Maxwell's equations

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}$$
$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho$$
$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c} \vec{J} + \frac{1}{c} \frac{\partial \vec{E}}{\partial t}$$
$$\vec{\nabla} \cdot \vec{B} = 0$$

In a medium it is convenient to explicitly introduce induced charges and currents

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} \qquad \qquad \vec{D} = \vec{E} + 4\pi \vec{P} \\ \vec{\nabla} \cdot \vec{D} = 4\pi\rho \\ \vec{\nabla} \times \vec{H} = \frac{4\pi}{c} \left( \vec{J} + \vec{J}_{ext} \right) + \frac{1}{c} \frac{\partial \vec{D}}{\partial t} \\ \vec{\nabla} \cdot \vec{B} = 0 \qquad \qquad \vec{\nabla} \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} \\ \vec{\nabla} \cdot \vec{D} = 0 \\ \vec{\nabla} \times \vec{H} = \frac{4\pi}{c} \vec{J} + \frac{1}{c} \frac{\partial \vec{D}}{\partial t} \\ \vec{\nabla} \cdot \vec{D} = 0 \\ \vec{\nabla} \times \vec{H} = \frac{4\pi}{c} \vec{J} + \frac{1}{c} \frac{\partial \vec{D}}{\partial t} \\ \vec{\nabla} \cdot \vec{B} = 0 \end{cases}$$

In a medium it is convenient to explicitly introduce induced charges and currents

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$$\vec{\nabla} \cdot \vec{D} = 4\pi\rho$$
  

$$\vec{\nabla} \times \vec{H} = \frac{4\pi}{c} \left( \vec{J} + \vec{J}_{ext} \right) + \frac{1}{c} \frac{\partial \vec{D}}{\partial t}$$
  

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In a medium it is convenient to explicitly introduce induced charges and currents



In a medium it is convenient to explicitly introduce induced charges and currents



 $\vec{P}$ ,  $\vec{M}$  and  $\vec{J}$  represent the response of the medium to the electromagnetic field If we assume the response is linear, we can write:

$$\vec{P} = \alpha \vec{E}$$
  
 $\vec{J} = \sigma E$   
 $\vec{M} = \chi \vec{B}$ 

where  $\alpha,\sigma$  e  $\chi$  are the polarizability, conductivity and susceptibility tensors, respectively.

For optical frequencies we can neglect susceptibility ( $\chi$ =0) so that  $\vec{B} = \vec{H}$ 

By introducing into the fourth of Maxwell's equations we get:

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c} \left( \sigma \vec{E} + \alpha \frac{\partial \vec{E}}{\partial t} \right) + \frac{1}{c} \frac{\partial \vec{E}}{\partial t}$$

Conductivity ( $\sigma$ ) and polarizability ( $\alpha$ ) both contain the material response giving rise to two induced currents, a polarization current:

$$\vec{J}_{pol} = \alpha \frac{\partial \vec{E}}{\partial t}$$

and a ohmic current

$$\vec{J}_{ohm} = \sigma \vec{E}$$

The absorbed power per unit volume is given by:

$$\left(\frac{\partial W}{\partial t}\right)_{abs} = \overline{\vec{J} \cdot \vec{E}} = \sigma \overline{E^2}$$

If we consider solutions of Maxwell's equations in the form  $\sin(\omega t)$  we see immediately that J<sub>ohm</sub> is in phase with E while J<sub>pol</sub> is out phase by  $\pi/2$ . Polarization current does not give rise to absorption and is responsible of *dispersion* (refraction index). Ohmic current, in turn produce an *absorption*:

$$\left(\frac{\partial W}{\partial t}\right)_{abs} = \overline{\vec{J}_{ohm} \cdot \vec{E}} = \sigma \overline{E^2}$$

We introduce the dielectric tensor  $\boldsymbol{\epsilon}$ 

$$\vec{D} = \epsilon \vec{E}$$
$$\epsilon = 1 + 4\pi\alpha$$

As with simple a.c. circuits, absorption and dispersion can be treated with a single *complex* quantity.

If we consider a field in the form

$$\vec{E} = \vec{E}_0 e^{-i\omega t}$$

we get

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c}\vec{J} + \frac{1}{c}\frac{\partial \vec{D}}{\partial t} = \frac{1}{c}\left[\epsilon\frac{\partial \vec{E}}{\partial t} - 4\pi\vec{E}\right] = \frac{\tilde{\epsilon}}{c}\frac{\partial \vec{E}}{\partial t}$$

in which we have introduced the complex dielectric function:

$$\tilde{\epsilon} = \epsilon_1 + i\epsilon_2 = \epsilon + i\frac{4\pi\sigma}{\omega}$$

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c} \left( \sigma \vec{E} + \alpha \frac{\partial \vec{E}}{\partial t} \right) + \frac{1}{c} \frac{\partial \vec{E}}{\partial t}$$

$$\vec{E} = \vec{E}_0 e^{-i\omega t}$$
$$\frac{\partial \vec{E}}{\partial t} = -i\omega \vec{E}_0 e^{-i\omega t} = -i\omega \vec{E}$$

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c} \sigma \vec{E} + \frac{1}{c} (4\pi\alpha + 1) \frac{\partial \vec{E}}{\partial t} = \frac{4\pi}{c} \sigma \vec{E} + \frac{\epsilon}{c} \frac{\partial \vec{E}}{\partial t}$$
$$= \left[ \frac{4\pi}{c} \sigma + (-i\omega) \frac{\epsilon}{c} \right] \frac{i}{\omega} \frac{\partial \vec{E}}{\partial t} = \left[ \frac{\epsilon}{c} + i \frac{4\pi\sigma}{c} \right] = \frac{\tilde{\epsilon}}{c} \frac{\partial \vec{E}}{\partial t}$$

By introducing the complex dielectric constant into Maxwell's equations we get

$$\nabla^2 \vec{E} - \frac{\tilde{\epsilon}}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

As well known a class of solutions of the wave equations are plane waves:

$$\vec{E} = \vec{E}_0 e^{i(\vec{q}\cdot\vec{r}-\omega t)} + c.c.$$

whose dispersion law

$$\omega^2 = \frac{c^2}{\tilde{\epsilon}}q^2$$

suggest a complex refraction

$$\tilde{n} = n + i\kappa$$

so that

$$\tilde{n}^2 = \tilde{\epsilon}$$

and therefore

$$\epsilon_1 = n^2 - \kappa^2$$
$$\epsilon_2 = 2n\kappa$$

A plane wave propagating along the x axis can be written in terms of the complex dielectric index:

$$\vec{E} = \vec{E}_0 e^{i(\vec{q} \cdot \vec{r} - \omega t)} + c.c. = \vec{E}_0 e^{-i\omega\left(t - \frac{\tilde{n}x}{c}\right)} + c.c. = \vec{E}_0 e^{-\frac{\omega\kappa x}{c}} e^{-i\omega\left(t - \frac{nx}{c}\right)} + c.c.$$



# Phase and group velocity



# Phase and group velocity



The absorption coefficient  $\eta$  is defined by the equation:

$$\overline{W} = \overline{W}_0 e^{-\eta x}$$

which describes the attenuation of the average energy flux, which is proportional to the square of the field, so:

$$\eta = \frac{2\omega\kappa}{c} = \frac{\omega\epsilon_2}{nc} = \frac{4\pi\sigma}{nc}$$

The complex reflection coefficient is given by the generalization of Frenel law:

$$r = \frac{\tilde{n} - 1}{\tilde{n} + 1} = \frac{(n - 1) + i\kappa}{(n + 1) + i\kappa}$$

So the reflectivity is:

$$R = r^* r = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2}$$

If  $\kappa >>n$ , R $\approx 1$  and thw wave is rapidly attenuated in the medium. This happens, for example in metals at low frequency (high  $\sigma$ )

The real and imaginary part of the dielectric function and in general of any function describing the linear response to a physical stimulus are **not** independent of each other. This is a consequence of the **causality principle**, which states that the response cannot occur in time preceding the stimulus.

Let us focus on polarization (response) and the electric field (stimulus). The following dependence will hold:

$$\vec{P}(t) = \int_{-\infty}^{t} G(t - t') \vec{E}(t') dt'$$

i.e. the polarization at a given time t depends on the history of the electric field weighted by the Green function G.

For a sinusoidal field (and a substitution of a variable) we ca write:

$$\vec{P}(t) = \int_{-\infty}^{t} G(t - t') \,\vec{E}_0 e^{-i\omega t'}(t') \,dt' = \vec{E}_0 e^{-i\omega t} \int_0^{\infty} G(\tau) \,e^{i\omega \tau} d\tau$$

so we the complex response function (polarizability in this case) can **always** be expressed as:

$$\tilde{\alpha}\left(\omega\right) = \int_{0}^{\infty} G\left(\tau\right) e^{i\omega\tau} d\tau$$

If  $\tilde{\alpha}(\omega)$  decreases to zero away from the real axis, the function  $\alpha(\omega)/(\omega-\omega_0)$  has a single pole in  $\omega_0$ .

And its integral along the path in the figure is zero, i.e. by applying Cauchy's theorem:



From:

$$\tilde{\alpha}\left(\omega\right) = \int_{0}^{\infty} G\left(\tau\right) e^{i\omega\tau} d\tau$$

we immediately obtain that

$$\epsilon\left(-\omega\right)=\epsilon^{*}\left(\omega\right)$$

we can therefore rewrite the integral and write the Kramers-Kronig dispersion relations between the real and imaginary part of the dielectric function:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$
$$\epsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\epsilon_1(\omega') - 1}{\omega'^2 - \omega^2} d\omega'$$

Dispersion relation for reflectivity

$$r\left(\omega\right) = \frac{(n-1) + i\kappa}{(n+1) + i\kappa} = |r\left(\omega\right)| e^{i\theta}$$

$$\mathsf{R}(\omega) = |r(\omega)|^2 = \left|\frac{(n-1) + i\kappa}{(n+1) + i\kappa}\right|^2$$

$$\ln (r(\omega)) = \ln (|r(\omega)|) + i\theta(\omega) = \frac{1}{2}\ln (\mathsf{R}(\omega)) + i\theta(\omega)$$

$$\theta\left(\omega\right) = -\frac{2\omega}{\pi} P \!\!\!\int\limits_{0}^{\infty} \frac{\ln\left(\left|r\left(\omega'\right)\right|\right)}{\omega'^{2} - \omega^{2}} d\omega' = -\frac{\omega}{\pi} P \!\!\!\int\limits_{0}^{\infty} \frac{\ln\left(\mathsf{R}\left(\omega'\right)\right)}{\omega'^{2} - \omega^{2}} d\omega'$$

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If we consider the natural logarithm of  $r(\omega)$ :

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Static sum rule. For  $\omega=0$  we have:

$$\epsilon_1(0) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\epsilon_2(\omega')}{\omega'} d\omega'$$

so, if the static dielectric constant is  $\neq 1$ , the imaginary part wil be  $\neq 0$  in some part of the spectrum, i.e the medium must absorb radiation. Because of the  $1/\omega$  factor in the integrand, the static dielectric function will be greater if the absorption occurs at low frequency.

# Absorption localized at $\omega = \omega_0$

$$\epsilon_2\left(\omega\right) = A\delta\left(\omega - \omega_0\right)$$

$$\epsilon_1\left(0\right) = 1 + \frac{2}{\pi} \frac{A}{\omega_0}$$

therefore:

$$\epsilon_1(\omega) = 1 + \frac{\omega_0^2 \left[\epsilon_1(0) - 1\right]}{\omega_0^2 - \omega^2}$$
$$\epsilon_2(\omega) = \frac{\pi}{2} \omega_0 \left[\epsilon_1(0) - 1\right] \delta(\omega - \omega_0)$$



Drude-Lorentz model.

We describe the medium as an ensemble of harmonic oscillators whose resonance frequency and damping are  $\omega_0$  and  $\gamma$ , respectively:

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$$\tilde{\epsilon}(\omega) = 1 + 4\pi\tilde{\alpha} = 1 + 4\pi\frac{P}{E} = 1 + \frac{4\pi e^2 N}{m} \frac{1}{(\omega_0^2 - \omega^2) - i\gamma\omega}$$

So:

$$\epsilon_1 = 1 + \frac{4\pi e^2 N}{m} \frac{\omega_0^2 - \omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma\omega\right)^2}$$
$$\epsilon_2 = \frac{4\pi e^2 N}{m} \frac{\gamma\omega}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma\omega\right)^2}$$





Integration by parts

$$\epsilon_{2}(\omega) = -\frac{1}{\pi} P \int_{0}^{\infty} \left[ \frac{d\epsilon_{1}(\omega')}{d\omega'} \right] \cdot \ln \left[ \frac{\omega' + \omega}{\omega' - \omega} \right] d\omega'$$



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By considering the complex refraction index, one can identify regions in which transmissivity, absorption or reflectivity are the main effects:



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Optical properties of metals can be obtained from the Lorentz-Drude model by setting  $\omega_0=0$  and by defining the *plasma frequency:* 

$$\omega_p^2 = \frac{4\pi N e^2}{m}$$

The dielectric functions becomes:

$$\tilde{\epsilon} = \left(1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right) + i \frac{\gamma \omega_p^2}{\omega^3 + \gamma^2 \omega}$$

Free electron metal with  $\hbar\omega_{\rm p}$ =8eV and  $\hbar\gamma$ =0.5 eV



The conductivity,  $\sigma$  is given by:

$$\sigma = \frac{\omega \epsilon_2}{4\pi}$$

which in the statc limit becomes:

$$\sigma_0 = \lim_{\omega \to 0} \frac{\omega \epsilon_2}{4\pi} = \frac{Ne^2}{m\gamma}$$

which can be compared with the expression derived in the transport theory to find that  $\gamma\!\!=\!\!1/\tau$ 

At very low frequencies ( $\omega << 1/\tau$ ) the reflectivity is:

$$R \cong 1 - 2\sqrt{\frac{\omega}{2\pi\sigma}} = 1 - 2\sqrt{\frac{2\omega}{\omega_p^2\tau}}$$

Free electron metal with  $\hbar\omega_{\rm p}$ =8eV and  $\hbar\gamma$ =0.5 eV



At frequencies much higher than the plasma frequency we get:

$$\epsilon_1 \cong 1 - \frac{\omega_p^2}{\omega^2}$$
$$\epsilon_2 \cong \frac{\omega_p^2 \gamma}{\omega^3}$$

which represent the behaviour of any material at high energy. If we now consider the KK relation:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$

At high energy we can neglect  $\omega^{2}$  in the integrand denominator because  $\varepsilon_{2}$  decreases very rapidly (as  $1/\omega^{3}$ , superconvergence theorem) and therefore:

$$\epsilon_1(\omega)_{\omega\to\infty} \cong 1 - \frac{2}{\omega^2 \pi} \int_0^\infty \omega' \epsilon_2(\omega') d\omega'$$

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$$\epsilon_1(\omega)_{\omega \to \infty} \cong 1 - \frac{2}{\omega^2 \pi} \int_0^\infty \omega' \epsilon_2(\omega') d\omega'$$

so we get the sum rule:

$$\int_{0}^{\infty} \omega' \epsilon_2(\omega') d\omega' = \frac{\pi}{2} \omega_p^2 = \frac{2\pi^2 e^2 N}{m}$$

which relates he dielectric function to the total number of electrons contributing to it. We can define the effective number of electrons contributing to the dielectric function up to a frequency  $\omega_{max}$ :

$$\int_{0}^{\omega_{max}} \omega' \epsilon_2(\omega') d\omega' \cong \frac{\pi}{2} \frac{4\pi e^2}{m} N_{eff}$$

The other KK relation

$$\epsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\epsilon_1(\omega') - 1}{\omega'^2 - \omega^2} d\omega'$$

at high frequency becomes

$$\epsilon_2(\omega)_{\omega\to\infty} = \frac{2}{\pi\omega} \int_0^\infty (\epsilon_1(\omega') - 1) d\omega'$$

and by comparison with the expression of the dielectric function at high energy we get:

$$\int_{0}^{\infty} \left(\epsilon_1\left(\omega\right) - 1\right) d\omega = 0$$

Free electron metal with  $\hbar\omega_{\rm p}$ =8eV and  $\hbar\gamma$ =0.5 eV



Normal incidence Ag experimental Reflectivity



Experimental dielectric function of Ag:



E x p e r i m e n t a l Reflectivity of Al



Reflection and refraction at an arbitrary angle



All waves have the same frequency,  $\omega$ , and  $|\vec{k}| = |\vec{k''}| = \frac{\omega}{c}$ 

The refracted wave has phase velocity  $v_{\phi} = \frac{\omega}{k'} = \frac{c}{n} \Rightarrow k' = \left|\vec{k'}\right| = \frac{\omega}{c}(1 - \delta + i\beta)$ 



Kinematic boundary conditions:

at the boundary (z=0):  $\vec{k} \cdot \vec{r_0} = \vec{k'} \cdot \vec{r_0} = \vec{k''} \cdot \vec{r_0}$ nothing occurs along x  $k_x = k'_x = k''_x$ so along z  $\begin{vmatrix} k_z \end{vmatrix} = \begin{vmatrix} k'_z \end{vmatrix} = \begin{vmatrix} k''_z \end{vmatrix}$   $k \sin \phi = k' \sin \phi' = k'' \sin \phi''$ therefore:  $\phi = \phi''; \quad \frac{\sin \phi}{\sin \phi'} = n$ 

If we write the complex index of refraction as

$$\tilde{n} = (1 - \delta + i\beta)$$



and assume  $\beta \rightarrow 0$  then  $n \approx 1-\delta$  and we can have total *external* reflection for angles above the critical angle

$$\phi_c = \arcsin\left(1 - \delta\right)$$

or, in terms of the glancing incidence



$$\vec{E} = \vec{E}_0 e^{-i\left(\omega t - \vec{k} \cdot \vec{r}\right)}$$

$$\vec{E'} = \vec{E'_0} e^{-i\left(\omega t - \vec{k'} \cdot \vec{r}\right)}$$



Wednesday, July 10, 2013

# Dynamic boundary conditions for an **s polarized** wave:

 $\vec{E} = \vec{E}_0 e^{-i\left(\omega t - \vec{k} \cdot \vec{r}\right)}$ 

$$\vec{E'} = \vec{E'_0} e^{-i\left(\omega t - \vec{k'} \cdot \vec{r}\right)}$$



Dynamic boundary conditions for an **s polarized** wave:

tangential electric and magnetic fields are continuos:

$$E_0 = E'_0 = E''_0$$

$$H_0 \cos \phi - H_0'' \cos \phi = H_0' \cos \phi'$$

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tangential electric and magnetic fields are continuos:

$$E_0 = E'_0 = E''_0$$

$$H_0 \cos \phi - H_0'' \cos \phi = H_0' \cos \phi'$$

since

$$\vec{H}\left(\vec{r},t\right) = \tilde{n}\frac{\vec{k}}{k} \times \vec{E}\left(\vec{r},t\right)$$

we obtain

$$(E_0 - E_0'')\cos\phi = \tilde{n}E_0'\cos\phi'$$

# For an **s polarized** wave:

$$\frac{E'_0}{E_0} = \frac{2\cos\phi}{\cos\phi + \sqrt{n^2 - \sin^2\phi}}$$
$$\frac{E''_0}{E_0} = \frac{\cos\phi - \sqrt{n^2 - \sin^2\phi}}{\cos\phi + \sqrt{n^2 - \sin^2\phi}}$$

# so the reflectivity is

$$R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2}$$





# Reflectivity as a function of $\phi$ and n



# **Brewster's angle**

Incident ray Reflected ray (unpolarised) (polarised) When the reflected and refracted  $\Theta_{\rm B}$ waves form an angle of 90° i.e. when:  $\theta_b = \arctan\left(\frac{n_2}{d}\right)$ the reflected wave is 100% s polarized Refracted ray (if no absorption (slightly polarised) occurs!)

# Ag s- and p- polarized reflectivity at $\hbar\omega$ =20eV



Wednesday, July 10, 2013

# Experimental reflectivity of Ag for p-polarized light



Glancing incidence reflection as a function of  $\beta/\delta$ 



- finite  $\beta/\delta$  rounds the sharp angular dependence
- cutoff angle and absorption edges can enhance the sharpness
- note the effects of oxide layers and surface contamination



(Henke, Gullikson, Davis)