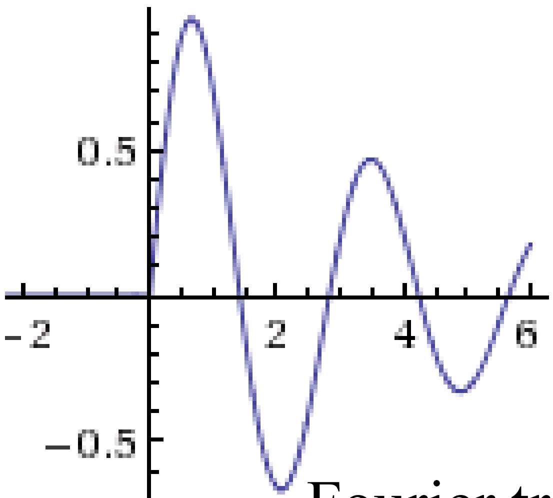
Linear response theory

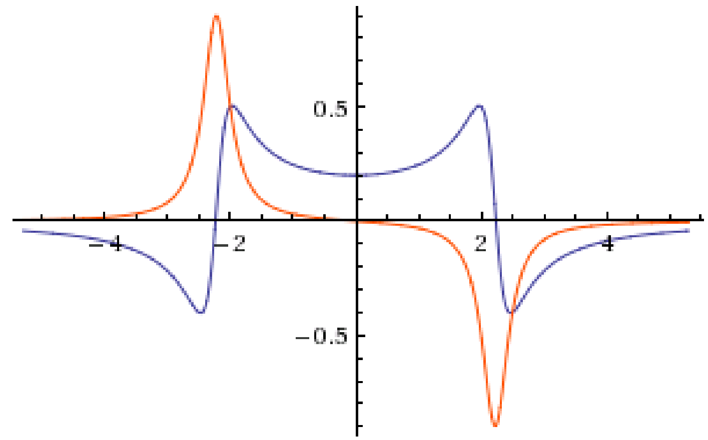
Damped mass-spring system

$$m\frac{d^2g}{dt^2}+b\frac{dg}{dt}+kg=\delta(t)$$

$$-\omega^2 m\chi+i\omega b\chi+k\chi=1$$

$$g=e^{\lambda t}\qquad \lambda_\pm=\frac{-b\pm\sqrt{b^2-4mk}}{2m}$$





Fourier transform pair

$$\chi=\left(\frac{1}{m}\right)\frac{\frac{k}{m}-\omega^2-i\omega\frac{b}{m}}{\left(\frac{k}{m}-\omega^2\right)^2+\left(\omega\frac{b}{m}\right)^2}$$

$$g(t)=H(t)\frac{1}{m}\exp\left(\frac{-bt}{2m}\right)\sin\left(\frac{\sqrt{4mk-b^2}}{2m}t\right)$$

More complex linear systems

Any coupled system of linear differential equations can be written as a set of first order equations

$$\frac{d\vec{x}}{dt} = M\vec{x}$$

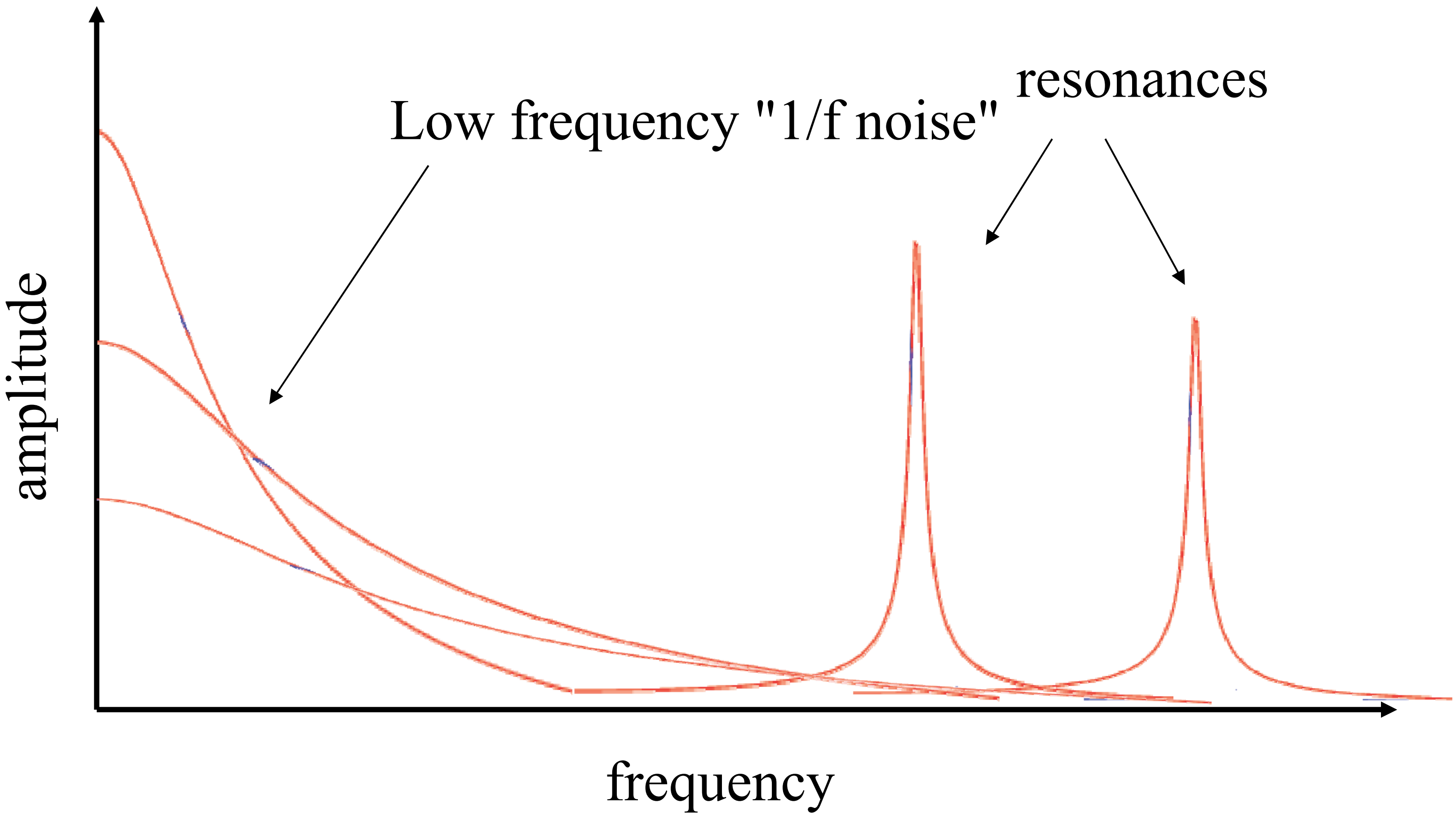
The solutions have the form $\vec{x}_i e^{\lambda_i t}$

where $\vec{x}_i$ are the eigenvectors and λ_i are the eigenvalues of matrix M.

$\mathrm{Re}(\lambda_i) < 0$ for stable systems

λ_i is either real and negative (overdamped) or comes in complex conjugate pairs with a negative real part (underdamped).

More complex linear systems



Odd and even components

Any function $f(t)$ can be written in terms of its odd and even components

$$E(t) = ½[f(t) + f(-t)]$$

$$O(t) = ½[f(t) - f(-t)]$$

$$f(t) = \mathrm{E}(t) + O(t)$$

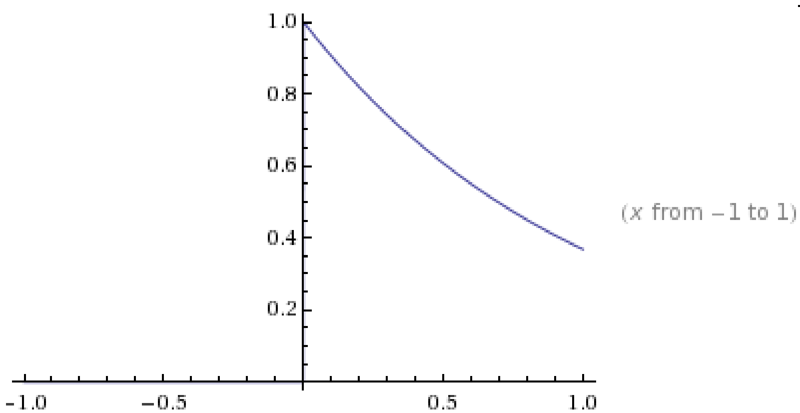
$$f(t) = ½[f(t) + f(-t)] + ½[f(t) - f(-t)]$$

$$\int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt = \int_{-\infty}^{\infty} \left(E(t) + O(t)\right)\left(\cos\omega t - i\sin\omega t\right)dt$$

$$= \int_{-\infty}^{\infty} E(t)\cos\omega t dt - i\int_{-\infty}^{\infty} O(t)\sin\omega t dt$$

The Fourier transform of $E(t)$ is real and even

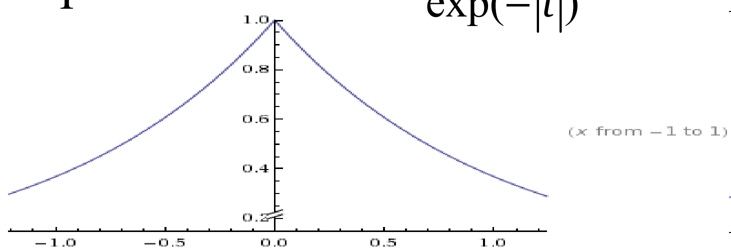
The Fourier transform of $O(t)$ is imaginary and odd

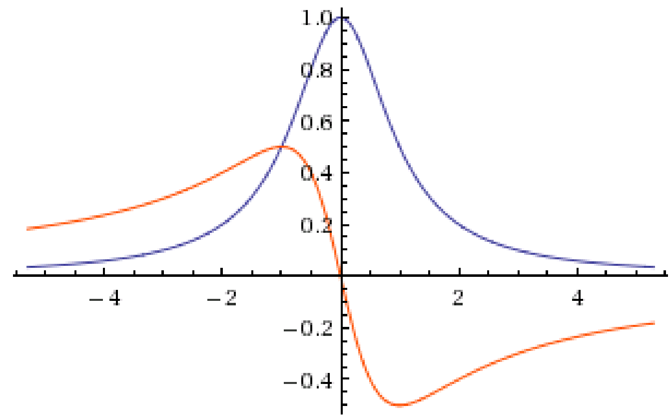


$$\chi(\omega) = \frac{1}{m}\frac{\frac{b}{m} - i\omega}{\left(\frac{b}{m}\right)^2 + \omega^2}$$

even component

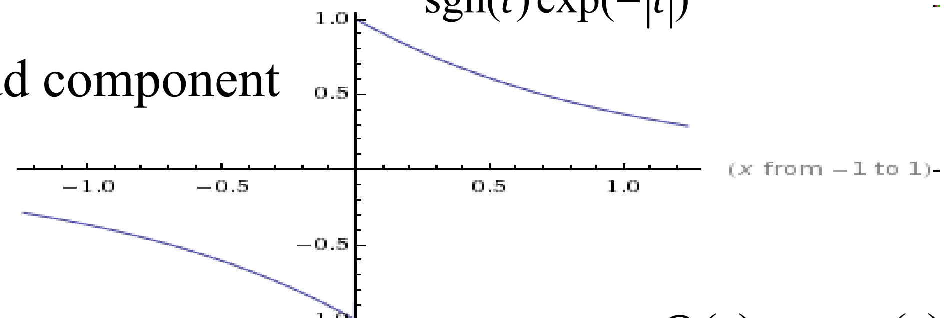
$\exp(-|t|)$





$\mathrm{sgn}(t)\exp(-|t|)$

odd component



$$O(t) = \mathrm{sgn}(t)E(t)$$

$$E(t) = \mathrm{sgn}(t)O(t)$$

Causality and the Kramers-Kronig relations (I)

$$\chi(\omega) = \int g(\tau) e^{-i\omega\tau} d\tau = \int E(\tau)\cos(\omega\tau) d\tau - i\int O(\tau)\sin(\omega\tau) d\tau = \chi'(\omega) + i\chi''(\omega)$$

The real and imaginary parts of the susceptibility are related.

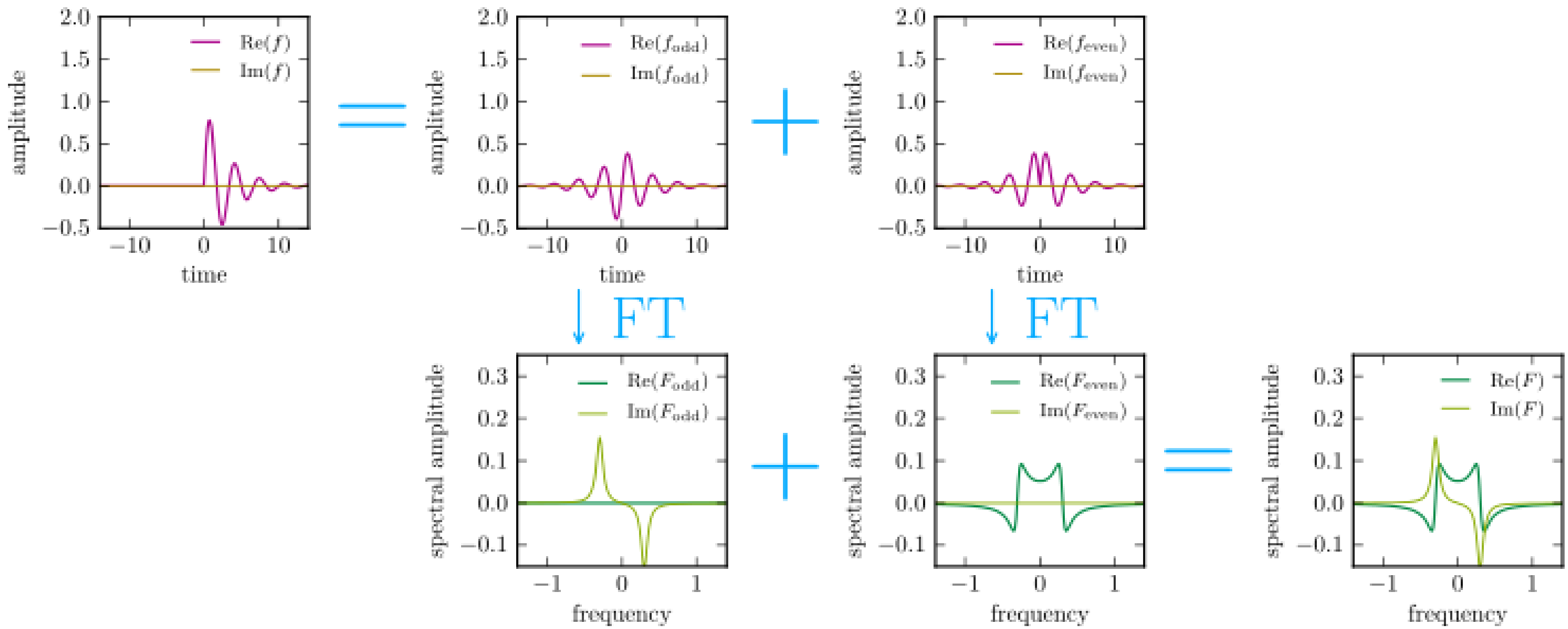
If you know χ', inverse Fourier transform to find $E(t)$. Knowing $E(t)$ you can determine $O(t) = \mathrm{sgn}(t)E(t)$. Fourier transform $O(t)$ to find χ''.

$$\chi'(\omega) = \int_{-\infty}^{\infty} E(t)\cos(\omega t) dt \qquad E(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \chi'(\omega)\cos(\omega t) d\omega$$

$$\boxed{O(t) = \mathrm{sgn}(t)E(t) \qquad E(t) = \mathrm{sgn}(t)O(t)}$$

$$\chi''(\omega) = -\int_{-\infty}^{\infty} O(t)\sin(\omega t) dt \qquad O(t) = \frac{-1}{2\pi}\int_{-\infty}^{\infty} \chi''(\omega)\sin(\omega t) d\omega$$

Kramers-Kronig relations



If you know any of these for just positive frequencies,
you can calculate all the others.

https://en.wikipedia.org/wiki/Kramers%E2%80%93Kronig_relations

Causality and the Kramers-Kronig relation (II)

Real space

$$E(t) = \mathrm{sgn}(t) O(t)$$

$$O(t) = \mathrm{sgn}(t) E(t)$$

Reciprocal space

$$\chi'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega'$$

$$\chi''(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega'$$

$$\chi' = \frac{-i}{\pi\omega} * i\chi'', \quad i\chi'' = \frac{-i}{\pi\omega} * \chi'$$

Take the Fourier transform, use the convolution theorem.

P: Cauchy principle value (go around the singularity and take the limit as you pass by arbitrarily close)

Singularity makes a numerical evaluation more difficult.

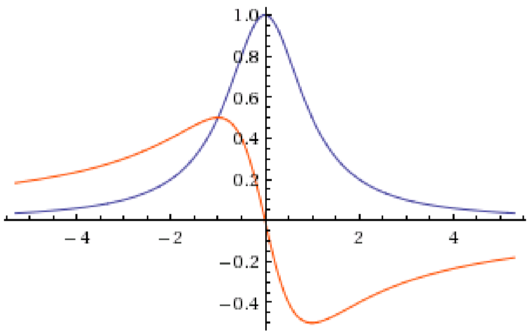
http://lamp.tu-graz.ac.at/~hadley/ss2/linearresponse/causality.php

Kramers-Kronig relations (III)

$$\chi''(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega'$$

$$\chi'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega'$$

Kramers-Kronig relations II



$$\chi'(\omega) = \chi'(-\omega)$$
$$\chi''(\omega) = -\chi''(-\omega)$$

Real part is even
Imaginary part is odd

$$\chi'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{0} \frac{\chi''(\omega')}{\omega' - \omega} d\omega' - \frac{1}{\pi} P \int_{0}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega'$$

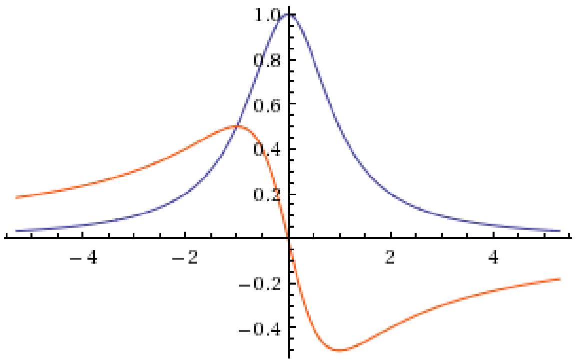
change variables ω'→-ω'
(4 minus signs)

Kramers-Kronig relations (III)

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

$$\frac{1}{\omega'+\omega} + \frac{1}{\omega'-\omega} = \frac{2\omega'}{(\omega')^2 - \omega^2}$$

$$\boxed{\begin{aligned} \chi'(\omega) &= \frac{2}{\pi} P\int_0^\infty \frac{\omega'\chi''(\omega')}{(\omega')^2-\omega^2} d\omega' \\ \chi''(\omega) &= -\frac{2}{\pi} P\int_0^\infty \frac{\omega\chi'(\omega')}{(\omega')^2-\omega^2} d\omega' \end{aligned}}$$



Singularity is stronger in this form.

Impulse response/generalized susceptibility

The impulse response function is the response of the system to a δ-function excitation. The response function must be zero before the excitation.

The generalized susceptibility is the Fourier transform of the impulse response function.

Any function that is zero before the excitation and nonzero afterwards must have both an odd component and an even component.

The generalized susceptibility must have a real and imaginary part. All information about the real part is contained in the imaginary part and vice versa.

Optical Properties of Insulators

Dielectric response of insulators

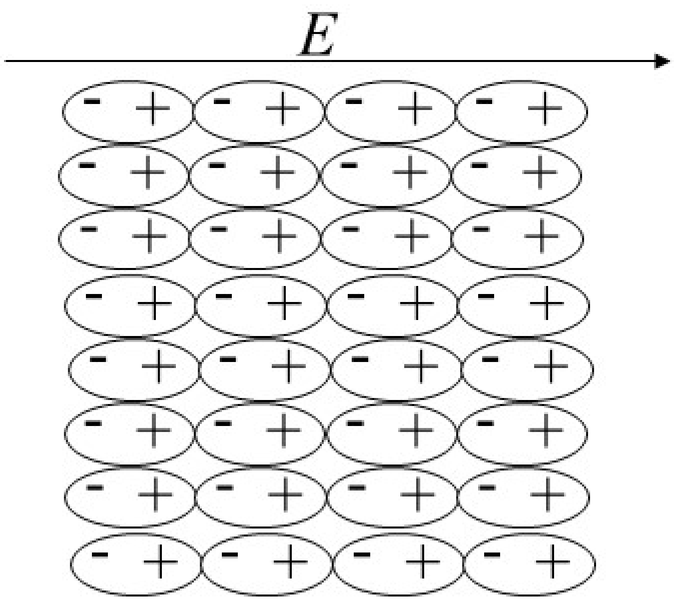
The electric polarization is related to the electric field

$$P_i = \varepsilon_0 \chi_{ij} E_j$$

The electric displacement vector D is also related to the electric field

$$D_i = P_i + \varepsilon_0 E_i = \varepsilon_0 (1 + \chi_{ij}) E_j = \varepsilon_0 \varepsilon_{ij} E_j$$

$$\varepsilon_{ij} = (1 + \chi_{ij})$$



E is decreased by a factor of the dielectric constant

Dielectric response of insulators

In an insulator, charge is bound. The response to an electric field can be modeled as a collection of damped harmonic oscillators

$$P = nex$$

Macroscopic polarization

electron density

ex = dipole moment

The core electrons of a metal respond to an electric field like this too.

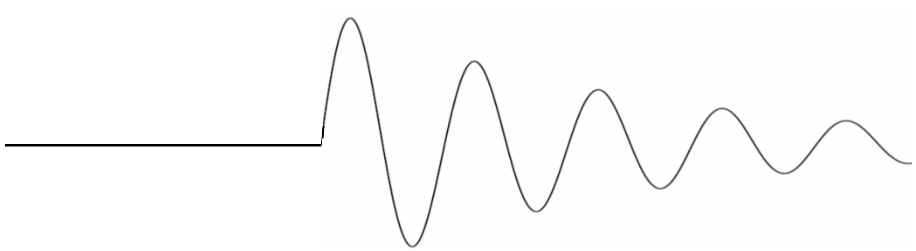
Dielectric response of insulators

The differential equation that describes how the position of the charge changes in time is:

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = -eE(t)$$

The impulse response function is:

$$g(t) = -\frac{1}{b}\exp\left(\frac{-bt}{2m}\right)\sin\left(\frac{\sqrt{4mk-b^2}}{2m}t\right) \qquad t > 0$$



Electric susceptibility

$$\vec{P} = \varepsilon_0 \chi_E \vec{E} \qquad\qquad \vec{P} = nq\vec{x}$$

$$\chi_E = \frac{P}{\varepsilon_0 E} = \frac{nqx}{\varepsilon_0 E}$$

Assume a solution of the form $x(\omega)e^{i\omega t}$, $E(\omega)e^{i\omega t}$

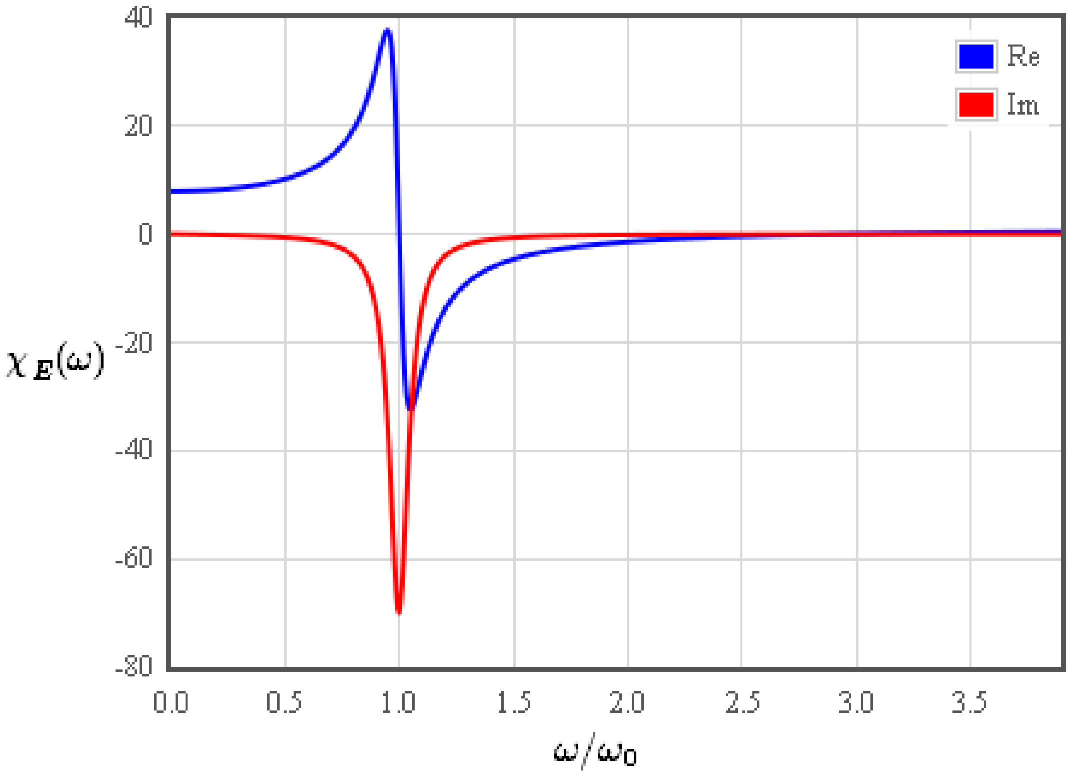
$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = qE(t)$$

$$\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \omega_0^2 x = -\frac{qE}{m}$$

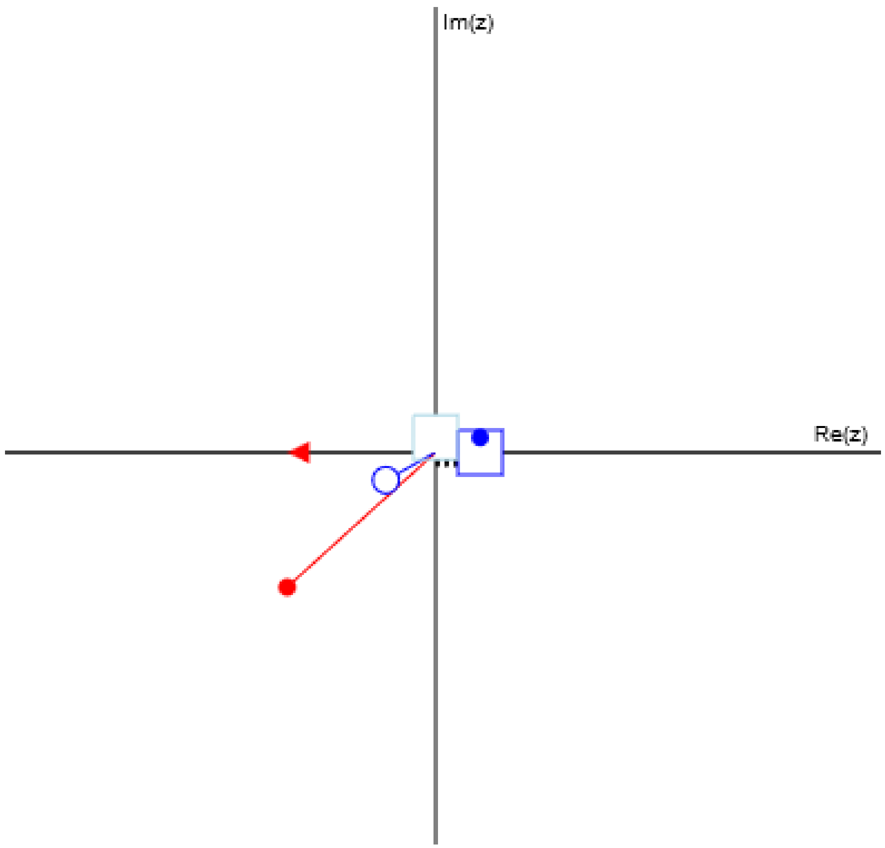
$$\omega_0 = \sqrt{\frac{k}{m}} \qquad\qquad \gamma = \frac{b}{m}$$

Electric susceptibility

$$\chi_E(\omega) = \frac{n_{\omega_0} q^2}{\varepsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 + i\gamma\omega}$$



Resonance of a damped driven harmonic oscillator



m =4 [kg]

b =1 [N s/m]

k =6 [N/m]

F_0 =0.9 [N]

ω =0.8 [rad/s]

$$\omega_0 = \sqrt{\frac{k}{m} - \frac{b^2}{4m^2}} = 1.22 \text{ [rad/s]} = 0.194 \text{ [Hz]}$$

$$\theta = \text{atan}\left(\frac{\omega b}{k - m\omega^2}\right) = 0.228 \text{ [rad]} = 13.1 \text{ [deg]}$$

$$|A| = \frac{F_0}{\sqrt{(k - m\omega^2)^2 + \omega^2 b^2}} = 0.255 \text{ [m]}$$

$$Q = \frac{\sqrt{mk}}{b} = 4.90$$

Display $F_0 e^{i\omega t}$: ☑ Display $|A|e^{i(\omega t - \theta)}$: ☑

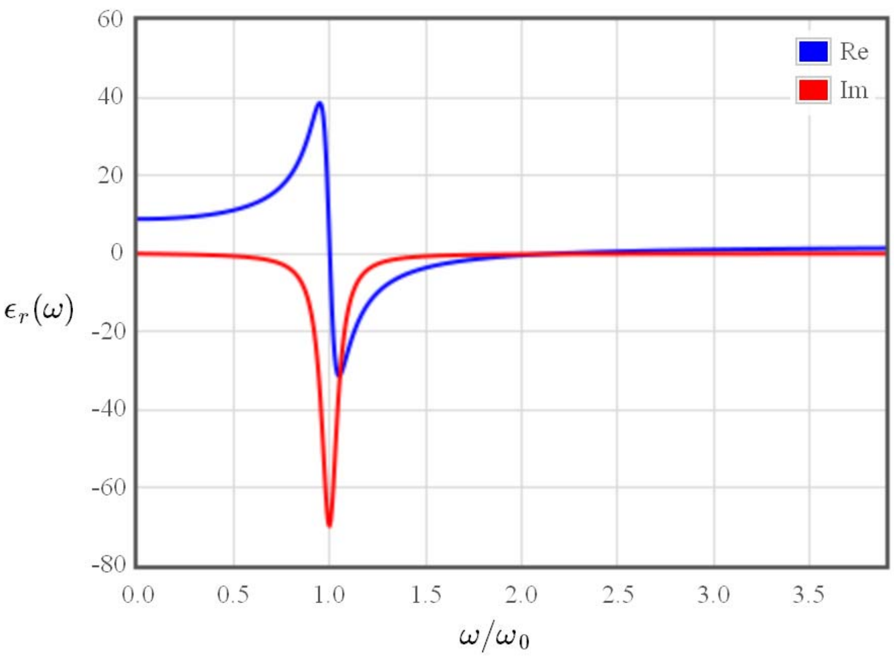
Display transients z: ☑ Display x_2: ☑

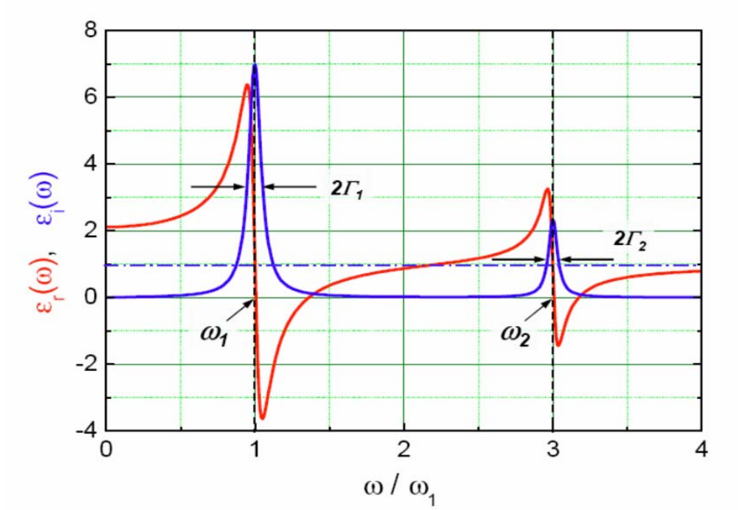
http://lamp.tu-graz.ac.at/~hadley/physikm/apps/resonance.en.php

Dielectric function

$$\vec{D} = \epsilon_r \epsilon_0 \vec{E} = \vec{P} + \epsilon_0 \vec{E}$$

$$\varepsilon_r(\omega) = 1 + \chi_E(\omega) = 1 + \frac{n_{\omega_0} q^2}{\varepsilon_0 m} \frac{1}{\omega_0^2 - \omega^2 + i\gamma\omega}$$

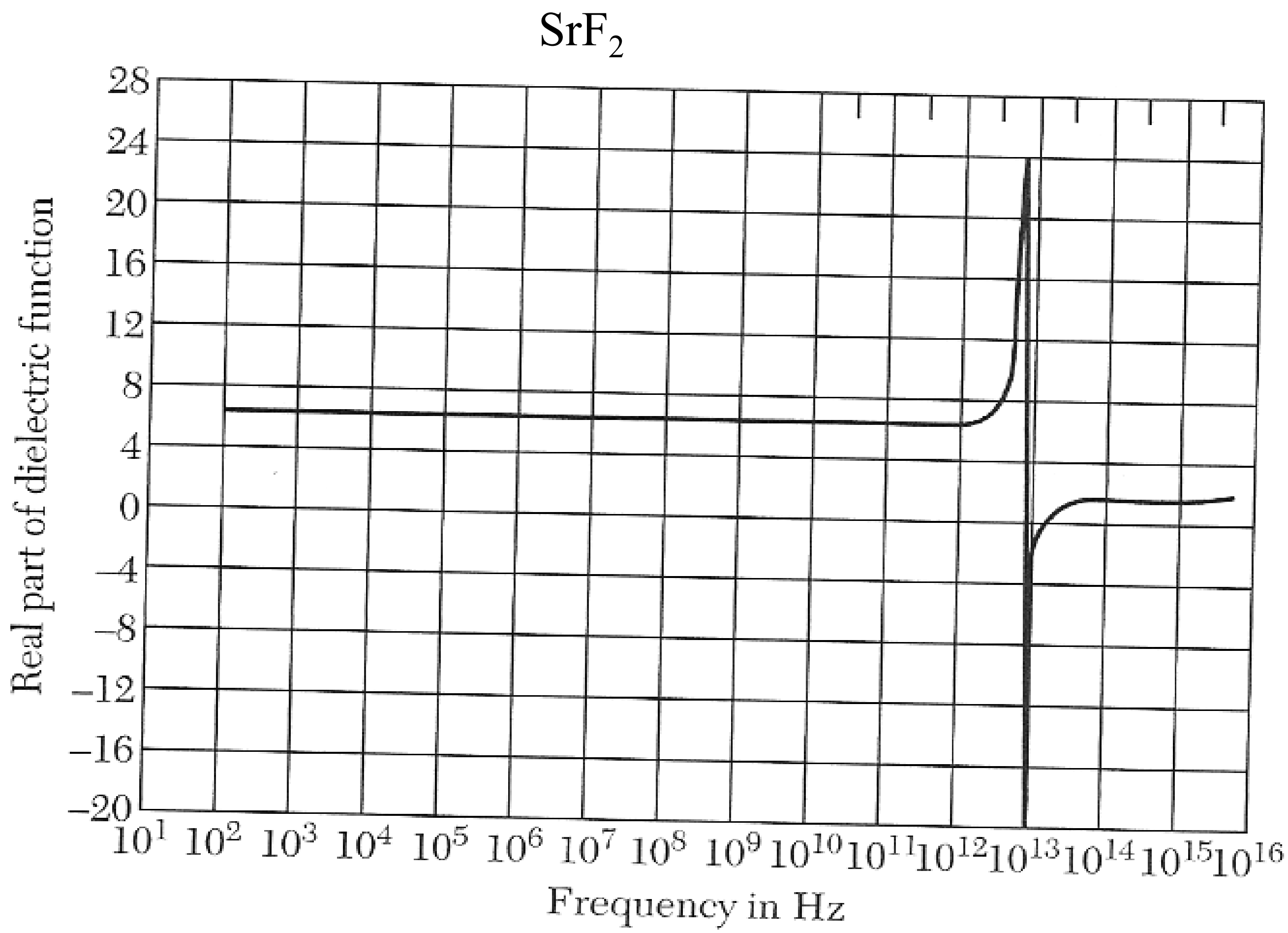




Gross and Marx

There can be more resonances.

Dielectric function of insulators



Insulators can often be modeled as a simple resonance.

Dispersion relation

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

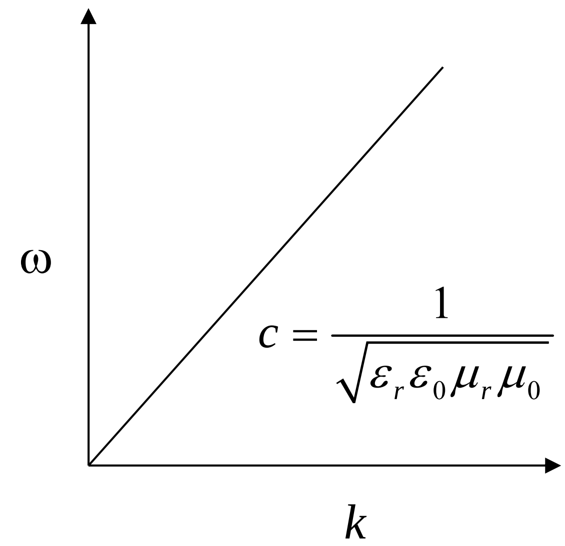
$$\vec{D} = \varepsilon \vec{E} \qquad \vec{B} = \mu \vec{H}$$

$$\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}$$

Take the curl $\quad \nabla \times \nabla \times \vec{E} = -\mu \frac{\partial \nabla \times \vec{H}}{\partial t}$

$$\nabla\left(\cancelto{0}{\nabla \cdot \vec{E}}\right) - \nabla^2 \vec{E} = -\mu \frac{\partial^2 \vec{D}}{\partial t^2}$$

$$\varepsilon_r \varepsilon_0 \mu_r \mu_0 \frac{\partial^2 \vec{D}}{\partial t^2} = \nabla^2 \vec{D}$$



The normal mode solutions are plane waves: $\vec{D} = \vec{D}_0 \exp\left(i\left(\vec{k} \cdot \vec{r} - \omega t\right)\right)$

$$\boxed{\varepsilon(\omega, k)\mu_0 \varepsilon_0 \omega^2 = k^2}$$

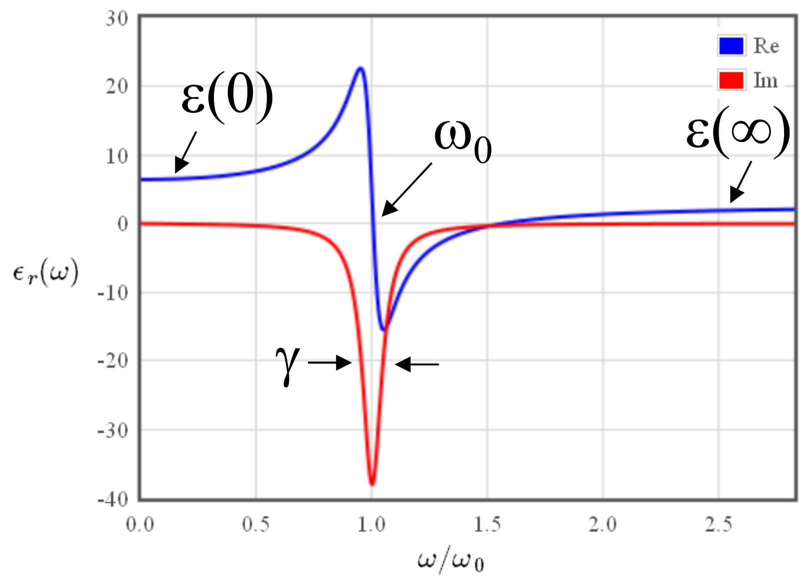
Dispersion relation

$$\varepsilon(\omega)\mu_0\varepsilon_0\omega^2 = k^2$$

If ε is real and positive: propagating electromagnetic waves $\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$

If $\varepsilon_r < 0$: decaying solutions $\exp(-\vec{k}\cdot\vec{r}-i\omega t)$

If ε is complex, $\varepsilon_r > 0$: decaying electromagnetic waves $\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)\exp(-\kappa r)$



Dielectric function

Dispersion relation: $\varepsilon_r \mu_0 \varepsilon_0 \omega^2 = k^2$

$$k = \sqrt{\varepsilon_r \mu_0 \varepsilon_0}\,\omega = \frac{\sqrt{\varepsilon_r}\,\omega}{c}$$

Measurable: $\sqrt{\varepsilon} = n + iK$

refractive index (n) extinction coefficient (K)

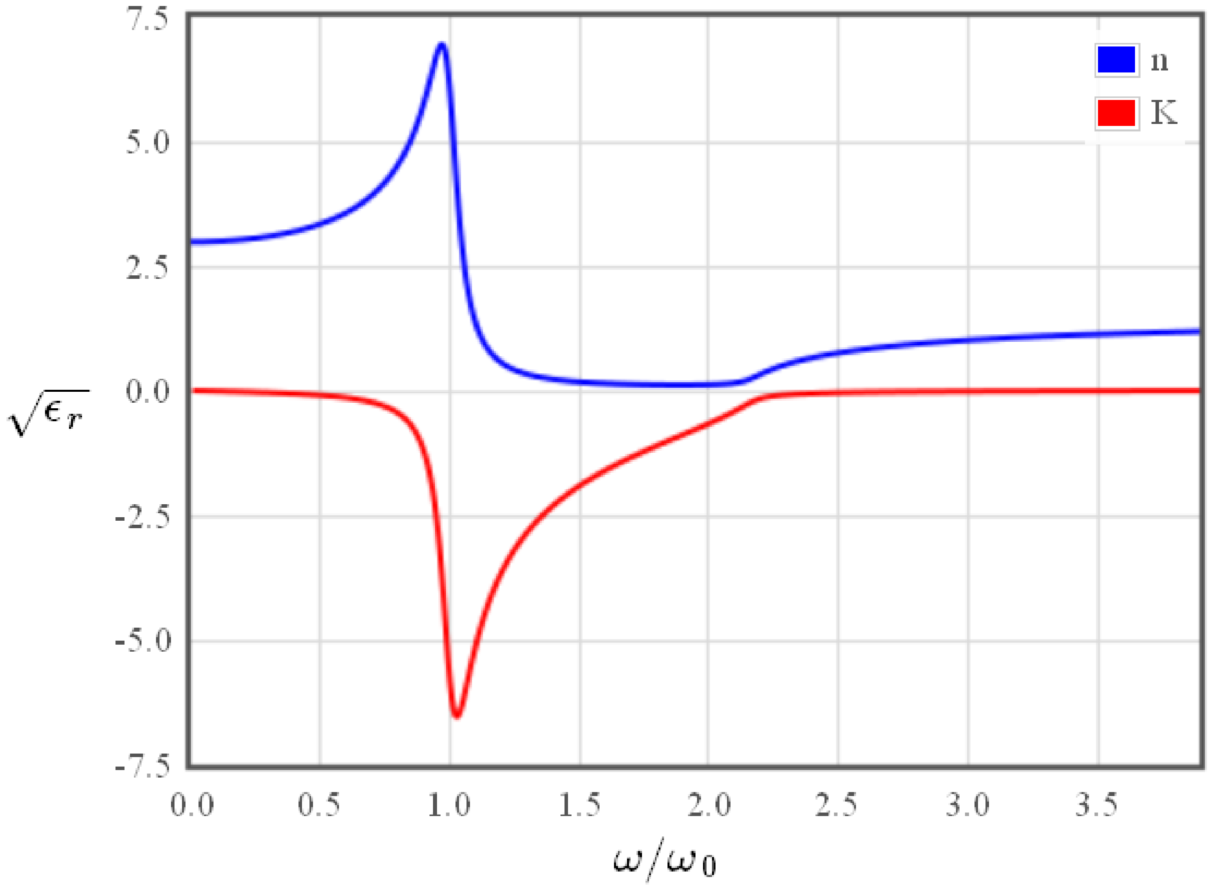
Vacuum	Dielectric
$\omega = ck$	$k = \frac{\sqrt{\varepsilon_r}\,\omega}{c}$
$\exp\left(i\left(\frac{\omega x}{c} - \omega t\right)\right)$	$\exp\left(i\left(\frac{(n+iK)\omega x}{c} - \omega t\right)\right)$ $= \exp\left(i\left(\frac{n\omega x}{c} - \omega t\right)\right)\exp\left(-\frac{\omega K x}{c}\right)$

Intensity $I(x) = I(0)\exp(-\alpha x)$ J m^{-2} s^{-1} Beer-Lambert

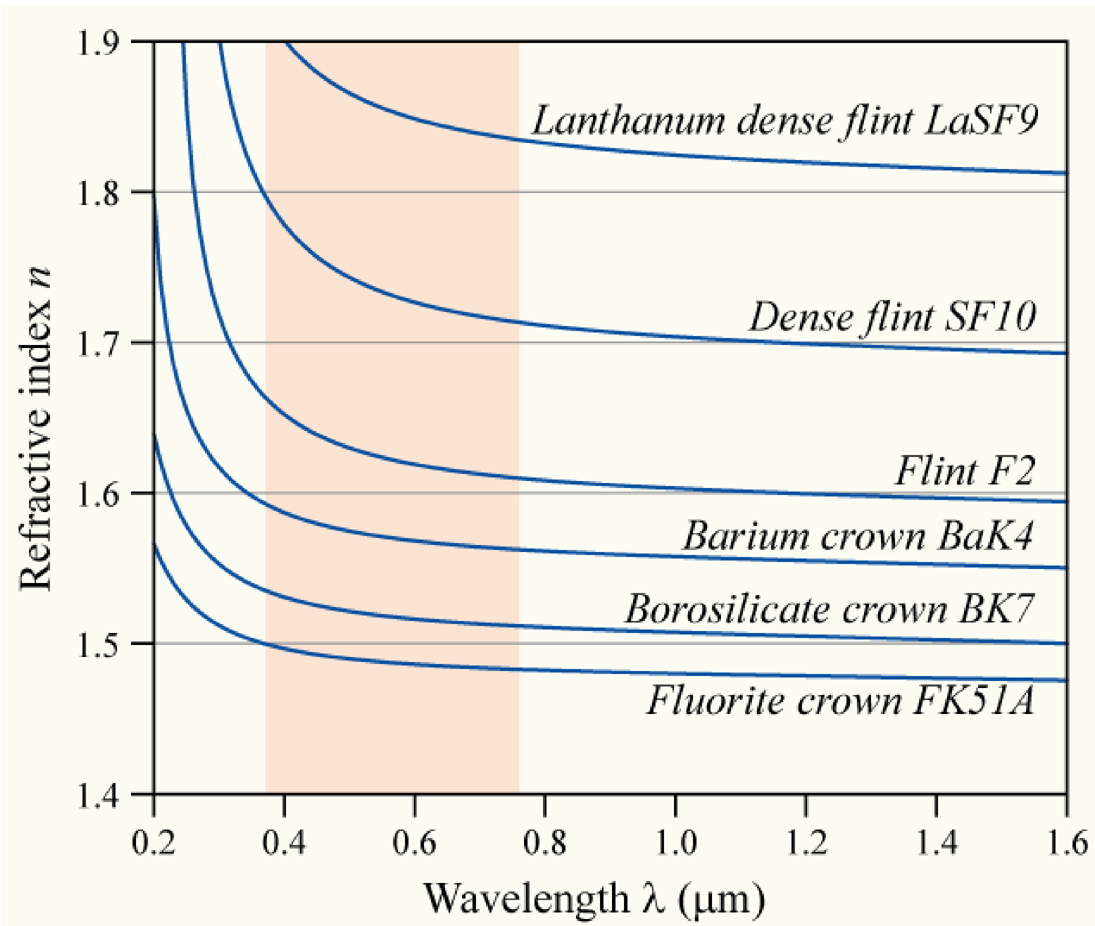
absorption coefficient $\longrightarrow$ $\alpha = \frac{2\omega K}{c}$

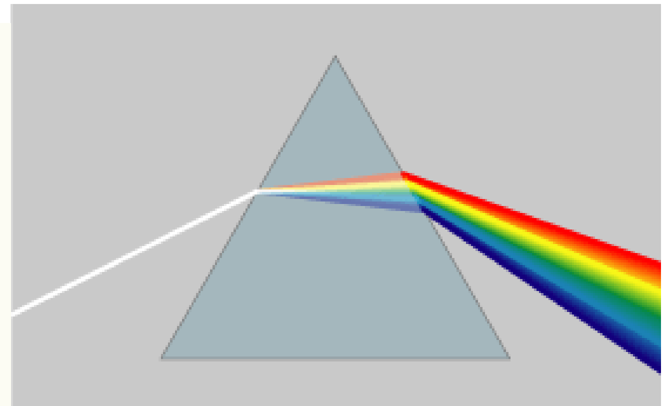
The index of refraction *n* and the extinction coefficient *K*

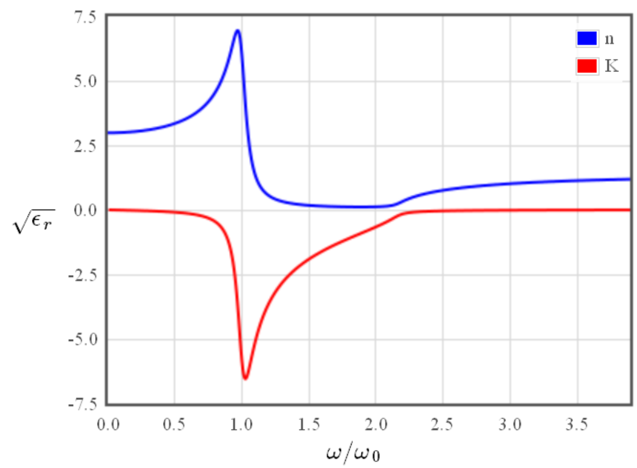
$$\sqrt{\epsilon_r} = n + iK$$



Dispersion







Cause of chromatic aberration in lenses.

http://en.wikipedia.org/wiki/Dispersion_%28optics%29#mediaviewer/File:Prism_rainbow_schema.png
http://en.wikipedia.org/wiki/Refractive_index