Theoretical Optics

Modelling material properties

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1.2 Material properties

phenomenological models for $\mathbf{P}(\mathbf{E})$ und $\mathbf{j}(\mathbf{E})$

$$\mathbf{E}(\mathbf{r},t) \rightarrow \textbf{medium} \text{ (response function)} \rightarrow \mathbf{P}(\mathbf{r},t)$$

$$\bar{\mathbf{E}}(\mathbf{r},\omega) \rightarrow \textbf{medium} \text{ (transfer function)} \rightarrow \bar{\mathbf{P}}(\mathbf{r},\omega)$$

1.2.1 Basic properties

biaxial anisotropic material

$$P_i(\mathbf{r},t) = \varepsilon_0 \sum_{j=1}^{3} \int_{-\infty}^{t} R_{ij}^{(1)}(\mathbf{r},t-t')E_j(\mathbf{r},t')dt'$$ $R(\mathbf{r},\tau)$ - response function

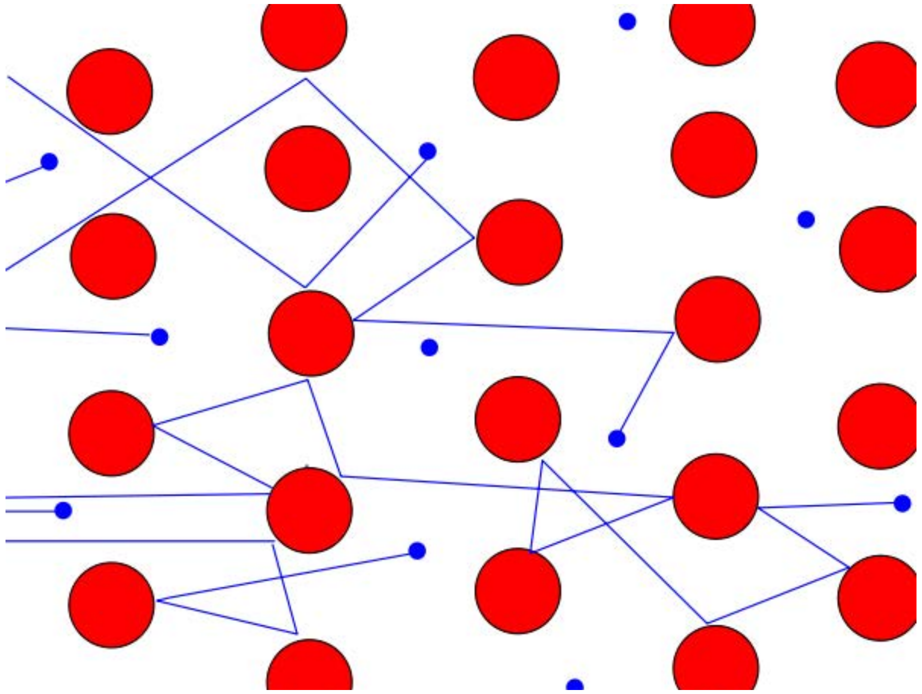
$$\bar{P}_i(\mathbf{r},\omega) = \varepsilon_0 \sum_{j=1}^{3} \chi_{ij}^{(1)}(\mathbf{r},\omega)\bar{E}_j(\mathbf{r},\omega)$$ $\chi^{(1)}(\mathbf{r},\omega)$- susceptibility

$$\boxed{\chi^{(1)}(\mathbf{r},\omega) \overset{FT}{\leftrightarrow} R(\mathbf{r},\tau)}$$

linear, homogenous, isotropic and dispersive media

$$R(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \chi^{(1)}(\omega) \mathrm{e}^{-i\omega t}\, d\omega$$

Drude model for free electrons



$$\frac{\partial^2}{\partial t^2}\mathbf{s}(\mathbf{r},t) + g\frac{\partial}{\partial t}\mathbf{s}(\mathbf{r},t) = -\frac{e}{m}\mathbf{E}(\mathbf{r},t)$$

$$\mathbf{j}(\mathbf{r},t) = -Ne\frac{\partial}{\partial t}\mathbf{s}(\mathbf{r},t)$$

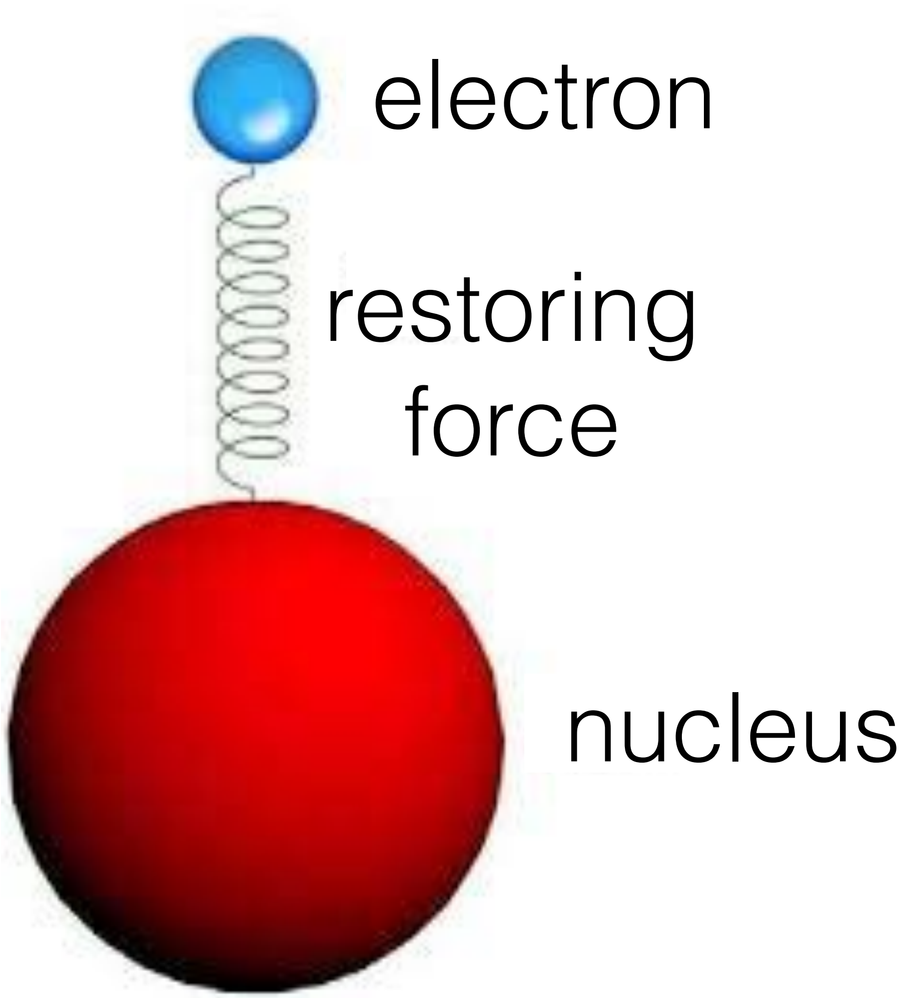
$$\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r},t) + g\mathbf{j}(\mathbf{r},t) = \frac{e^2N}{m}\mathbf{E}(\mathbf{r},t) = \varepsilon_0 f\mathbf{E}(\mathbf{r},t) = \varepsilon_0\omega_p^2\mathbf{E}(\mathbf{r},t)$$

$$\omega_p^2 = f = \frac{1}{\varepsilon_0}\frac{e^2N}{m}$$

$$-i\omega\bar{\mathbf{j}}(\mathbf{r},\omega) + g\bar{\mathbf{j}}(\mathbf{r},\omega) = \varepsilon_0\omega_p^2\bar{\mathbf{E}}(\mathbf{r},\omega)$$

$$\bar{\mathbf{j}}(\mathbf{r},\omega) = \frac{\varepsilon_0\omega_p^2}{g - i\omega}\bar{\mathbf{E}}(\mathbf{r},\omega) = \sigma(\mathbf{r},\omega)\bar{\mathbf{E}}(\mathbf{r},\omega)$$

Lorentz model for bound charges



$$\frac{\partial^2}{\partial t^2}\mathbf{s}(\mathbf{r},t) + g\frac{\partial}{\partial t}\mathbf{s}(\mathbf{r},t) + \omega_0^2\mathbf{s}(\mathbf{r},t) = \frac{q}{m}\mathbf{E}(\mathbf{r},t)$$

$$\mathbf{p}(\mathbf{r},t) = q\mathbf{s}(\mathbf{r},t)$$

$$\mathbf{P}(\mathbf{r},t) = N\mathbf{p}(\mathbf{r},t) = Nq\mathbf{s}(\mathbf{r},t)$$

$$\frac{\partial^2}{\partial t^2}\mathbf{P}(\mathbf{r},t) + g\frac{\partial}{\partial t}\mathbf{P}(\mathbf{r},t) + \omega_0^2\mathbf{P}(\mathbf{r},t) = \frac{q^2N}{m}\mathbf{E}(\mathbf{r},t) = \varepsilon_0 f\mathbf{E}(\mathbf{r},t)$$

$$f = \frac{1}{\varepsilon_0}\frac{q^2N}{m}$$

$$-\omega^2\overline{\mathbf{P}}(\mathbf{r},\omega) - ig\omega\overline{\mathbf{P}}(\mathbf{r},\omega) + \omega_0^2\overline{\mathbf{P}}(\mathbf{r},\omega) = \varepsilon_0 f\overline{\mathbf{E}}(\mathbf{r},\omega)$$

$$\boxed{\overline{\mathbf{P}}(\mathbf{r},\omega) = \frac{\varepsilon_0 f}{(\omega_0^2-\omega^2) - ig\omega}\overline{\mathbf{E}}(\mathbf{r},\omega) = \varepsilon_0\chi(\omega)\overline{\mathbf{E}}(\mathbf{r},\omega)}$$

1.2.2 Complex dielectric function

$$\mathbf{rot}\,\mathbf{rot}\,\bar{\mathbf{E}}(\mathbf{r},\omega) - \frac{\omega^2}{c_0^2}\,\bar{\mathbf{E}}(\mathbf{r},\omega) = \omega^2\mu_0\bar{\mathbf{P}}(\mathbf{r},\omega) + i\omega\mu_0\bar{\mathbf{j}}(\mathbf{r},\omega)$$

$$= [\mu_0\varepsilon_0\omega^2\chi(\omega) + i\omega\mu_0\sigma(\mathbf{r},\omega)]\bar{\mathbf{E}}(\mathbf{r},\omega)$$

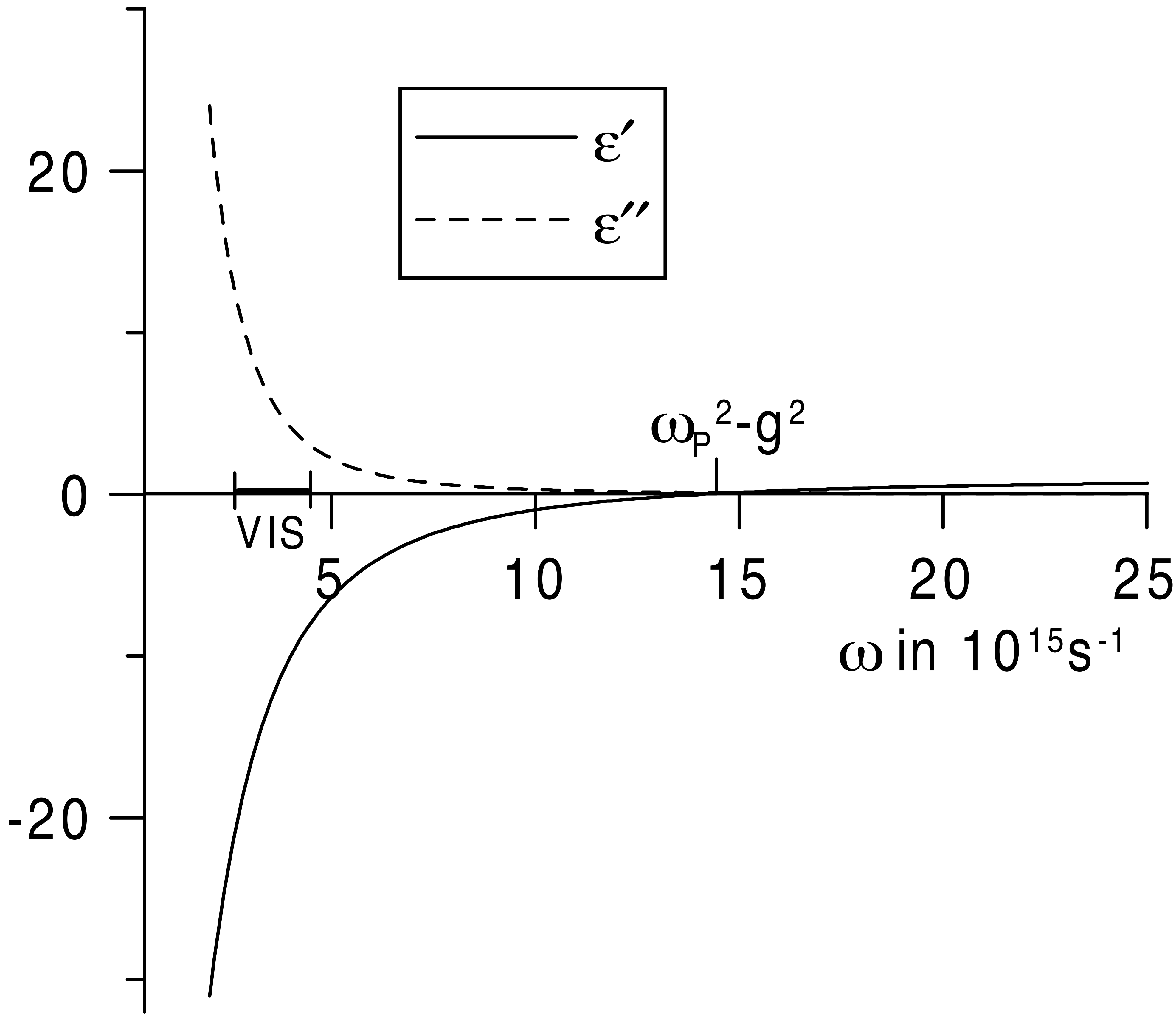
$$\mathbf{rot}\,\mathbf{rot}\,\bar{\mathbf{E}}(\mathbf{r},\omega) = \frac{\omega^2}{c_0^2}\left\{\mathbf{1} + \chi(\omega) + \frac{i}{\omega\varepsilon_0}\sigma(\mathbf{r},\omega)\right\}\bar{\mathbf{E}}(\mathbf{r},\omega)$$

$$= \frac{\omega^2}{c_0^2}\varepsilon(\omega)\bar{\mathbf{E}}(\mathbf{r},\omega)$$

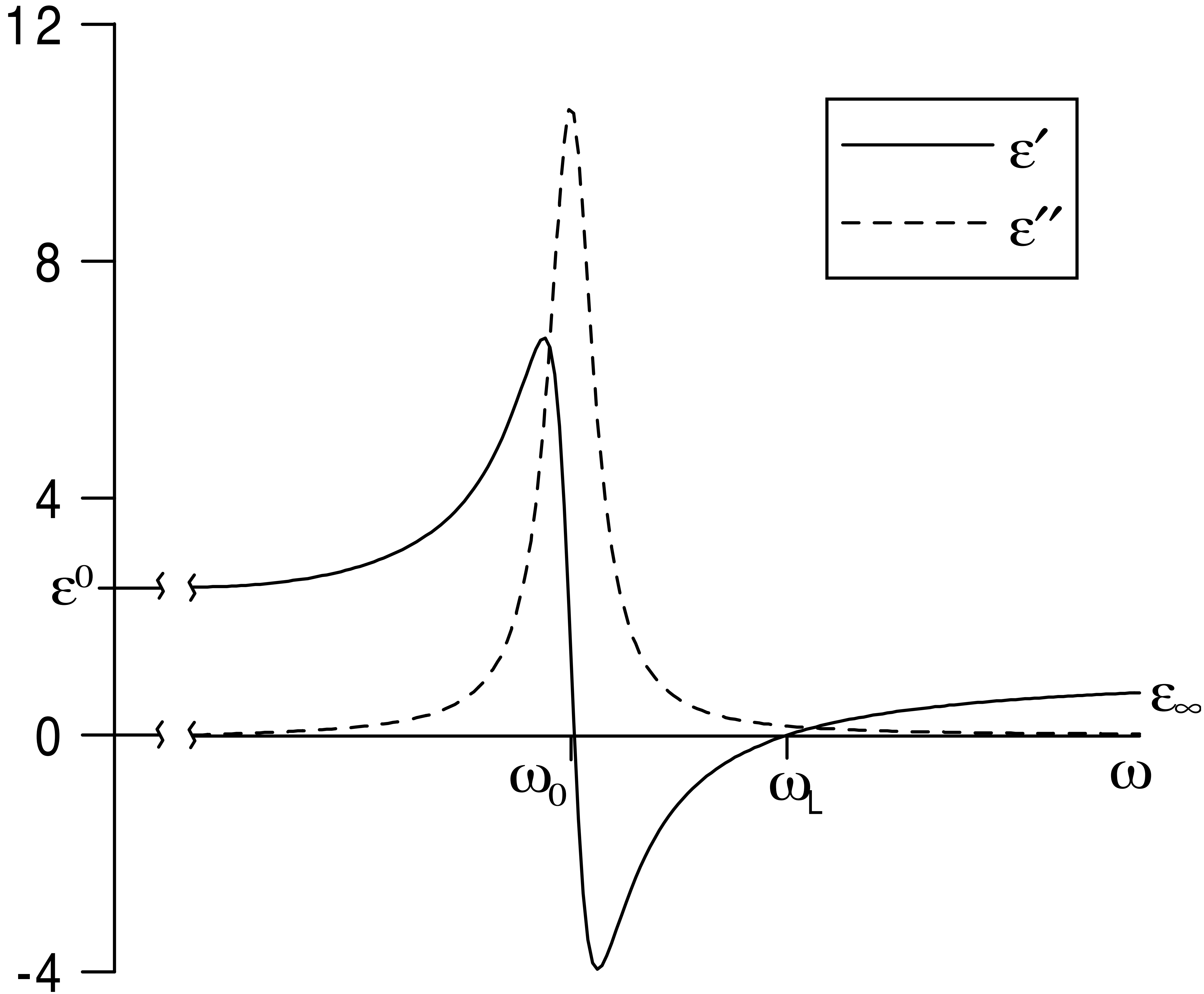
Generalized complex dielectric function

$$\varepsilon(\omega) = \mathbf{1} + \chi(\omega) + \frac{i}{\omega\varepsilon_0}\sigma(\mathbf{r},\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$$

$$\varepsilon(\omega) = 1 + \sum_j \frac{f_j}{(\omega_{0j}^2 - \omega^2) - ig_j\omega} + \frac{\omega_p^2}{-\omega^2 - ig\omega}$$



ε′
ε″
20
0
-20
VIS
5
10
15
20
25
ωP²-g²
ω in 10¹⁵s⁻¹



12
8
4
0
-4
ε′
ε″
ε⁰
ε∞
ω0
ωL
ω

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Kramers-Kronig Relation

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1.2.3 Kramers-Kronig dispersion relation

real and imaginary part of transfer function are linked by an integral

Applies when the response function is:

- time invariant
- real valued
- when causality applies.

Time invariance

$$\mathbf{P}(r,t) = \varepsilon_0 \int_{-\infty}^{t} R(t-t')\mathbf{E}(r,t')dt' \quad \leftrightarrow \quad \mathbf{P}(r,t) = \varepsilon_0 \int_{0}^{\infty} R(\tau)\mathbf{E}(r,t-\tau)d\tau$$

Real valued

$$R(\tau) = \int_{-\infty}^{\infty} \chi(\omega)\mathrm{e}^{-i\omega\tau}\, d\omega = \int_{-\infty}^{\infty} \chi^*(\omega)\mathrm{e}^{i\omega\tau}\, d\omega$$

$$\rightarrow \quad \chi(\omega) = \chi^*(-\omega)$$

Causality

$$R(\tau) = \theta(\tau) y(\tau) \quad \text{with} \quad \theta(\tau) = \begin{cases} 1 & \text{for } \tau > 0 \\ 1/2 & \text{for } \tau = 0 \\ 0 & \text{for } \tau < 0 \end{cases}$$ Heaviside distribution

$$\chi(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} R(\tau)\mathrm{e}^{i\omega\tau}\, d\tau = \frac{1}{2\pi}\int_{-\infty}^{\infty} \theta(\tau) y(\tau)\mathrm{e}^{i\omega\tau}\, d\tau$$

$$= \int_{-\infty}^{\infty} \bar{\theta}(\omega - \bar{\omega})\bar{y}(\bar{\omega})\, d\bar{\omega}$$

$$2\pi\bar{\theta}(\omega) = \int_{-\infty}^{\infty} \theta(t) e^{i\omega t} dt = \lim_{\varepsilon\to 0} \frac{i}{\omega + i\varepsilon} = P\frac{i}{\omega} + \pi\delta(\omega)$$

proof in tutorials

Delta distribution: $\int_{-\infty}^{\infty} \delta(\omega - \omega_0) f(\omega) d\omega = f(\omega_0)$

Cauchy principal value:

$$P \int_{-\infty}^{\infty} d\omega \frac{i}{\omega} f(\omega) = \lim_{\alpha \to 0} \left[\int_{-\infty}^{-\alpha} d\omega \frac{i}{\omega} f(\omega) + \int_{\alpha}^{\infty} d\omega \frac{i}{\omega} f(\omega) \right]$$

$$\chi(\omega) = \frac{1}{2\pi} P \int_{-\infty}^{\infty} d\bar{\omega} \, \frac{i \, \bar{y}(\bar{\omega})}{\omega - \bar{\omega}} + \frac{\bar{y}(\omega)}{2} \qquad \textbf{(*)}$$

(1) $y(-\tau) = y(\tau)$ even function

(2) $y(-\tau) = -y(\tau)$ odd function

(1) Even function

$$\bar{y}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, y(\tau) e^{i\omega\tau} = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, y(\tau) e^{-i\omega\tau} = \bar{y}^*(\omega)$$

$\bar{y}(\omega)$ real valued $\longrightarrow$

$$\chi^*(\omega) = -\frac{1}{2\pi} P \int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega - \bar{\omega}} + \frac{\bar{y}(\omega)}{2}$$

$$\chi(\omega) + \chi^*(\omega) = \frac{1}{2\pi} P \int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega - \bar{\omega}} + \frac{\bar{y}(\omega)}{2} - \frac{1}{2\pi} P \int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega - \bar{\omega}} + \frac{\bar{y}(\omega)}{2} = \bar{y}(\omega) \quad \text{(a)}$$

$$\chi(\omega) - \chi^*(\omega) = \cdots = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega - \bar{\omega}} \quad \text{(b)}$$

inserting (a) into the right hand side of (b)

$$\Im[\chi(\omega)] = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\bar{\omega}\, \frac{\Re[\chi(\bar{\omega})]}{\bar{\omega} - \omega}$$

(2) Odd function

$$\bar{y}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, y(\tau) e^{i\omega\tau} = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, y(\tau) e^{-i\omega\tau} = -\bar{y}^*(\omega)$$

$$\boxed{\chi^*(\omega) = \frac{1}{2\pi} P\int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega - \bar{\omega}} - \frac{\bar{y}(\omega)}{2}}$$

$$\chi(\omega) - \chi^*(\omega) = \frac{1}{2\pi} P\int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega-\bar{\omega}} + \frac{\bar{y}(\omega)}{2} - \frac{1}{2\pi} P\int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega-\bar{\omega}} + \frac{\bar{y}(\omega)}{2} = \bar{y}(\omega) \quad \text{(a)}$$

$$\chi(\omega) + \chi^*(\omega) = \cdots = \frac{1}{\pi} P\int_{-\infty}^{\infty} d\bar{\omega}\, \frac{i\,\bar{y}(\bar{\omega})}{\omega-\bar{\omega}} \quad \text{(b)}$$

inserting (a) into the right hand side of (b)

$$\boxed{\Re[\chi(\omega)] = \frac{1}{\pi} P\int_{-\infty}^{\infty} d\bar{\omega}\, \frac{\Im[\chi(\bar{\omega})]}{\bar{\omega} - \omega}}$$

Using

$$\chi(\omega) = \chi^*(-\omega) \quad \rightarrow \quad \chi'(\omega) = \chi'(-\omega) \quad \text{and} \quad \chi''(\omega) = -\chi''(-\omega)$$

and

$$\chi(\omega) = \varepsilon(\omega) - 1 = [\varepsilon'(\omega) - 1] + i\varepsilon''(\omega)$$

it follows for the two Kramers-Kronig relations for the permittivity that

$$\varepsilon'(\omega) - 1 = \frac{2}{\pi} P \int_0^\infty d\overline{\omega}\, \frac{\overline{\omega}\varepsilon''(\overline{\omega})}{\overline{\omega}^2 - \omega^2}$$

$$\varepsilon''(\omega) = -\frac{2}{\pi}\omega P \int_0^\infty d\overline{\omega}\, \frac{[\varepsilon'(\overline{\omega}) - 1]}{\overline{\omega}^2 - \omega^2}$$

Example: absorption line at a discrete frequency.

$\varepsilon''(\omega) \sim \delta(\omega - \omega_0)$.

Contribution to the integral $\overline{\omega} = \omega_0$.

Real part $\varepsilon'(\omega) - 1 \sim \frac{\omega_0}{\omega_0^2 - \omega^2}$.

Lorentzian line

Kramers-Kronig Relation

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