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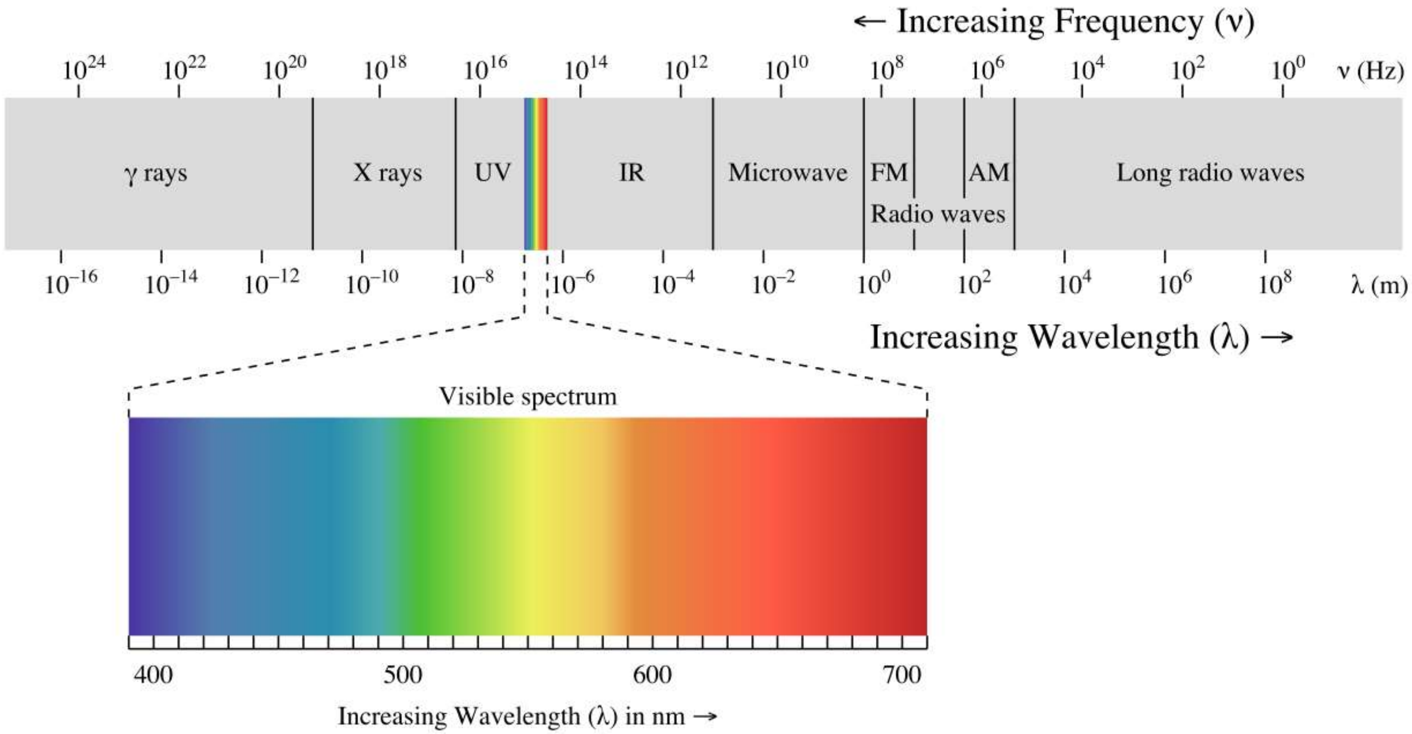
Optical Spectroscopy in Materials Science

<u>Recommended litrature</u>

Kamarás K.: Spektroszkópia és anyagszerkezet. Bevezetés a modern optikába V. kötet, (Műegyetemi Kiadó, 2000.)
D.B. Tanner: Optical Effects in Solids
(Cambridge University Press, Cambridge, 2019.)
G. Grüner, M. Dressel: Electrodynamics of Solids
(Cambridge University Press, Cambridge, 2003.)
H. Kuzmany: Solid State Spectroscopy, an Introduction
(Springer, Berlin, Heidelberg, 1998.)

Optical spectroscopy: study of light-matter interaction as a function of the frequency of the radiation



Conversion of units: $h\nu = hc\frac{1}{\lambda} = eU = k_B T$ ☠ Wavenumber (hullámszám)

	THz	cm^{-1}	meV	K
1 THz	1	33.333	4.13	47.96
1 cm^{-1}	0.03	1	0.124	1.439
1 meV	0.24	8.0655	1	11.6
1 K	0.02086	0.695	0.0862	1

Optical spectroscopy: study of light-matter interaction as a function of the frequency of the radiation

Microscopic model of materials

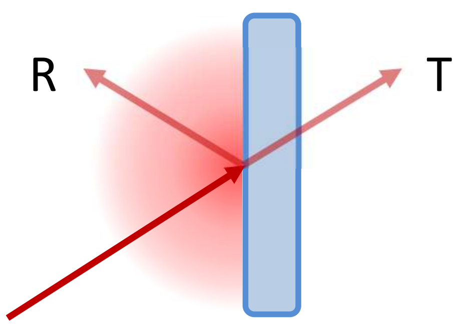
- Classical equation of motion of charges (magnetic moments): free electron gas, vibrations of molecules
- Quantum mechanics: excitation of electrons in atoms

↕ Linear response theory

Optical response functions

- Refractive index, absorption coefficient, polarizability

↕ Maxwell's equations



Directly measured quantities

- Reflected, transmitted, scattered intensity

Experimental setups, methods

Electromagnetic wave propagation in vacuum

Maxwell's equations in vacuum:

$$\nabla \cdot \mathrm{E} = \frac{1}{\varepsilon_0}\rho \qquad \nabla \cdot \mathrm{B} = 0$$

$$\nabla \times \mathrm{E} = -\partial_t \mathrm{B} \qquad \nabla \times \mathrm{B} = \mu_0\left(\mathrm{j} + \varepsilon_0 \partial_t \mathrm{E}\right)$$

Wave equations with sources:

$$\nabla\times\left(\nabla\times\boldsymbol{E}\right) = -\partial_t\left(\nabla\times\boldsymbol{B}\right)$$

$$\nabla\left(\nabla\cdot\boldsymbol{E}\right) - \nabla^2\boldsymbol{E} = -\mu_0\partial_t\boldsymbol{j} - \frac{1}{c^2}\partial_t^2\boldsymbol{E} \qquad \nabla\times\left(\nabla\times\boldsymbol{B}\right) = \mu_0\nabla\times\boldsymbol{j} + \frac{1}{c^2}\partial_t\left(\nabla\times\boldsymbol{E}\right)$$

$$\boxed{\nabla^2\boldsymbol{E} - \frac{1}{c^2}\partial_t^2\boldsymbol{E} = \nabla\frac{\rho}{\varepsilon_0} + \mu_0\partial_t\boldsymbol{j}} \qquad \boxed{\nabla^2\boldsymbol{B} - \frac{1}{c^2}\partial_t^2\boldsymbol{B} = -\mu_0\nabla\times\boldsymbol{j}}$$

Speed of the wave/light:

$$c = \frac{1}{\sqrt{\varepsilon_0\mu_0}}$$

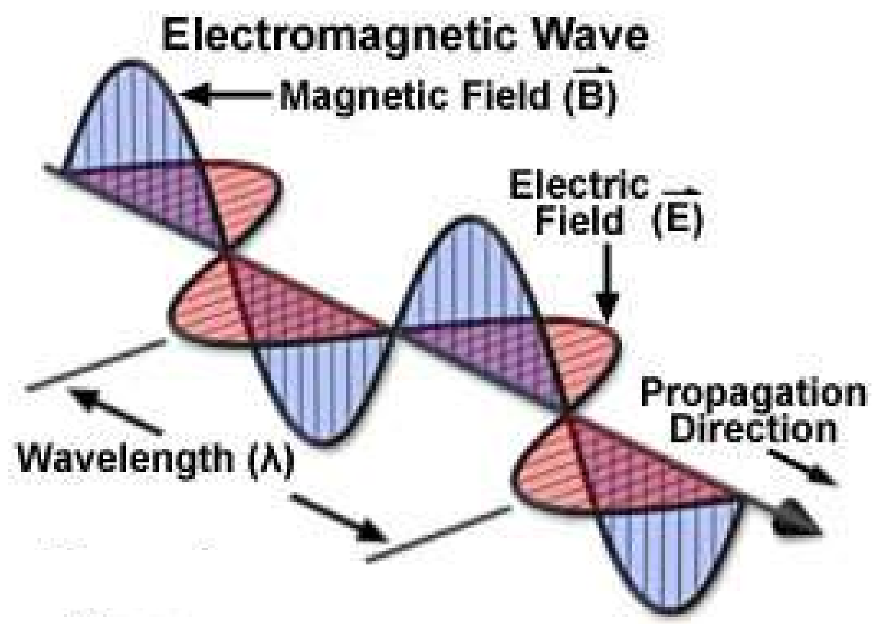
Electromagnetic wave propagation in vacuum

Plane wave solution in free space:

$$\boldsymbol{E}(\boldsymbol{r},t)=\frac{1}{(2\pi)^4}\int d^3\boldsymbol{q}\,d\omega\,\boldsymbol{E}(q,\omega)e^{-i(\omega t-\boldsymbol{qr})}$$

$$\boldsymbol{B}(\boldsymbol{r},t)=\frac{1}{(2\pi)^4}\int d^3\boldsymbol{q}\,d\omega\,\boldsymbol{B}(q,\omega)e^{-i(\omega t-\boldsymbol{qr})}$$

$$q^2\boldsymbol{E}(\boldsymbol{q},\omega)-\frac{\omega^2}{c^2}\boldsymbol{E}(\boldsymbol{q},\omega)=0$$



Isotropic dispersion relation:

$$\boxed{\omega = cq}$$

E, **B** and **q** are orthogonal to each other:

$$\mathrm{q}\cdot\mathrm{E}=0 \qquad \mathrm{q}\cdot\mathrm{B}=0$$

$$\mathrm{q}\times\mathrm{E}=\omega\mathrm{B} \qquad \mathrm{q}\times\mathrm{B}=-\frac{1}{c^2}\omega\mathrm{E}$$

Characteristic ratio of **E** and **H** fields:

$$\boxed{Z_0=\frac{E}{H}=\sqrt{\frac{\mu_0}{\varepsilon_0}}\approx 377\Omega}$$

Z_0 vacuum impedance

Energy flux and intensity

From Maxwell's II and IV equations:

$$\mathrm{B}\cdot(\nabla\times\mathrm{E}) = -\frac{1}{2}\partial_t \mathrm{B}^2$$

$$\mathrm{E}\cdot(\nabla\times\mathrm{B}) = \mu_0\left(\mathrm{E}\cdot\mathrm{j} + \varepsilon_0\frac{1}{2}\partial_t \mathrm{E}^2\right)$$

Energy balance:

$$\partial_t\left(\frac{\varepsilon_0 \mathrm{E}^2}{2} + \frac{\mathrm{B}^2}{2\mu_0}\right) = -\nabla\cdot\left(\mathrm{E}\times\frac{\mathrm{B}}{\mu_0}\right) - \mathrm{E}\cdot\mathrm{j}$$

Energy density   Poynting vector   Dissipation by free charges

$$u = \frac{\varepsilon_0 \mathrm{E}^2}{2} + \frac{\mathrm{B}^2}{2\mu_0} \qquad \boxed{S = \mathrm{E}\times\frac{\mathrm{B}}{\mu_0} = E\times H}$$

Time averaged Poynting vector of a plane wave:

$$\langle S\rangle = \langle E\times H\rangle = \left\langle \Re e\left(Ee^{-i\omega t}\right)\times \Re e\left(He^{-i\omega t}\right)\right\rangle = \left\langle \frac{Ee^{-i\omega t} + E^* e^{i\omega t}}{2}\right\rangle \times \left\langle \frac{He^{-i\omega t} + H^* e^{i\omega t}}{2}\right\rangle$$

$$\langle S\rangle = \frac{1}{2}\Re e\left(E\times H^*\right) \qquad [S] = \frac{W}{m^2}$$

Magnitude of typical E and B fields in light

5 mW LASER pointer:

collimated beam with 1 mm² diameter

$$E_\omega \sim \sqrt{Z_0 \frac{P}{A}} \sim \sqrt{Z_0 \frac{5mW}{1mm^2}} \sim 1\frac{kV}{m} \qquad B_\omega = \frac{E_\omega}{c} \sim 10\mu T$$

focused to a 1 μm² spot

$$E_\omega \sim \sqrt{Z_0 \frac{P}{A}} \sim \sqrt{Z_0 \frac{5mW}{1\mu m^2}} \sim 1\frac{MV}{m} \qquad B_\omega = \frac{E_\omega}{c} \sim 10mT$$

Linear optics is applicable below E<1MV/m

Compare these values to static fields:

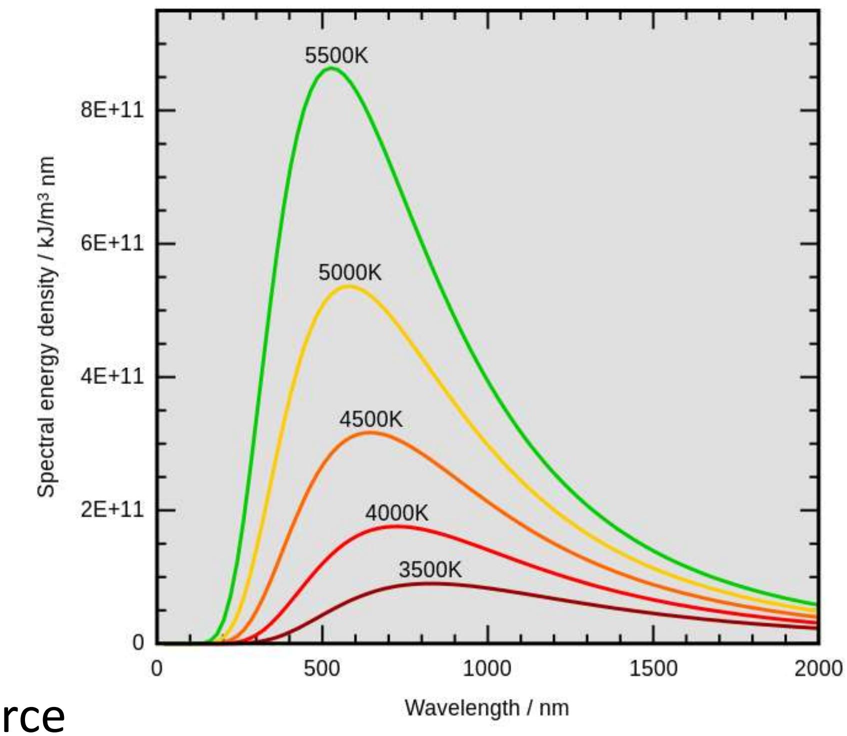
- dielectric strength of air: 3 MV/m (lightning)
- Earth's magnetic field: 25 .. 65 μT

Magnitude of typical E and B fields in light

Thermal sources:

$$B_\nu d\nu = h\nu \frac{1}{e^{\beta h\nu}-1} 2\frac{\nu^2}{c^2} d\nu$$

photon energy   population   photon DOS



Total emitted power per unit area

$$\int\int B_\nu d\nu d\Omega = \sigma T^4 \qquad \sigma=5.67\ 10^{-8}\ \mathrm{W/m^2/K^4}$$

Wien's law: $\nu_{\max} \propto T$ high frequencies → high T source

Raighly-Jeans (small ν limit): $B_\nu d\nu \approx kT 2\frac{\nu^2}{c^2} d\nu$ small frequencies → high T source

Example: a halogen lamp with T~3000 K and area of ~1 mm^2 emits P~5 W light over π solid angle

At around 600 nm in a ~1 nm broad spectra window the emitted power is ~2 mW for this lamp

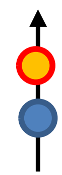
Maxwell's equations in materials

Maxwell's equations:

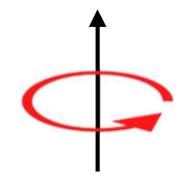
$$\nabla \cdot \mathrm{E} = \frac{1}{\varepsilon_0}\rho \qquad \nabla \cdot \mathrm{B} = 0$$

$$\nabla \times \mathrm{E} = -\partial_t \mathrm{B} \qquad \nabla \times \mathrm{B} = \mu_0\left(\mathrm{j} + \varepsilon_0 \partial_t \mathrm{E}\right)$$

Electric dipole density: $P = \dfrac{d}{\delta V}$



Magentic dipole density: $M = \dfrac{m}{\delta V}$



Free and bound charges: $\rho = \rho_f + \rho_b = \rho_f - \nabla P$

Free and bound currents: $j = j_f + j_b = j_f + \partial_t P + \nabla \times M$

Electric displacement: $D = \varepsilon_0 E + P$

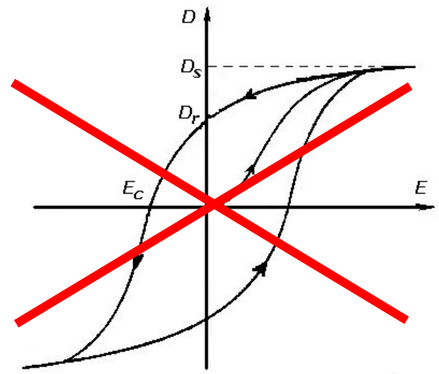
Magnetic induction: $B = \mu_0\left(H + M\right)$

$$\nabla \cdot \mathrm{D} = \rho_f \qquad \nabla \cdot \mathrm{B} = 0$$

$$\nabla \times \mathrm{E} = -\partial_t \mathrm{B} \qquad \nabla \times \mathrm{H} = \mathrm{j_f} + \partial_t \mathrm{D}$$

Electromagnetic wave propagation in linear materials

Linear response for **P**(**E**) and **M**(**H**):



$$P_\alpha = \chi^{ee}_{\alpha\beta} E_\beta$$

$$M_\alpha = \chi^{mm}_{\alpha\beta} H_\beta$$

Further response functions:

$$D_\alpha = \varepsilon_0 \varepsilon_{\alpha\beta} E_\beta = \varepsilon_0 \left(1 + \chi^{ee}_{\alpha\beta}\right) E_\beta$$

$$j_\alpha = \sigma_{\alpha\beta} E_\beta$$

$$B_\alpha = \mu_0 \mu_{\alpha\beta} H_\beta = \mu_0 \left(1 + \chi^{mm}_{\alpha\beta}\right) H_\beta$$

Charge conservation:

$$\partial_t \rho_f = -\nabla \cdot j_f$$

$$\omega \rho_f = q \cdot j_f = q_\alpha \sigma_{\alpha\beta} E_\beta$$

$$iq \cdot \left(\varepsilon_0 \varepsilon \mathrm{E}\right) = \rho_f = \frac{1}{\omega} q \cdot \left(\sigma \mathrm{E}\right)$$

$$iq \cdot \left(\varepsilon \mathrm{E} + i \frac{\sigma \mathrm{E}}{\varepsilon_0 \omega}\right) = 0$$

$$q \times \mathrm{H} = \mathrm{j_f} + \partial_t \mathrm{D} = -i\sigma E - \omega \varepsilon_0 \varepsilon E$$

$$q \times \mathrm{H} = \mathrm{j_f} + \partial_t \mathrm{D} = -\varepsilon_0 \omega \left(\varepsilon E + i \frac{\sigma E}{\varepsilon_0 \omega}\right)$$

Electromagnetic wave propagation in linear materials

Linear response for **P**(**E**) and **M**(**H**):

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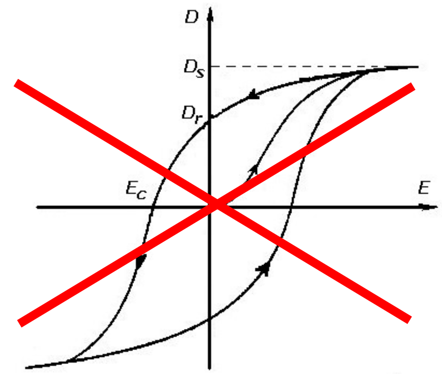


Further response functions:

$$D_\alpha = \varepsilon_0 \varepsilon_{\alpha\beta} E_\beta = \varepsilon_0 \left(1 + \chi^{ee}_{\alpha\beta}\right) E_\beta$$

$$j_\alpha = \sigma_{\alpha\beta} E_\beta$$

$$B_\alpha = \mu_0 \mu_{\alpha\beta} H_\beta = \mu_0 \left(1 + \chi^{mm}_{\alpha\beta}\right) H_\beta$$

Charge conservation:

$$\partial_t \rho_f = -\nabla \cdot j_f$$

$$\omega \rho_f = q \cdot j_f = q_\alpha \sigma_{\alpha\beta} E_\beta$$

$$iq \cdot \left(\varepsilon \mathrm{E} + i \frac{\sigma \mathrm{E}}{\varepsilon_0 \omega} \right) = 0$$

$$q \cdot \mathrm{B} = 0$$

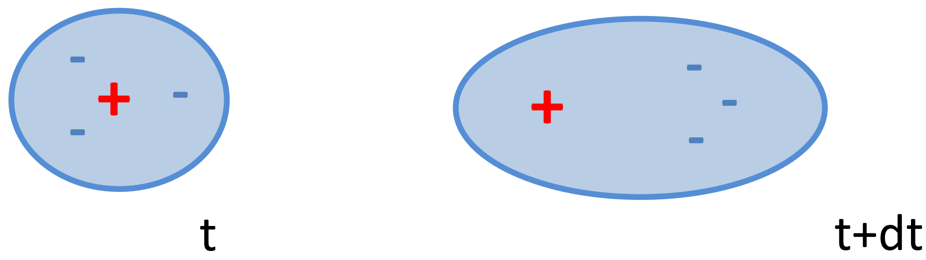
$$q \times \mathrm{E} = \omega \mathrm{B}$$

$$q \times \mathrm{H} = \mathrm{j_f} + \partial_t \mathrm{D} = -\varepsilon_0 \omega \left(\varepsilon E + i \frac{\sigma E}{\varepsilon_0 \omega} \right)$$

Complex response functions

At finite frequencies charge susceptibility and conductivity appears similarly:

$$\chi_{\alpha\beta}^{ee} = \frac{i\sigma_{\alpha\beta}}{\varepsilon_0 \omega}$$



Further response functions:

$$\varepsilon_{\alpha\beta} = 1 + \chi_{\alpha\beta}^{ee} = 1 + \frac{i\sigma_{\alpha\beta}}{\varepsilon_0 \omega}$$

$$\varepsilon_0 = 8.85 \ldots 10^{-8} s\Omega^{-1} m^{-1}$$

Electromagnetic wave propagation in isotropic materials

Isotropic, linear materials: $\varepsilon_{\alpha\beta} = \varepsilon\delta_{\alpha\beta}$

$$\mathrm{q}\cdot\varepsilon_0\varepsilon\mathrm{E} = 0$$
$$\mathrm{q}\times\mathrm{E} = \omega\mu_0\mu H$$
$$\mathrm{q}\cdot\mu_0\mu H = 0$$
$$\mathrm{q}\times\mathrm{H} = -\omega\varepsilon_0\varepsilon\mathrm{E}$$

$$q\times(q\times E) = \omega\mu_0\mu(q\times H)$$

$$\boxed{q\cdot(q\cdot E) - q^2 E = -\frac{\omega^2}{c^2}\varepsilon\mu E}$$

To satisfy Maxwell I, either ε=0 (comes latter), or q·E=0 (transverse solution)

$$q^2 E = \frac{\omega^2}{c^2}\varepsilon\mu E$$

Isotropic dispersion relation with renormalized speed of light:

$$\boxed{\omega = \frac{c}{N}q}$$

refractive index $N = \sqrt{\varepsilon\mu} = n + i\kappa$

Ratio of **E** and **H** fields:

$$\boxed{\frac{E}{H} = \sqrt{\frac{\mu_0}{\varepsilon_0}}\sqrt{\frac{\mu}{\varepsilon}} = Z_0 Z}$$

Electromagnetic wave propagation in isotropic materials

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$$\mathrm{q}\cdot\varepsilon_0\varepsilon\mathrm{E} = 0$$

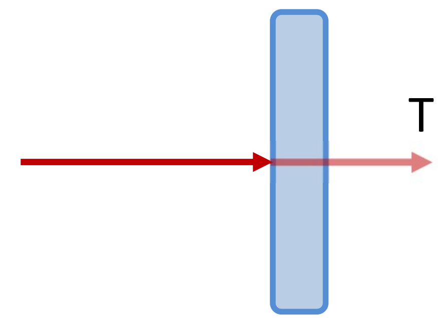
$$\mathrm{q}\times\mathrm{E} = \omega\mu_0\mu H$$

$$\mathrm{q}\cdot\mu_0\mu H = 0$$

$$\mathrm{q}\times\mathrm{H} = -\omega\varepsilon_0\varepsilon\mathrm{E}$$

$$q\times\left(q\times E\right) = \omega\mu_0\mu\left(q\times H\right)$$

$$\boxed{q\cdot(q\cdot E) - q^2 E = -\frac{\omega^2}{c^2}\varepsilon\mu E}$$



Propagation along the z direction

$$E = E_0 e^{-i\left(\omega t - qz\right)} = E_0 e^{i\frac{N\omega}{c}z} e^{-i\omega t} = E_0 e^{i\frac{n\omega}{c}z} e^{-\frac{\kappa\omega}{c}z} e^{-i\omega t}$$

phase shift attenuation

Intensity

$$I(z) = \left\langle S\right\rangle = \left\langle \Re e\left(E\right)\times\Re e\left(H\right)\right\rangle = \frac{1}{2}\frac{\left|E_0\right|^2}{Z_0 Z^*} e^{-\frac{2\kappa\omega}{c}z} = I(0)e^{-\frac{2\kappa\omega}{c}z}$$

Comparing with the Beer-Lambert law

$$\boxed{\alpha = \frac{2\omega\kappa}{c}}$$

Electromagnetic wave propagation in isotropic materials

Isotropic, linear materials: $\varepsilon_{\alpha\beta} = \varepsilon\delta_{\alpha\beta}$

$$\mathrm{q}\cdot\varepsilon_0\varepsilon\mathrm{E} = 0$$

$$\mathrm{q}\times\mathrm{E} = \omega\mu_0\mu H$$

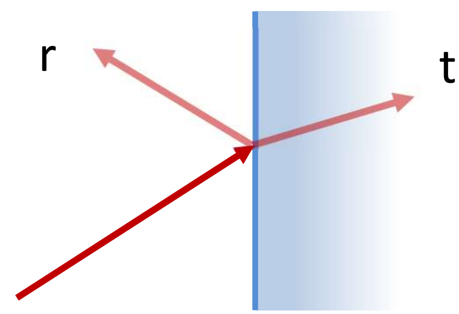
$$\mathrm{q}\cdot\mu_0\mu H = 0$$

$$\mathrm{q}\times\mathrm{H} = -\omega\varepsilon_0\varepsilon\mathrm{E}$$

$$q\times(q\times E) = \omega\mu_0\mu(q\times H)$$

$$\boxed{q\cdot(q\cdot E) - q^2 E = -\frac{\omega^2}{c^2}\varepsilon\mu E}$$

(Near) normal incidence reflection from semi-infinite sample:



match fields at the bounday

$$E_i + E_r = E_t$$

$$H_i - H_r = H_t \longrightarrow \frac{E_i}{Z_0} - \frac{E_r}{Z_0} = \frac{E_t}{Z_0 Z}$$

$$R = \frac{I_r}{I_i} = \left|\frac{E_r}{E_i}\right|^2 = \left|\frac{Z-1}{Z+1}\right|^2$$

$$r = \frac{E_r}{E_i} = \frac{Z-1}{Z+1} \approx \frac{1-N}{1+N}$$

$$\boxed{R \approx \left|\frac{1-N}{1+N}\right|^2}$$

(far from spin resonances)

Electromagnetic wave propagation in isotropic materials

Isotropic, linear materials: $\varepsilon_{\alpha\beta} = \varepsilon\delta_{\alpha\beta}$

$$\mathrm{q}\cdot\varepsilon_0\varepsilon\mathrm{E} = 0$$

$$\mathrm{q}\times\mathrm{E} = \omega\mu_0\mu H$$

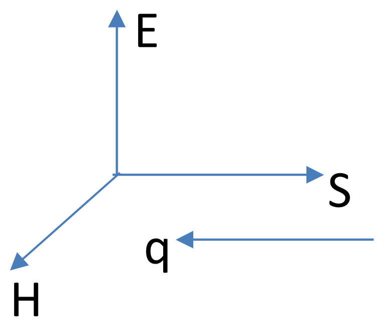
$$\mathrm{q}\cdot\mu_0\mu H = 0$$

$$\mathrm{q}\times\mathrm{H} = -\omega\varepsilon_0\varepsilon\mathrm{E}$$

$$q\times\left(q\times E\right) = \omega\mu_0\mu\left(q\times H\right)$$

$$\boxed{q\cdot(q\cdot E) - q^2 E = -\frac{\omega^2}{c^2}\varepsilon\mu E}$$

Both ε and μ are negative (for simplicity they are real)

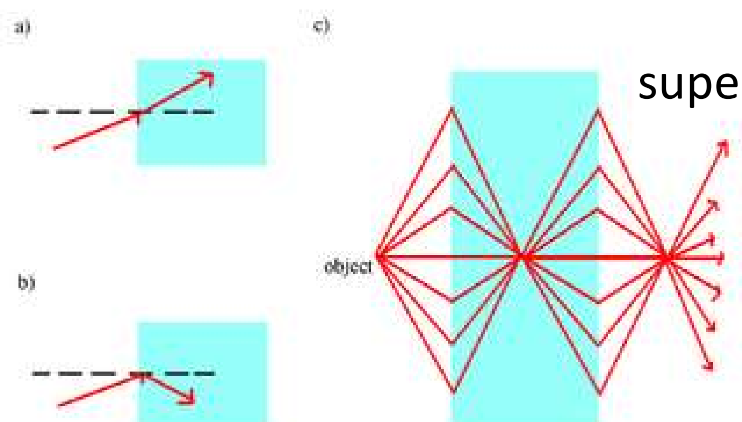


$$S = E\times H$$

Refractive index is negativ!

$$E = E_0 e^{-i\left(\omega t - qz\right)} = E_0 e^{i\frac{n\omega}{c}z} e^{-i\omega t} \qquad n = -\sqrt{\varepsilon\mu}$$

Snell's law in (a) ordinary and (b) negativ index or left-handed materials:



superlens

[wikipedia]

Complex response functions

Summary of response functions:

$$\boxed{\begin{aligned}
\varepsilon_{\alpha\beta} &= 1+\chi_{\alpha\beta}^{ee} = 1+\frac{i\sigma_{\alpha\beta}}{\varepsilon_0\omega} \\
\mu_{\alpha\beta} &= 1+\chi_{\alpha\beta}^{mm} \approx 1 \\
N &= \sqrt{\varepsilon\mu} \approx \sqrt{\varepsilon} \\
\alpha &= \frac{2\omega\kappa}{c}
\end{aligned}}$$

(far from spin resonances)

(isotropic materials)

General linear response function:

$$\langle A(r,t)\rangle = \int dr'\,dt'\,\chi(r,r',t,t')B(r',t')$$

Homogenous in material and time-independent:

$$\langle A(r,t)\rangle = \int dr'\,dt'\,\chi(r-r',t-t')B(r',t')$$

Fourier space

$$\langle A(q,\omega)\rangle = \chi(q,\omega)B(q,\omega)$$

Long-wavelength limit (a<<λ), q=0

$$\boxed{\langle A(\omega)\rangle = \chi(\omega)B(\omega)}$$

Complex response functions

If χ(t) is real then χ(ω)=χ(-ω)*

$$\chi(t)=\chi(t)^*$$

$$\chi(t)=\int\chi(\omega)e^{-i\omega t}\frac{d\omega}{2\pi} \longrightarrow \boxed{\begin{aligned}&\chi=\chi'+i\chi''\\&\chi'(\omega)=\chi'(-\omega)\\&\chi''(\omega)=-\chi''(-\omega)\end{aligned}}$$

$$\chi(t)^*=\int\chi(\omega)^*e^{i\omega t}\frac{d\omega}{2\pi}=\int\chi(-\omega)^*e^{-i\omega t}\frac{d\omega}{2\pi}$$

If a response is causal χ(ω)’ and χ(ω)” are connected by the Kramers-Kroning relation

$$\chi(t)=p(t)+q(t)$$

$$p(t)=p(-t)$$

$$q(t)=-q(-t)$$

$$\chi(\omega)=\int\chi(t)e^{i\omega t}dt=\underbrace{\int p(t)e^{i\omega t}dt}_{\chi'(\omega)}+\underbrace{\int q(t)e^{i\omega t}dt}_{\chi''(\omega)}$$

Causality: χ(t)=0 if t<0, thus p(t)=sgn(t)q(t)

$$F\left[p(t)\right]=F\left[\mathrm{sgn}(t)q(t)\right]$$

$$F\left[p(t)\right]=F\left[\mathrm{sgn}(t)\right]*F\left[q(t)\right]$$

Complex response functions

If χ(t) is real then χ(ω)=χ(-ω)*

$$\chi(t) = \chi(t)^*$$

$$\chi(t) = \int \chi(\omega) e^{-i\omega t} \frac{d\omega}{2\pi}$$

$$\chi(t)^* = \int \chi(\omega)^* e^{i\omega t} \frac{d\omega}{2\pi} = \int \chi(-\omega)^* e^{-i\omega t} \frac{d\omega}{2\pi}$$

$$\chi = \chi' + i\chi''$$

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

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

If a response is causal χ(ω)' and χ(ω)" are connected by the Kramers-Kroning relation

$$F\left[\operatorname{sgn}(t)\right] = \frac{2i}{\omega}$$

$$\boxed{\begin{aligned} \chi'(\omega) &= \frac{1}{\pi} \wp \int \frac{\chi''(\omega')}{\omega' - \omega} d\omega' \\ \chi''(\omega) &= -\frac{1}{\pi} \wp \int \frac{\chi'(\omega')}{\omega' - \omega} d\omega' \end{aligned}}$$

Kramers-Kronig transformation

Often only positive frequencies are known (absorption is measured)

$$\chi'(\omega) = \frac{1}{\pi}\wp\int \frac{\omega'+\omega}{\omega'+\omega}\frac{\chi''(\omega')}{\omega'-\omega}d\omega' = \frac{1}{\pi}\wp\int \frac{\omega'}{\omega'^2-\omega^2}\chi''(\omega')d\omega' + \frac{1}{\pi}\wp\int \frac{\omega}{\omega'^2-\omega^2}\chi''(\omega')d\omega'$$

even in ω' odd in ω'

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

For numerical evaluation we should remove divergences by adding $\int_0^\infty \frac{\omega\chi''(\omega)}{\omega'^2-\omega^2}d\omega' = 0$

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

Kramers-Kronig transformation

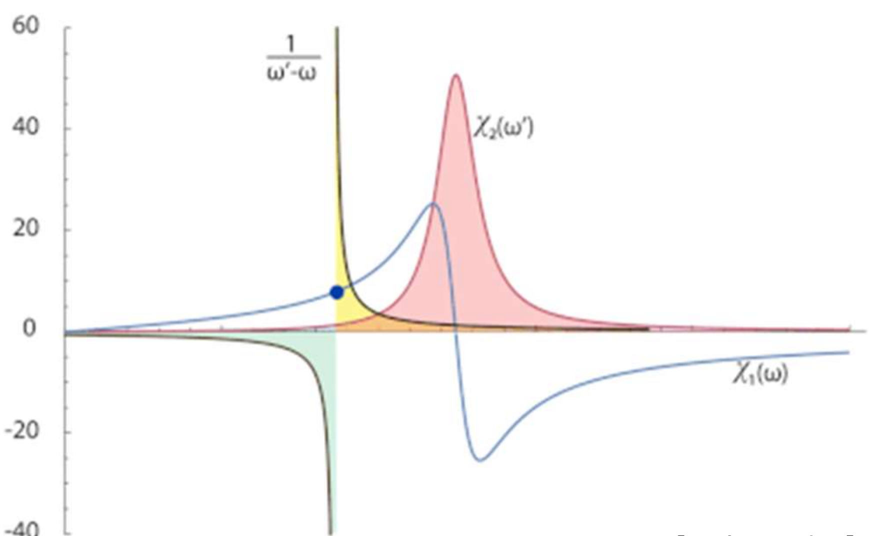
Titchmarsh theorem:

The following statements are equivalent

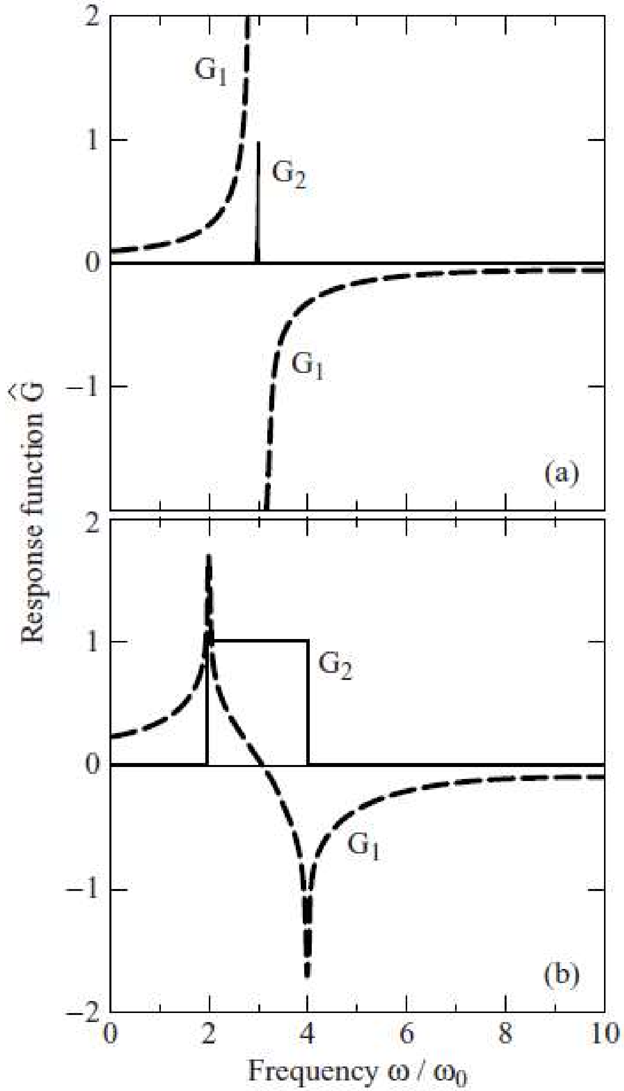
- The real and imaginary part of χ(ω) are related by Kramers-Kronig transformation
- χ(ω) is causal (χ(t)=0 if t<0)
- χ(ω) is analytic in the complex upper half-plane

$$\chi'(\omega) = \frac{1}{\pi}\wp\int \frac{\chi''(\omega')}{\omega' - \omega} d\omega'$$

$$\chi''(\omega) = -\frac{1}{\pi}\wp\int \frac{\chi'(\omega')}{\omega' - \omega} d\omega'$$



[wikipedia]



[Grüner&Dressel]

Kramers-Kronig transformation: applications

No strong static response without high-frequency losses:

$$\chi'(0)=\frac{2}{\pi}\wp\int_0^\infty \frac{\chi''(\omega')}{\omega'}d\omega'$$

Restore phase, ϕ in the measurement of normal incidence reflectivity:

$$E_r = rE_i$$

$$r=\rho e^{i\phi}$$

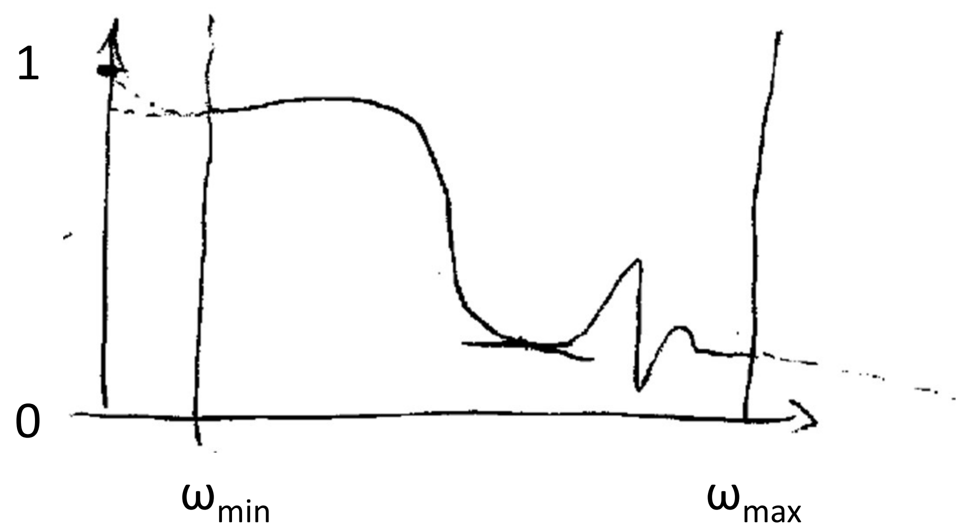
$$\ln(r)=\ln(\rho)+i\phi$$

$$R=\rho^2$$

$$\ln(r)=\frac{\ln(R)}{2}+i\phi$$

$$\phi(\omega)=-\frac{\omega}{\pi}\wp\int_0^\infty \frac{\ln\left(R(\omega')\right)}{\omega'^2-\omega^2}d\omega'$$

Then the complex refractive index can be deduced $r=\dfrac{1-N}{1+N}$ $\quad N=\dfrac{1-\sqrt{R}e^{i\phi}}{1+\sqrt{R}e^{i\phi}}$



Cook book for practical Kramers-Kronig:

- Reflectivtiy should be measured in a broad frequency range
- Join spectra in the different ranges
- Extrapolate below ω_{min} and above ω_{max} using plausible models