7.10 Causality, Kramers–Kronig relations

Observe that having a frequency-dependent $\epsilon(\omega)$ implies nonlocal effects in time.

Aside: in QM, a LOCAL potential $\hat{V}^{\text{local}}$ only involves one point in space, i.e.

$$\hat{V}^{\text{local}}\psi \longrightarrow V(\vec{r})\,\psi(\vec{r})$$

whereas a nonlocal potential $\hat{V}^{\text{nonlocal}}$ involves different $\vec{r}\,'$, i.e. $\hat{V}^{\text{nonlocal}}\psi \to \int d^3x'\, V(\vec{x},\vec{x}\,')\,\psi(\vec{x}\,')$

$\Rightarrow$ Here our starting assumption is the local relationship in ω, namely $\vec{D}(\omega)=\epsilon(\omega)\vec{E}(\omega)$, implying that the time-dependences look like:

$$\vec{D}(\vec{x},t)=\int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{2\pi}}\,e^{-i\omega t}\,D(\vec{x},\omega)$$

$$=\int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{2\pi}}\,e^{-i\omega t}\,\epsilon(\omega)\,\vec{E}(\vec{x},\omega)$$

and plugging in $\vec{E}(\vec{x},\omega)=\int\frac{dt'}{\sqrt{2\pi}}\,e^{i\omega t'}\,\vec{E}(\vec{x},t')$

$$\Rightarrow \vec{D}(\vec{x},t)=\int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{dt'}{\sqrt{2\pi}}\,e^{-i\omega t}\,\epsilon(\omega)\,e^{i\omega t'}\,\vec{E}(\vec{x},t')$$

$$=\int_{-\infty}^{\infty}\frac{dt'}{\sqrt{2\pi}}\,\epsilon(t-t')\,\vec{E}(\vec{x},t')$$

(F.T. of $\epsilon(\omega)$)

which can be rewritten as:

$$\boxed{\vec{D}(\vec{x},t) = \int_{-\infty}^{\infty} \frac{d\tau}{\sqrt{2\pi}}\, \epsilon(\tau)\, \vec{E}(\vec{x}, t-\tau)} \quad (*)$$

This is a practical example of the Fourier transform "convolution" or "Faltung" theorem.

It is useful to recast the preceding result as:

$$\vec{D}(\vec{x},t) = \epsilon_0 \vec{E}(\vec{x},t) + \epsilon_0 \int_{-\infty}^{\infty} G(\tau)\, \vec{E}(\vec{x}, t-\tau)\, d\tau$$

where

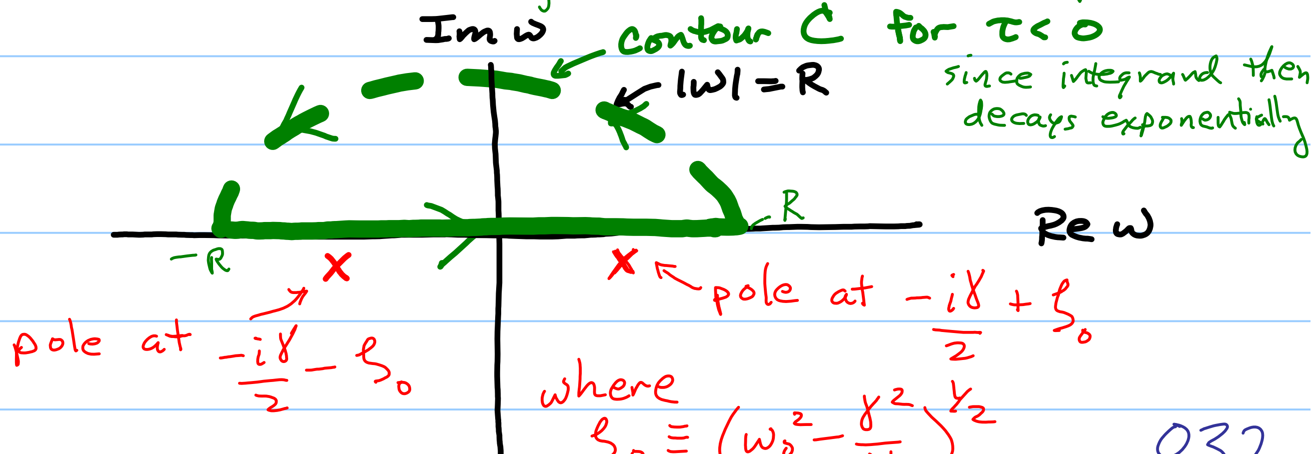
$$G(\tau) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\frac{\epsilon(\omega)}{\epsilon_0} - 1 \right) e^{-i\omega\tau}\, d\omega$$

The implications of these results can be explored by considering the single resonance model for $\epsilon(\omega)$, namely

$$\frac{\epsilon(\omega)}{\epsilon_0} - 1 = \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

$$\Rightarrow G(\tau) = \frac{\omega_p^2}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

The structure of this integral in the complex plane is:



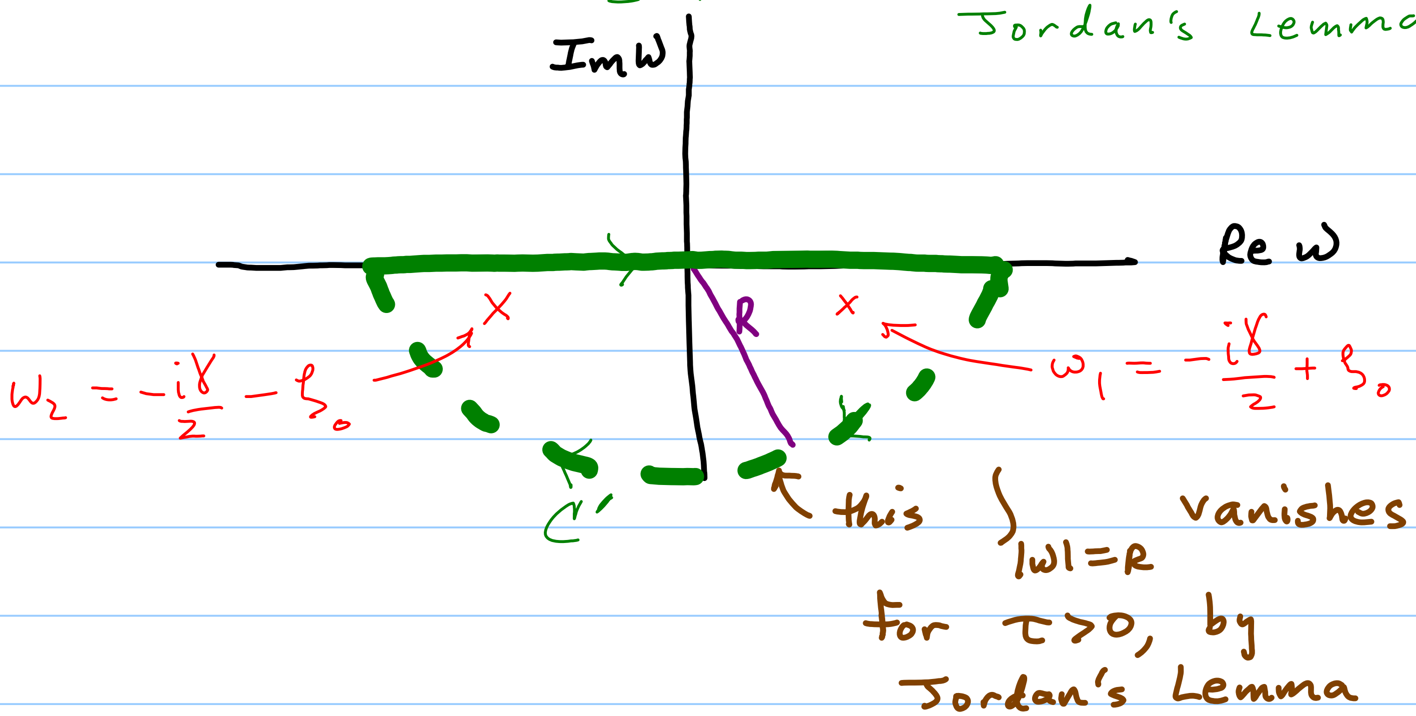
Thus for $\tau < 0$, $G(\tau) = \frac{\omega_p^2}{2\pi} \oint_C \frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega} d\omega$

Since by Jordan's Lemma, the $\int_{|\omega|=R}$ vanishes @ $R \to \infty$

Thus, since we have a closed-contour integral, with an integrand analytic within C,

$$\Rightarrow \quad G(\tau) = 0 \quad \text{for } \tau < 0$$

But for $\tau > 0$, we must close the contour in the LOWER $\frac{1}{2}$-plane, in order to use Jordan's Lemma:



Thus,

$$G(\tau) = \frac{\omega_p^2}{2\pi} \oint_{C'} \frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega} d\omega$$

$$= \frac{\omega_p^2}{2\pi}(-2\pi i)\left\{ \mathrm{Res}\left(\frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega}, \omega_1\right) + \mathrm{Res}\left(\frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega}, \omega_2\right)\right\}$$

Aside: to evaluate $\operatorname{Res} \frac{Q(z)}{P(z)}$ at a simple zero of $P(z_0)$, if $Q(z_0) \neq 0$ is analytic,

is equal to $\frac{Q(z_0)}{P'(z_0)}$

Hence we have

$$G(\tau) = -i\omega_p^2 \left\{ \frac{e^{-i\tau(\xi_0 - \frac{i\gamma}{2})}}{-i\gamma - 2(\xi_0 - \frac{i\gamma}{2})} + \frac{e^{-i\tau(-\xi_0 - \frac{i\gamma}{2})}}{-i\gamma - 2(-\xi_0 - \frac{i\gamma}{2})} \right.$$

$$= \frac{\omega_p^2}{\xi_0} e^{-\gamma\tau/2} \sin(\xi_0 \tau)$$

or in summary,

$$G(\tau) = \begin{cases} 0, & \tau < 0 \\ \omega_p^2 e^{-\frac{\gamma\tau}{2}} \frac{\sin \xi_0 \tau}{\xi_0}, & \tau > 0 \end{cases}$$

or

$$G(\tau) = \omega_p^2 e^{-\frac{\gamma\tau}{2}} \frac{\sin \xi_0 \tau}{\xi_0} \Theta(\tau)$$

where $\Theta(\tau) = \begin{cases} 1, & \tau > 0 \\ 0, & \tau < 0 \end{cases}$

$\Rightarrow$ Since typical damping constants are in the range $\gamma \simeq 10^{7}$ to $10^{9}\ s^{-1}$, the <u>nonlocality</u> in time is limited to short durations of order 10^{-7} to 10^{-9} sec.

Causality implications

We saw that $G(\tau)=0$ for $\tau<0$, which makes sense since this means that Eq. (*) above implies that $\vec{D}(\vec{x},t)$ only depends on $\vec{E}(\vec{x},t')$ at earlier times $t'<t$. In our math, this reasoning was not tied to our specific model for $\epsilon(\omega)$.

$\Rightarrow$ In fact, it was just necessary to have $\frac{\epsilon(\omega)}{\epsilon_0}$ ANALYTIC on the REAL ω-AXIS and in the UPPER $\frac{1}{2}$-Plane, and also,

$$\frac{\epsilon(\omega)}{\epsilon_0}-1 \xrightarrow[|\omega|\to\infty]{} 0$$

which allows us to use Jordan's Lemma to say $\int_{|\omega|=R} \to 0$

and this in turn allows us to write

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1+\int_0^\infty G(\tau)e^{i\omega\tau}\,d\tau$$

with $G(\tau)=$ REAL

since $\vec{D}$ and $\vec{E}$ are real in:

$$\vec{D}(\vec{x},t) = \epsilon_0\vec{E}(\vec{x},t)+\epsilon_0\int_0^\infty G(\tau)\vec{E}(\vec{x},t-\tau)\,d\tau$$

$$\Rightarrow \epsilon^*(\omega^*) = 1+\int_0^\infty G(\tau)e^{-i\omega\tau}\,d\tau = \epsilon(-\omega)$$

$$\Rightarrow \epsilon^*(\omega^*) = \epsilon(-\omega)$$

Kramers – Kronig relations

We have now seen that CAUSALITY implies that $\frac{\epsilon(\omega)}{\epsilon_0}$ is analytic in the upper $\frac{1}{2}$-plane.

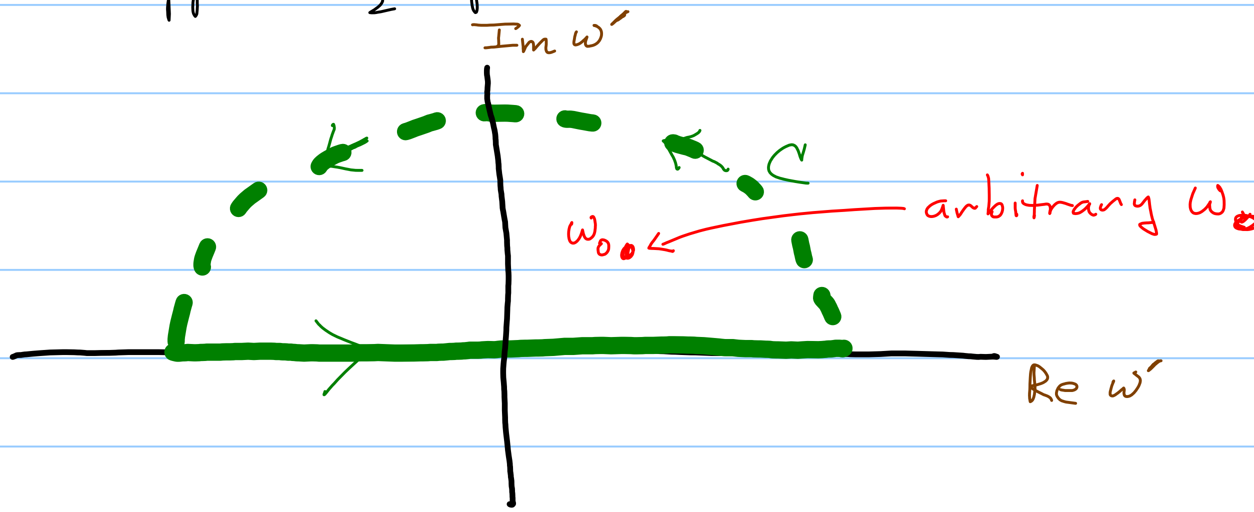
This simple fact enables us to relate

$$\mathrm{Re}(\epsilon(\omega)) \text{ to } \mathrm{Im}(\epsilon(\omega)),$$

by starting from the following identity:

$$\frac{\epsilon(\omega_0)}{\epsilon_0} - 1 = \frac{1}{2\pi i} \oint_C \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega_0} \, d\omega'$$

For any ω_0 having $\mathrm{Im}\,\omega_0 > 0$ where closed contour C is along the real ω'-axis and then closed at ∞ in the upper $\frac{1}{2}$-plane.



The semicircle portion vanishes here since:

$$\left| \frac{\epsilon(\omega')}{\epsilon_0} - 1 \right| \xrightarrow[|\omega'| \to \infty]{} \lesssim O(|\omega'|^{-2})$$

And therefore we also have:

$$\frac{\epsilon(\omega_0)}{\epsilon_0} - 1 = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega_0}\, d\omega'$$

Next, let $\omega_0 = \omega + i\delta$ with $\delta \to 0^+$

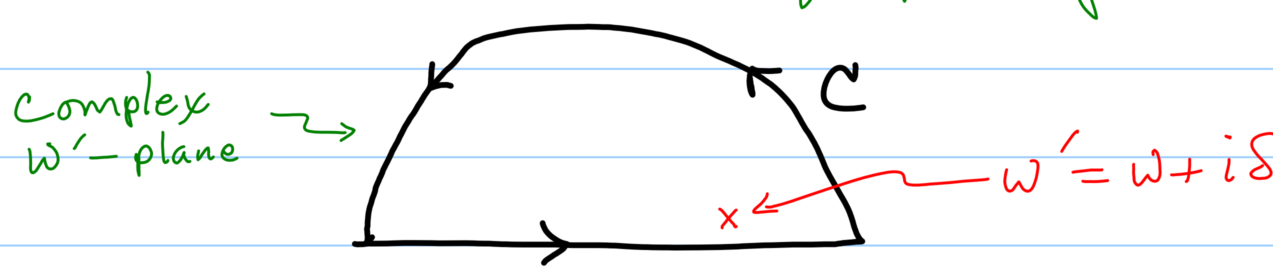
$$\Rightarrow \frac{\epsilon(\omega)}{\epsilon_0} - 1 = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega - i\delta}\, d\omega'$$

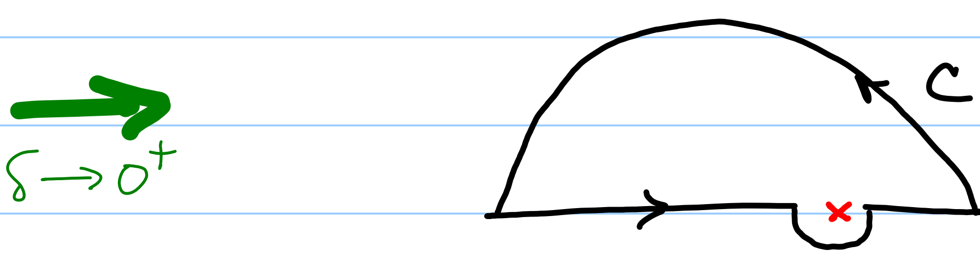
Before proceeding, consider a brief aside. The following identity is useful,

$$\frac{1}{\omega' - \omega - i\delta} = \mathcal{P}\frac{1}{\omega' - \omega} + i\pi\delta(\omega' - \omega)$$

where $\mathcal{P}$ merely signals that any integration carried out over the point of singularity is to be handled as a PRINCIPAL VALUE.

This can be illustrated graphically as follows,

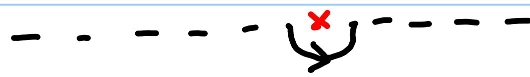




which equals

 $= \mathcal{P}\dfrac{1}{\omega'-\omega}$

$+$

 $= \dfrac{2i\pi}{2}\delta(\omega-\omega')$

Plugging this identity into the above integral gives:

$$\frac{\epsilon(\omega)}{\epsilon_0} - 1 = \frac{1}{2\pi i}\mathcal{P}\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega'-\omega}\,d\omega' + \frac{1}{2}\left(\frac{\epsilon(\omega)}{\epsilon_0} - 1\right)$$

or

$$\frac{\epsilon(\omega)}{\epsilon_0} - 1 = \frac{1}{\pi i}\mathcal{P}\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega'-\omega}\,d\omega'$$

Next, simply take the real and imaginary parts of this equation:

$$\mathrm{Re}\,\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right)}{\omega'-\omega}\,d\omega'$$

and
$$\mathrm{Im}\,\frac{\epsilon(\omega)}{\epsilon_0} = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\mathrm{Re}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right) - 1}{\omega'-\omega}\,d\omega'$$

Now recall the symmetry properties $\epsilon^*(\omega^*) = \epsilon(-\omega)$

$\Rightarrow \boxed{\mathrm{Re}\,\epsilon(-\omega) = \mathrm{Re}\,\epsilon(\omega)}$ and $\mathrm{Im}\,\epsilon(-\omega) = -\mathrm{Im}\,\epsilon(\omega)$

⇒ we can recast these as integrals only over positive ω only, as

$$\boxed{\begin{aligned} \mathrm{Re}\left(\frac{\epsilon(\omega)}{\epsilon_0}\right) &= 1 + \frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{\omega' \,\mathrm{Im}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right]}{\omega'^2 - \omega^2}\, d\omega' \\ \mathrm{Im}\left(\frac{\epsilon(\omega)}{\epsilon_0}\right) &= -\frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{\mathrm{Re}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] - 1}{\omega'^2 - \omega^2}\, d\omega' \end{aligned}}$$

These are the Kramers – Kronig dispersion relations, which reflect little more physics than causality and analyticity.

Derivation of those last form(s):

$$\mathrm{Re}\,\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right)}{\omega' - \omega}\, d\omega'$$

$$= 1 + \frac{1}{\pi}\mathcal{P}\int_0^\infty \frac{\mathrm{Im}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right) d\omega'}{\omega' - \omega} + \frac{\mathcal{P}}{\pi}\int_{-\infty}^{0} \frac{\mathrm{Im}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right) d\omega'}{\omega' - \omega}$$

set $\omega' = -\omega''$, $d\omega' = -d\omega''$

$$-\frac{\mathcal{P}}{\pi}\int_\infty^0 \frac{\mathrm{Im}\left(\frac{\epsilon(-\omega'')}{\epsilon_0}\right) d\omega''}{-\omega'' - \omega}$$

$$-\frac{\mathcal{P}}{\pi}\int_0^\infty \frac{-\mathrm{Im}\left(\frac{\epsilon(\omega'')}{\epsilon_0}\right) d\omega''}{\omega'' + \omega}$$

$$= 1 + \frac{1}{\pi}\mathcal{P}\int_0^\infty \mathrm{Im}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right)\left(\frac{1}{\omega' - \omega} + \frac{1}{\omega' + \omega}\right) d\omega'$$

or finally,

$$\text{Re}\,\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{2}{\pi} P\int_0^\infty \frac{\omega' \,\text{Im}\left(\frac{\epsilon(\omega')}{\epsilon_0}\right)}{\omega'^2 - \omega^2}$$

checks! ✓

Note also that since $\epsilon^*(\omega^*) = \epsilon(-\omega)$

$$= \epsilon_r(\omega^*) - i\,\epsilon_i(\omega^*) = \epsilon_r(-\omega) + i\,\epsilon_i(-\omega)$$

and if we evaluate this for <u>real ω</u>,
this gives immediately

$$\epsilon_r(\omega) = \epsilon_r(-\omega) \qquad \text{(real part is even)}$$

whereas

$$\epsilon_i(\omega) = -\epsilon_i(-\omega) \qquad \text{(imag. part is odd)}$$

<u>**Implications**</u> Knowledge of $\text{Im}\,\epsilon(\omega)$, e.g. from light absorption experiments at <u>all</u> ω, determines $\text{Re}\,\epsilon(\omega)$, or vice versa!

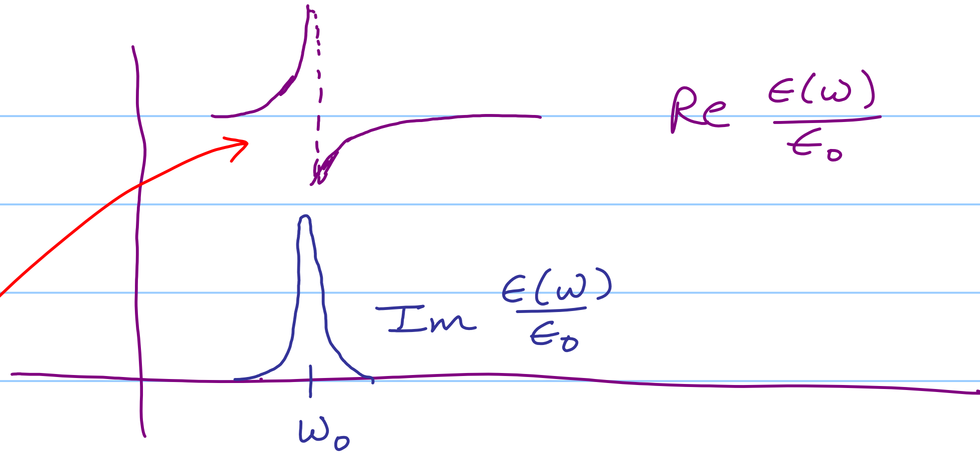
e.g. for a single narrow absorption line,

$$\text{Im}\,\epsilon(\omega') \simeq \frac{\pi K}{2\omega_0}\,\delta(\omega' - \omega_0) + \text{smooth stuff}$$

$$\Rightarrow \text{Re}\,\epsilon(\omega) \cong \frac{K}{\omega_0^2 - \omega^2} + \bar{\epsilon}$$

contributions from the smooth, nonresonant parts of $\text{Im}\,\epsilon(\omega')$

See, e.g. Fig. 7.8, p. 311



This type of interference, of opposite signs below and above the resonance, arises in other contexts, especially the "Fano lineshape" characterizing the interaction between a discrete (bound) state and a continuum state in quantum mechanics.

See U. Fano, Phys. Rev. 124, 1866 (1961)

"autoionizing line shape" — 6191 citations to date

also Fano, Nuovo Cimento 12, 154 (1935)
or translated in J. Res. NIST 110, 583 (2005)

Aside EM-waves in conductors, and/or materials with constant, complex ϵ, μ

$$\Rightarrow \nabla\cdot\vec{E} = \frac{\rho_f}{\epsilon}, \quad \nabla\cdot\vec{B} = 0, \quad \vec{J} = \sigma\vec{E}$$

$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t} \qquad \nabla\times\vec{B} = \mu\sigma\vec{E} + \mu\epsilon\frac{\partial\vec{E}}{\partial t}$$

$$\Rightarrow \nabla\times(\nabla\times\vec{E}) = \nabla(\nabla\cdot\vec{E}) - \nabla^2\vec{E} = -\frac{\partial}{\partial t}\left(\mu\sigma\vec{E} + \mu\epsilon\frac{\partial\vec{E}}{\partial t}\right)$$

$$\Rightarrow \boxed{\begin{aligned} \nabla^2\vec{E} &= \mu\sigma\frac{\partial\vec{E}}{\partial t} + \mu\epsilon\frac{\partial^2\vec{E}}{\partial t^2} \\ \nabla^2\vec{B} &= \mu\sigma\frac{\partial\vec{B}}{\partial t} + \mu\epsilon\frac{\partial^2\vec{B}}{\partial t^2} \end{aligned}}$$

As before, consider any single component of $\vec{E}$ or $\vec{B}$, denoted now by $u(\vec{x},t)$, so a 1D plane wave obeys

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \mu\sigma \frac{\partial u}{\partial t} + \mu\epsilon \frac{\partial^2 u}{\partial t^2}$$

$\Rightarrow$ Try solution $u(x,t) = u_0 e^{i(kx-\omega t)}$

$$\Rightarrow \quad -k^2 u_0 e^{i(kx-\omega t)} = (-i\omega\mu\sigma - \omega^2\mu\epsilon) u_0 e^{i(kx-\omega t)}$$

$$\Rightarrow \quad \boxed{k^2 = \omega^2\mu\epsilon + i\mu\sigma\omega}$$

or

$$k = (\omega^2\mu\epsilon + i\mu\sigma\omega)^{1/2} \equiv k_r + i k_i$$

where $k_r > 0$, $k_i \geq 0$

This expression shows that k_i is nonzero if EITHER $\sigma \neq 0$ OR if $\mathrm{Im}(\epsilon\mu) \neq 0$ in which case

$$u(x,t) \rightarrow u_0 e^{-k_i x} e^{i(k_r x - \omega t)}$$