Kramers - Kronig Overview

In this section we will describe the Kramers - Kronig relation. Points to take away

1. For any causal response function, e.g. $\sigma(\omega)$ and $\chi(\omega)$, $\varepsilon(\omega)$, etc The real and imaginary parts are related by a specific integral relation

   The real part of $\varepsilon(\omega)$ determines the phase and group velocities of the wave

   The imag part of $\varepsilon(\omega)$ determines the damping of the wave.

2. The Kramers Kronig relations show that the (correct) qualitative features of the Lorenz model for $\chi_e(\omega)$ are very generic, dictated by causality.

Causality, Analyticity, & Kramers - Kronig Relations

Recall that $\sigma(t)$ is a causal function:

$$j(t) = \int_{-\infty}^{\infty} dt' \, \sigma(t-t') \, E(t') \quad \leftarrow \text{Depends on past values of } E$$

i.e. $\sigma(t) = 0$ for $t < 0$ (or $\sigma(t-t')$ vanishes when $t' > t$)

Similary $\chi(t-t')$ is also causal:

$$j(t) = \int_{-\infty}^{\infty} \chi(t-t') \, \partial_{t'} E(t') \, dt'$$

i.e. $\chi(t) = 0$ for $t < 0$.

The Fourier transform of a causal function is

$$(1) \quad \boxed{\chi(\omega) = \int_{0}^{\infty} dt \, e^{i\omega t} \, \chi(t)}$$

The fourier integral guarantees that $\sigma(\omega)$ is an analytic function of ω for ω in the Upper Half Plane (UHP), $\mathrm{Im}\,\omega \geq 0$. To see this...

... note that the exponential becomes increasingly convergent for ω in UHP and $t > 0$ (causality)

$$e^{i\omega t} = e^{i(\mathrm{Re}\,\omega + i\,\mathrm{Im}\,\omega)t} = e^{i(\mathrm{Re}\,\omega)t}\, e^{-\overbrace{(\mathrm{Im}\,\omega)}^{\text{greater than zero}} t}$$

Thus the fourier integral provides an analytic continuation of χ for ω complex.

For such causal functions, which are always analytic in UHP, have a relation between the real and imaginary parts

Principal value (see below)

$$\boxed{\begin{aligned} \mathrm{Re}\,\chi(\omega) &= -\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{P}{\omega-\omega'}\, \mathrm{Im}\,\chi(\omega) \\ \mathrm{Im}\,\chi(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{P}{\omega-\omega'}\, \mathrm{Re}\,\chi(\omega) \end{aligned}}$$

Kramers Kronig relations (Proof Below)

From Eq. (1) on previous page

$$\mathrm{Re}\,\chi(-\omega) = \mathrm{Re}\,\chi(\omega)$$

$$\mathrm{Im}\,\chi(-\omega) = -\mathrm{Im}\,\chi(\omega)$$

So these can be written:

$$\text{Re}\,\chi(\omega) = -\frac{2}{\pi}\int_0^\infty \frac{P}{\omega^2-(\omega')^2}\,\omega'\,\text{Im}\,\chi(\omega')$$

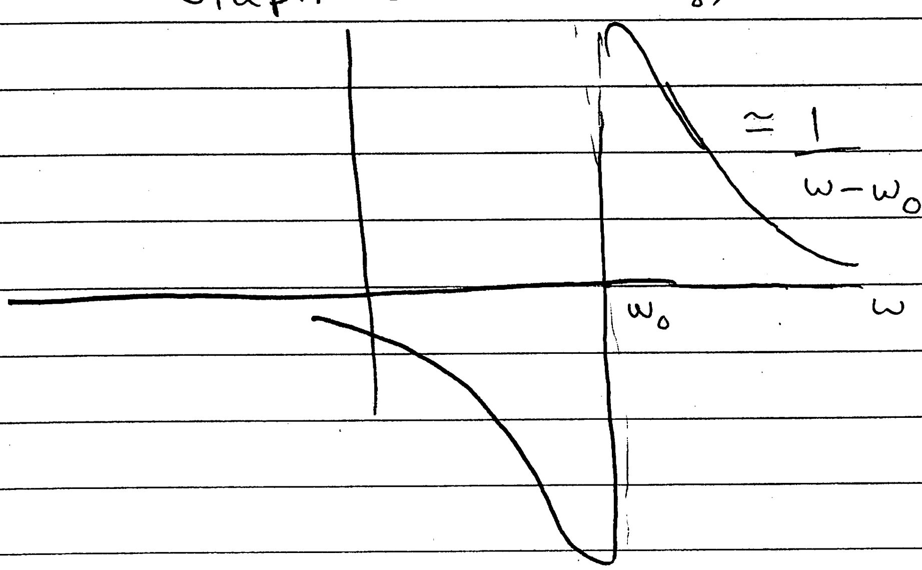
$$\text{Im}\,\chi(\omega) = +\frac{2\omega}{\pi}\int_0^\infty \frac{P}{(\omega')^2-\omega^2}\,\text{Re}\,\chi(\omega')$$

Here, $\frac{P}{\omega-\omega_0}$, denotes the "principal value function"

Much like a δ-fcn, it should be thought of as the limit of a sequence of functions.

$$\frac{P}{\omega-\omega_0} = \lim_{\varepsilon\to 0}\frac{(\omega-\omega_0)}{(\omega-\omega_0)^2+\varepsilon^2} = \frac{1}{\omega-\omega_0}$$ everywhere except right near ω_0

Graph of $P/(\omega-\omega_0)$

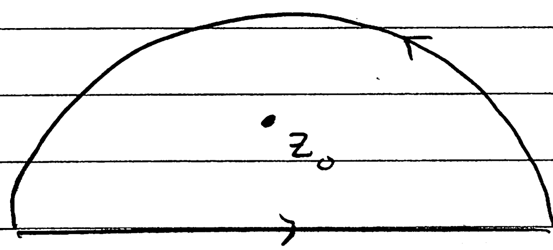


Here we have shown one of many ways to represent the principal value.

Proof of Kramers - Kronig

Since $\chi(z)$ is analytic in the UHP we can use cauchy theorem

$$\chi(z_0) = \int_C \frac{dz}{2\pi i} \frac{\chi(z)}{z - z_0}$$



Here the only pole is at z_0, since $\chi(z)$ is analytic in UHP.

Now let $z_0 = \omega_0 + i\varepsilon$. Then, assuming that the arc at infinity gives no contribution,

$$\mathrm{Re}\,\chi(\omega_0) + i\,\mathrm{Im}\,\chi(\omega_0)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{\mathrm{Re}\,\chi(\omega) + i\,\mathrm{Im}\,\chi(\omega)}{(\omega - (\omega_0 + i\varepsilon))}$$

Now

$$\frac{1}{\omega - \omega_0 - i\varepsilon} = \frac{\omega - \omega_0}{[(\omega-\omega_0)^2 + \varepsilon^2]} + i\frac{\varepsilon}{[(\omega-\omega_0)^2 + \varepsilon^2]}$$

So

$$\lim_{\varepsilon \to 0} \frac{1}{\omega - \omega_0 - i\varepsilon} = \frac{P}{\omega - \omega_0} + i\pi\,\delta(\omega - \omega_0)$$

Yielding

$$\mathrm{Re}\,\chi(\omega_0) + i\,\mathrm{Im}\,\chi(\omega_0)$$

$$= \frac{1}{2}\mathrm{Re}\,\chi(\omega_0) + \frac{i}{2}\mathrm{Im}\,\chi(\omega_0)$$

$$+ P\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\frac{-i\,\mathrm{Re}\,\chi(\omega) + \mathrm{Im}\,\chi(\omega)}{\omega - \omega_0}$$

So comparing

$$\mathrm{Im}\,\chi(\omega_0) = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi}\,\frac{P}{\omega-\omega_0}\,\mathrm{Re}\,\chi(\omega_0)$$

$$\mathrm{Re}\,\chi(\omega_0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\,\frac{P}{\omega-\omega_0}\,\mathrm{Im}\,\chi(\omega_0)$$

This is the same as quoted with the subs $\omega_0 \to \omega$ and $\omega \to \omega'$.

Kramers Kronig Relations + Qualitative Features

We can now see why the Lorenz model gives a reasonable qualitative description of real dielectrics

Suppose the material has a strong absorption band at $\omega \simeq \omega_*$

$$\operatorname{Im} \chi(\omega) \simeq C\pi\,\delta(\omega-\omega_*) + \text{regular}$$

absorption at ω_*

Then $$\operatorname{Re} \chi(\omega) = -\int \frac{d\omega'}{\pi} \frac{P}{\omega-\omega'} \operatorname{Im}\chi(\omega')$$

$$\simeq \frac{-P}{\omega-\omega_*} + \text{regular}$$

So, qualitatively we will always see the following structure:

This explains the success of the Lorenz Model.