electromagnetic field:

$$\hat{H} = \hat{H}_o + \frac{q A_o \left[e^{i\vec{q}\,.\,\hat{\vec{r}} - i\,\omega\, t} + e^{-i\vec{q}\,.\,\hat{\vec{r}} + i\,\omega\, t} \right]}{2m} \hat{\vec{P}} \,.\, \hat{n}$$

$$\hat{H}_o \left| \psi_{n,\vec{k}} \right\rangle = E_n\left(\vec{k}\right) \left| \psi_{n,\vec{k}} \right\rangle$$



2) Find out how the electron wavefunctions (i.e. Bloch functions) get modified using standard first order perturbation theory:

$$\left| \psi_{n,\vec{k}} \right\rangle_{new} = \left| \psi_{n,\vec{k}} \right\rangle + \sum_{m} \sum_{\vec{k}'} c_{m,\vec{k}'}(t) \left| \psi_{m,\vec{k}'} \right\rangle$$

3) From the modified wavefunctions, calculate the electron charge density, and then the dipole density

The above procedure, although doable, is a little complicated and we will use an alternate approach!

Refractive Index of Solids

The refractive index of a material is defined as: $n(\omega) = \sqrt{\dfrac{\varepsilon(\omega)}{\varepsilon_o}}$

The wave dispersion relation is then: $\omega = q \dfrac{c}{n(\omega)}$

And the electric field phasor can be written as:

$$\vec{E}(\vec{r},\omega) = \hat{n}\, E_o\, e^{i\,\vec{q}\,.\,\vec{r}} = \hat{n}\, E_o\, e^{i \frac{\omega\, n(\omega)}{c} \hat{q}\,.\,\vec{r}}$$

The refractive index usually has real and imaginary parts:

$$n(\omega) = n'(\omega) + i\, n''(\omega)$$

The electric field phasor is then:

$$\vec{E}(\vec{r},\omega) = \hat{n}\, E_o\, e^{i \frac{\omega\, n'(\omega)}{c} \hat{q}\,.\,\vec{r}} \underbrace{e^{-\frac{\omega\, n''(\omega)}{c} \hat{q}\,.\,\vec{r}}}$$

The imaginary part of the index describes wave decay (or wave amplification if gain is present)

Imaginary Part of the Refractive Index and the Loss Coefficient

We have already seen that stimulated absorption results in a wave to decay in a medium (optical loss):

$$\vec{E}(\vec{r},\omega) \propto e^{-\frac{\alpha(\omega)}{2}\hat{q}\,.\,\vec{r}}$$

Where:

$$\alpha(\omega) = \frac{\hbar\omega\,(R_{\uparrow} - R_{\downarrow})}{P}$$

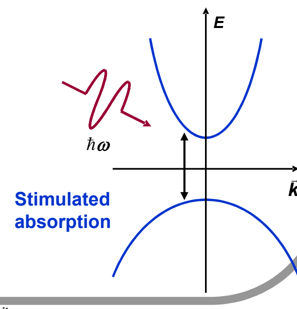
$$= \left(\frac{q}{m}\right)^2 \frac{\pi}{\varepsilon_o n'\omega\, c} \left\langle \left|\vec{P}_{cv}\,.\,\hat{n}\right|^2 \right\rangle \; 2\times \int_{\text{FBZ}} \frac{d^3\vec{k}}{(2\pi)^3} \left[f_v(\vec{k}) - f_c(\vec{k})\right] \delta\left(E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega\right)$$

But we also have:

$$\vec{E}(\vec{r},\omega) \;\propto\; e^{-\frac{\omega\, n''(\omega)}{c}\hat{q}\,.\,\vec{r}}$$

This means the imaginary part of the refractive index is:

$$\boxed{n''(\omega) = \frac{c}{\omega}\frac{\alpha(\omega)}{2}}$$



Imaginary Part of the Refractive Index and the Loss Coefficient

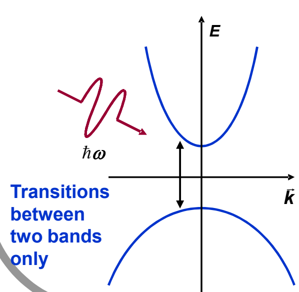
Transitions between just two bands:

$$\alpha(\omega) = \left(\frac{q}{m}\right)^2 \frac{\pi}{\varepsilon_o n'\omega\, c} \; 2\times \int_{\text{FBZ}} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{cv}\,.\,\hat{n}\right|^2 \left[f_v(\vec{k}) - f_c(\vec{k})\right] \delta\left(E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega\right)$$

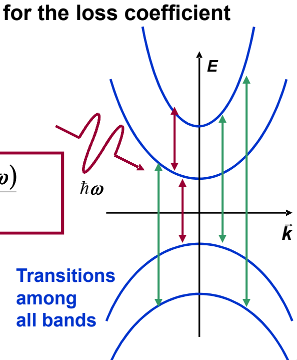
Transitions among all bands:

$$\alpha(\omega) = \left(\frac{q}{m}\right)^2 \frac{\pi}{\varepsilon_o n'\omega\, c} \sum_{r,s} 2\times \int_{\text{FBZ}} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{rs}\,.\,\hat{n}\right|^2 \left[f_s(\vec{k}) - f_r(\vec{k})\right] \delta\left(E_r(\vec{k}) - E_s(\vec{k}) - \hbar\omega\right)$$

The above is a more general and complete expression for the loss coefficient



$$\boxed{n''(\omega) = \frac{c}{\omega}\frac{\alpha(\omega)}{2}}$$



High Frequency Dielectric Constant of Solids: Imaginary Part

The refractive index of a material is defined as: $n(\omega)=\sqrt{\frac{\varepsilon(\omega)}{\varepsilon_o}}$

Therefore, using the fact that: $|n''(\omega)| << |n'(\omega)|$

$$\varepsilon(\omega)=\varepsilon_o\, n^2(\omega)=\varepsilon_o\,[\,n'(\omega)+in''(\omega)\,]^2 \approx \varepsilon_o\,[\,n'(\omega)\,]^2+i2\,\varepsilon_o n'(\omega)n''(\omega)$$
$$\Rightarrow \varepsilon'(\omega)+i\varepsilon''(\omega)=\varepsilon_o\,[\,n'(\omega)\,]^2+i2\,\varepsilon_o n'(\omega)n''(\omega)$$

This implies:

$$\boxed{\varepsilon''(\omega)\approx 2\varepsilon_o n'(\omega)n''(\omega)} \quad \text{and} \quad \boxed{\varepsilon'(\omega)\approx \varepsilon_o[\,n'(\omega)\,]^2}$$

$$\Rightarrow \varepsilon''(\omega)\approx \frac{\varepsilon_o n'(\omega)c}{\omega}\alpha(\omega)$$

Using the expression for the absorption coefficient we get:

$$\varepsilon''(\omega)=\left(\frac{q}{m}\right)^2\frac{\pi}{\omega^2}\sum_{r,s}\;2\times\int_{\text{FBZ}}\frac{d^3\vec{k}}{(2\pi)^3}\left|\vec{P}_{rs}\cdot\hat{n}\right|^2\left[f_s(\vec{k})-f_r(\vec{k})\right]\delta\left(E_r(\vec{k})-E_s(\vec{k})-\hbar\omega\right)$$

Question: What is the real part of the dielectric constant?

Linear Response Functions

Linear Response Functions:

In a linear time invariant (LTI) system, the stimulus phasor $S(\omega)$ is related to the response phasor $R(\omega)$ by a linear response function $\gamma(\omega)$:

$$R(\omega)=\gamma(\omega)\,S(\omega) \qquad \left\{\;\gamma(\omega)=\gamma'(\omega)+i\,\gamma''(\omega)\right.$$

The linear system must satisfy the following two properties:

i) It must be causal (system cannot respond before the stimulus is applied)
ii) A real stimulus $S(t)$ must result in a real response $R(t)$ (with no imaginary component)

The second condition gives:

$$\gamma(-\omega)=\gamma^*(\omega) \;\Rightarrow\; \gamma'(-\omega)=\gamma'(\omega) \quad \text{and} \quad \gamma''(-\omega)=-\gamma''(\omega)$$

Most responses of solids are expressed in terms of linear response functions. Examples include:

Conductivity: $\sigma(\omega) \longrightarrow \vec{J}(\vec{r},\omega)=\sigma(\omega)\,\vec{E}(\vec{r},\omega)$
Dielectric Constant: $\varepsilon(\omega) \longrightarrow \vec{D}(\vec{r},\omega)=\varepsilon(\omega)\,E(\vec{r},\omega)$

Linear Response Functions and Kramers-Kronig Relations

The two conditions, listed on previous slide, dictate that the real and imaginary parts of any response function cannot be independent – they must be RELATED!

$$R(\omega)=\gamma(\omega)\,S(\omega) \qquad \left\{ \gamma(\omega)=\gamma'(\omega)+i\,\gamma''(\omega) \right.$$

This relationship between the real and the imaginary parts of the response functions is captured by the Kramers-Kronig relations:

$$\boxed{\begin{aligned} \gamma''(\omega) &= 4\int_0^{\infty}\frac{d\omega'}{2\pi}\,\left[\gamma'(\omega')-\gamma'(\infty)\right]\frac{\omega}{\omega^2-\omega'^2} &\longrightarrow \quad (1) \\ \gamma'(\omega)-\gamma'(\infty) &= -4\int_0^{\infty}\frac{d\omega'}{2\pi}\,\gamma''(\omega')\frac{\omega'}{\omega^2-\omega'^2} &\longrightarrow \quad (2) \end{aligned}}$$

- **If one knows the real part for all frequencies, then one can find the imaginary part using Kramers-Kronig relations**

- **Conversely, if one knows the imaginary part for all frequencies, then one can find the real part using Kramers-Kronig relations**

PROOF OF KRAMERS-KRONIG RELATIONS GIVEN IN APPENDIX

High Frequency Dielectric Constant of Solids: Real Part

We have:

$$\boxed{\varepsilon''(\omega)=\left(\frac{q}{m}\right)^2\frac{\pi}{\omega^2}\sum_{r,s}2\times\int_{FBZ}\frac{d^3\vec{k}}{(2\pi)^3}\left|\vec{P}_{rs}\cdot\hat{n}\right|^2\left[f_s(\vec{k})-f_r(\vec{k})\right]\delta\left(E_r(\vec{k})-E_s(\vec{k})-\hbar\omega\right)}$$

And from the Kramers-Kronig relations we know:

$$\varepsilon'(\omega)-\varepsilon'(\infty)=-4\int_0^{\infty}\frac{d\omega'}{2\pi}\,\varepsilon''(\omega')\frac{\omega'}{\omega^2-\omega'^2} \longrightarrow \left\{ \varepsilon'(\infty)=\varepsilon_o \right.$$

$$\Rightarrow \varepsilon'(\omega)-\varepsilon_o=-2\left(\frac{q}{m}\right)^2\hbar^2\sum_{r,s}2\times\int_{FBZ}\frac{d^3\vec{k}}{(2\pi)^3}\left|\vec{P}_{rs}\cdot\hat{n}\right|^2\left[f_s(\vec{k})-f_r(\vec{k})\right]\frac{\left(E_r(\vec{k})-E_s(\vec{k})\right)^{-1}}{\omega^2-\left(E_r(\vec{k})-E_s(\vec{k})\right)^2}$$

$$\boxed{\Rightarrow \varepsilon'(\omega)=\varepsilon_o-2\left(\frac{q}{m}\right)^2\hbar^2\sum_{r,s}2\times\int_{FBZ}\frac{d^3\vec{k}}{(2\pi)^3}\left|\vec{P}_{rs}\cdot\hat{n}\right|^2\left[f_s(\vec{k})-f_r(\vec{k})\right]\frac{\left(E_r(\vec{k})-E_s(\vec{k})\right)^{-1}}{\omega^2-\left(E_r(\vec{k})-E_s(\vec{k})\right)^2}}$$

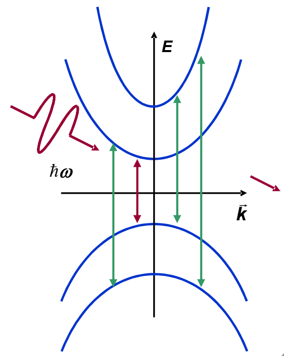
High Frequency Dielectric Constant of Solids

$$\varepsilon'(\omega) = \varepsilon_o - 2\left(\frac{q}{m}\right)^2 \hbar^2 \sum_{r,s} 2\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{rs}\,.\,\hat{n}\right|^2 \left[f_s(\vec{k}) - f_r(\vec{k})\right] \frac{\left(E_r(\vec{k})-E_s(\vec{k})\right)^{-1}}{\omega^2 - \left(E_r(\vec{k})-E_s(\vec{k})\right)^2}$$

$$\varepsilon''(\omega) = \left(\frac{q}{m}\right)^2 \frac{\pi}{\omega^2} \sum_{r,s} 2\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{rs}\,.\,\hat{n}\right|^2 \left[f_s(\vec{k}) - f_r(\vec{k})\right] \delta\left(E_r(\vec{k}) - E_s(\vec{k}) - \hbar\omega\right)$$

- The low frequency dielectric constant would also include contributions from the lattice (phonons) in polar materials (like GaAs, NaCl)

- The most important contributions to the dielectric constant will come from those two bands whose energy separation is close to the frequency ω and where the lower band is full and the top band is empty

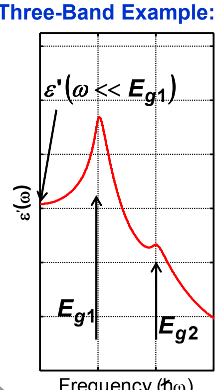


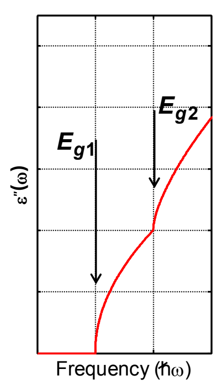
Bandgaps and the High Frequency Dielectric Constant

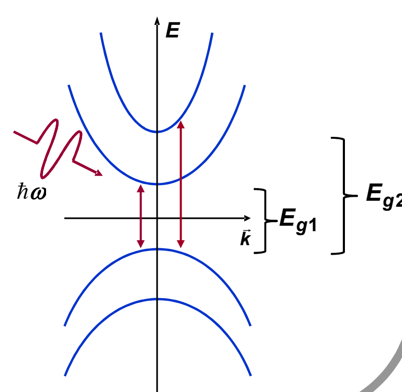
$$\varepsilon'(\omega) = \varepsilon_o - 2\left(\frac{q}{m}\right)^2 \hbar^2 \sum_{r,s} 2\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{rs}\,.\,\hat{n}\right|^2 \left[f_s(\vec{k}) - f_r(\vec{k})\right] \frac{\left(E_r(\vec{k})-E_s(\vec{k})\right)^{-1}}{\omega^2 - \left(E_r(\vec{k})-E_s(\vec{k})\right)^2}$$

$$\varepsilon''(\omega) = \left(\frac{q}{m}\right)^2 \frac{\pi}{\omega^2} \sum_{r,s} 2\times \int_{FBZ} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{rs}\,.\,\hat{n}\right|^2 \left[f_s(\vec{k}) - f_r(\vec{k})\right] \delta\left(E_r(\vec{k}) - E_s(\vec{k}) - \hbar\omega\right)$$

A Three-Band Example:



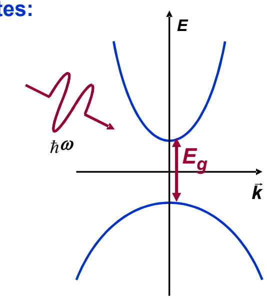




Bandgaps and the High Frequency Dielectric Constant

$$\varepsilon'(\omega) = \varepsilon_o - 2\left(\frac{q}{m}\right)^2 \hbar^2 \left\langle \left|\vec{P}_{cv} \cdot \hat{n}\right|^2 \right\rangle \; 2\times \int_{\text{FBZ}} \frac{d^3\vec{k}}{(2\pi)^3} \left[f_v(\vec{k}) - f_c(\vec{k})\right] \frac{\left(E_c(\vec{k}) - E_v(\vec{k})\right)^{-1}}{\omega^2 - \left(E_c(\vec{k}) - E_v(\vec{k})\right)^2}$$

Include just two bands and make some very rough estimates:



Suppose : $\hbar\omega << E_g$

$$E_c(\vec{k}) - E_v(\vec{k}) \approx E_g$$

$$f_v(\vec{k}) \approx 1 \qquad f_c(\vec{k}) \approx 0$$

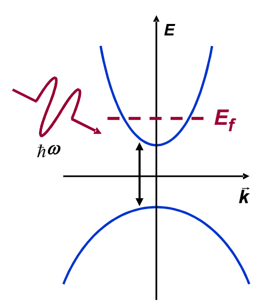
$$\Rightarrow \varepsilon'(\omega) \approx \varepsilon_o + 2\left(\frac{q}{m}\right)^2 \hbar^2 \frac{\left\langle \left|\vec{P}_{cv} \cdot \hat{n}\right|^2 \right\rangle}{E_g^3} \; 2\times \int_{\text{FBZ}} \frac{d^3\vec{k}}{(2\pi)^3} \; f_v(\vec{k})$$

$$\approx \varepsilon_o + 2\left(\frac{q}{m}\right)^2 \hbar^2 \frac{\left\langle \left|\vec{P}_{cv} \cdot \hat{n}\right|^2 \right\rangle}{E_g^3} \; n_v$$

⇒ Materials with larger bandgaps will have smaller real part of dielectric constants (and, therefore, smaller real part of refractive indices)

High Frequency Dielectric Constant: Case of Non-Zero Conductivity

We have obtained an expression for the dielectric constant that incorporated interband optical processes



What if the material also contained large densities of electrons or holes or both (i.e. what if the material was doped and conductive)?

Go back to Maxwell equations:

$$\nabla \times \vec{E}(\vec{r},\omega) = i\omega\,\mu_o \vec{H}(\vec{r},\omega) \qquad \text{Faraday's Law}$$

$$\nabla \times \vec{H}(\vec{r},\omega) = \vec{J}(\omega) - i\omega\,\varepsilon(\omega)\,\vec{E}(\vec{r},\omega) \qquad \text{Ampere's Law}$$

New term (current density due to electrons or holes or both)

$$\vec{J}(\omega) = \sigma(\omega)\,\vec{E}(\omega)$$

$$\Rightarrow \nabla \times \vec{H}(\vec{r},\omega) = \sigma(\omega)\,\vec{E}(\omega) - i\omega\,\varepsilon(\omega)\,\vec{E}(\vec{r},\omega)$$

$$\Rightarrow \nabla \times \vec{H}(\vec{r},\omega) = -i\omega\,\varepsilon_{\text{total}}(\omega)\,\vec{E}(\vec{r},\omega)$$

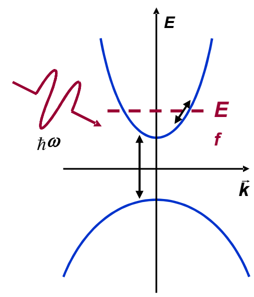
Where:

$$\varepsilon_{\text{total}}(\omega) = \varepsilon(\omega) + i\,\frac{\sigma(\omega)}{\omega}$$

High Frequency Dielectric Constant: Drude Model for Conductivity

We have:

$$\varepsilon_{\text{total}}(\omega) = \varepsilon(\omega) + i\,\frac{\sigma(\omega)}{\omega}$$



Drude model for the frequency dependent conductivity:

The equation for the electron velocity is (assuming parabolic/isotropic bands in 3D):

$$m_e \frac{d\vec{v}}{dt} + \frac{m_e \vec{v}}{\tau_e} = -q\,\vec{E}$$

In phasor notation (assuming a sinusoidal electric field):

$$\vec{v}(\omega) = -\frac{q\tau_e / m_e}{1 - i\omega\tau_e}\,\vec{E}(\omega)$$

The current density is:

$$\vec{J}(\omega) = n\,(-q)\,\vec{v}(\omega) = \sigma(\omega)\,\vec{E}(\omega)$$

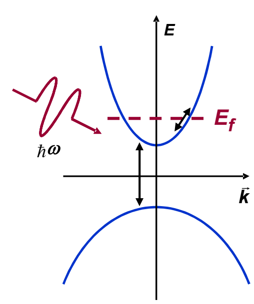
Where:

$$\sigma(\omega) = \frac{n\,q^2\tau_e / m_e}{1 - i\omega\tau_e} \qquad \text{(Drude model)}$$

High Frequency Dielectric Constant : Non-Zero Conductivity

Assuming non-zero densities for both electrons and holes the total conductivity becomes:

$$\sigma(\omega) = \frac{n\,q^2\tau_e / m_e}{1 - i\omega\tau_e} + \frac{p\,q^2\tau_h / m_h}{1 - i\omega\tau_h}$$



We have:

$$\varepsilon_{\text{total}}(\omega) = \varepsilon(\omega) + i\,\frac{\sigma(\omega)}{\omega}$$

Therefore:

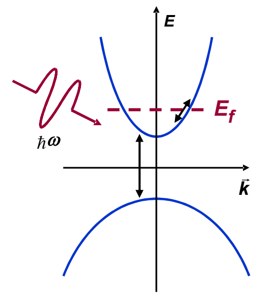
$$\boxed{\varepsilon_{\text{total}}(\omega) = \underbrace{\varepsilon(\omega)}_{\text{Interband optical processes}} + \underbrace{i\,\frac{nq^2\tau_e / m_e}{\omega(1 - i\omega\tau_e)} + i\,\frac{pq^2\tau_h / m_h}{\omega(1 - i\omega\tau_h)}}_{\text{Intraband optical processes}}}$$

The Plasma Frequency

Suppose we have a metal or a n-doped semiconductor for which:

$$\omega\tau >> 1$$

$$\hbar\omega << E_g$$



Then we have:

$$\varepsilon_{\text{total}}(\omega) = \varepsilon(\omega) + i\frac{nq^2\tau_e/m_e}{\omega(1-i\omega\tau_e)} + \cancelto{0}{i\frac{pq^2\tau_h/m_h}{\omega(1-i\omega\tau_h)}}$$

$$= \varepsilon + i\frac{nq^2\tau_e/m_e}{\omega(1-i\omega\tau_e)} \approx \varepsilon - \frac{nq^2/m_e}{\omega^2}$$

$$= \varepsilon\left(1-\frac{\omega_p^2}{\omega^2}\right)$$

Where the plasma frequency is defined as:

$$\omega_p = \sqrt{\frac{nq^2}{\varepsilon\, m_e}}$$

For metals:

$\omega_p/2\pi \sim 4\times10^{15}$ Hz (UV-blue light frequency)

For semiconductors:

$\omega_p/2\pi \sim 10^{11} - 10^{13}$ Hz (Terahertz frequency)

The Complete Absorption Coefficient

Now that we have the complete dielectric constant, we can find the complete absorption coefficient:

$$\varepsilon_{\text{total}}(\omega) = \varepsilon_{\text{inter}}(\omega) + \varepsilon_{\text{intra}}(\omega) = \underbrace{\varepsilon_{\text{inter}}(\omega)}_{\text{Interband optical processes}} + \underbrace{i\frac{nq^2\tau/m_e}{\omega(1-i\omega\tau_e)} + i\frac{pq^2\tau/m_h}{\omega(1-i\omega\tau_h)}}_{\text{Intraband optical processes}}$$

$$\varepsilon''_{\text{total}}(\omega) \approx 2\varepsilon_o n'(\omega) n''(\omega) = \frac{\varepsilon_o c n'(\omega)}{\omega}\alpha(\omega)$$

$$\Rightarrow \varepsilon''_{\text{inter}}(\omega) + \frac{nq^2\tau_e/m_e}{\omega\left(1+\omega^2\tau_e^2\right)} + \frac{pq^2\tau_h/m_h}{\omega\left(1+\omega^2\tau_h^2\right)} = \frac{\varepsilon_o c n'(\omega)}{\omega}\alpha(\omega)$$

Interband optical absorption

$$\alpha(\omega) = \left(\frac{q}{m}\right)^2 \frac{\pi}{\varepsilon_o n'(\omega)\omega c} \sum_{r,s} 2\times\int_{\text{FBZ}} \frac{d^3\vec{k}}{(2\pi)^3} \left|\vec{P}_{rs}\cdot\hat{n}\right|^2 \left[f_s(\vec{k}) - f_r(\vec{k})\right]\delta\left(E_r(\vec{k}) - E_s(\vec{k}) - \hbar\omega\right)$$

$$+ \frac{1}{\varepsilon_o c n'(\omega)}\left[\frac{nq^2\tau_e/m_e}{\left(1+\omega^2\tau_e^2\right)} + \frac{pq^2\tau_h/m_h}{\left(1+\omega^2\tau_h^2\right)}\right]$$

Intraband optical absorption

APPENDIX: Kramers-Kronig Relations (Proof)

In a linear time invariant (LTI) system, the stimulus phasor $S(\omega)$ is related to the response phasor $R(\omega)$ by:

$$R(\omega) = \gamma(\omega)\, S(\omega)$$

The linear response function is $\gamma(\omega)$: $\quad \gamma(\omega) = \gamma'(\omega) + i\,\gamma''(\omega)$

Reality:

Real inputs must result in a real response. This condition gives:

$$\gamma(-\omega) = \gamma^*(\omega) \quad \Rightarrow \quad \gamma'(-\omega) = \gamma'(\omega) \quad \text{and} \quad \gamma''(-\omega) = -\gamma''(\omega)$$

Causality:

Inverse FT gives: $\quad R(t) = \int_{-\infty}^{\infty} dt'\; \gamma(t-t')\, S(t') \qquad \left\{ \gamma(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \gamma(\omega)\, e^{-i\,\omega\,(t-t')} \right.$

Causality implies that the system cannot exhibit response to an input before the input occurs:

$$\gamma(t-t') = 0 \qquad \text{for} \quad t < t'$$

which gives:

$$R(t) = \int_{-\infty}^{t} dt'\; \gamma(t-t')\, S(t')$$

Infinite Frequency Response:

No physical system can respond at infinite frequencies, so:

$$\gamma(\omega \to \infty) = 0$$

Kramers-Kronig Relations (Proof)

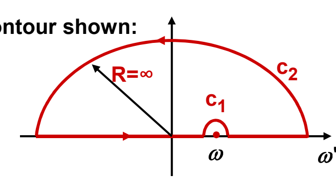
The causality condition is:

$$\gamma(t) = 0 \qquad \text{for} \quad t < 0$$

The function $\gamma(\omega)$, when considered as an analytic function in the complex plane, cannot have any pole in the upper half of the complex plane for the causality condition to hold

Consider the following contour integral over the contour shown:

$$\oint \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'}$$



Since there are no poles in the upper half plane, the closed contour contains no poles, and the contour integral must be zero

$$\oint \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'} = 0$$

$$\Rightarrow \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'} + \int_{c_1} \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'} + \cancelto{0}{\int_{c_2} \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'}} = 0$$

$$\Rightarrow \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'} + \frac{i}{2}\gamma(\omega) = 0$$

Kramers-Kronig Relations (Proof)

$$\Rightarrow \quad \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\gamma(\omega')}{\omega - \omega'} = -\frac{i}{2}\gamma(\omega)$$

Matching the real and imaginary parts on both sides gives:

$$\gamma'(\omega) = -2\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\gamma''(\omega')}{\omega - \omega'} = -4\int_{0}^{\infty} \frac{d\omega'}{2\pi}\, \gamma''(\omega')\, \frac{\omega'}{\omega^2 - \omega'^2}$$

$$\gamma''(\omega) = 2\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\gamma'(\omega')}{\omega - \omega'} = 4\int_{0}^{\infty} \frac{d\omega'}{2\pi}\, \gamma'(\omega')\, \frac{\omega}{\omega^2 - \omega'^2}$$

Where the following relations have been used to get the second integrals:

$$\gamma'(-\omega) = \gamma'(\omega) \quad \text{and} \quad \gamma''(-\omega) = -\gamma''(\omega)$$

In cases where the real part of $\gamma(\omega)$ may not be zero at infinite frequencies, as it happened in the case of the dielectric constant, we just repeat the entire procedure from the beginning with $\gamma(\omega) - \gamma'(\infty)$ instead of $\gamma(\omega)$ to get:

$$\gamma''(\omega) = 4\int_{0}^{\infty} \frac{d\omega'}{2\pi}\, [\gamma'(\omega') - \gamma'(\infty)]\, \frac{\omega}{\omega^2 - \omega'^2}$$

$$\gamma'(\omega) - \gamma'(\infty) = -4\int_{0}^{\infty} \frac{d\omega'}{2\pi}\, \gamma''(\omega')\, \frac{\omega'}{\omega^2 - \omega'^2}$$