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. $\sigma(w)$ and $\chi(w)$, $\varepsilon(w)$, etc. The real and imaginary parts are related by a specific integral relation.

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

   The imaginary part of $\varepsilon(w)$ determines the damping of the wave.

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

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

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

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

Similarly, $\chi(t-t')$ 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

$$\chi(w) = \int_{0}^{\infty} \ dt \ e^{iwt} \chi(t)$$

The Fourier integral guarantees that $\sigma(w)$ is an analytic function of $w$ for $w$ in the Upper Half Plane (UHP), $\text{Im} \ w > 0$. To see this...
Note that the exponential becomes increasingly convergent for $w$ in UHP and $t > 0$ (causality)

$$e^{iwt} = e^{i(Re w + iIm w)t} = e^{i(Re w)t} e^{-(Im w)t}$$

Thus the Fourier integral provides an analytic continuation of $x$ for $w$ complex.

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

$$\text{Re} x(w) = -\int_{-\infty}^{\infty} \frac{dw'}{\pi} \text{Im} x(w')$$

$$\text{Im} x(w) = \int_{-\infty}^{\infty} \frac{dw'}{\pi} \text{Re} x(w')$$

From Eq. (1) on previous page:

$$\text{Re} x(-w) = \text{Re} x(w)$$

$$\text{Im} x(-w) = -\text{Im} x(w) \quad \text{(Proof Below)}$$

Kramers Kronig relations
So these can be written:

\[
\text{Re } x(w) = -2 \int_0^\infty \frac{P}{\pi} \frac{w'}{w^2 - (w')^2} \text{Im } x(w')
\]

\[
\text{Im } x(w) = 2w \int_0^\infty \frac{P}{\pi} \frac{\text{Re } x(w')}{(w')^2 - w^2}
\]

Here, \( P \) denotes the "principal value function" \( \frac{1}{w-w_0} \).

Much like a \( \delta \)-function, it should be thought of as the limit of a sequence of functions.

\[
P = \lim_{\varepsilon \to 0} \frac{(w - w_0)}{(w-w_0)^2 + \varepsilon^2} = \frac{1}{w-w_0}
\]

except right near \( w_0 \).

Graph of \( \frac{P}{(w-w_0)} \):

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's theorem

$$\chi(z) = \frac{1}{2\pi i} \oint_C \frac{\chi(z)}{z - z_0} dz$$

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,

$$\Re \chi(\omega_0) + i \Im \chi(\omega_0)$$

$$= \int_{-\infty}^{\infty} dw \frac{\Re \chi(w) + i \Im \chi(w)}{2\pi i}$$

$$\int_{\omega - \omega_0 - i\varepsilon}^{\omega - \omega_0 + i\varepsilon} \frac{\chi(z)}{z - (\omega_0 + i\varepsilon)} dz$$

Now

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

So

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

\[ \text{Re } \chi(w_0) + i \text{Im } \chi(w_0) \]

\[ = \frac{1}{2} \text{Re } \chi(w_0) + i \frac{1}{2} \text{Im } \chi(w_0) \]

\[ + \mathcal{P} \int_{-\infty}^{\infty} \frac{dw}{2\pi} \frac{-i \text{Re } \chi(w) + \text{Im } \chi(w)}{w-w_0} \]

So comparing

\[ \text{Im } \chi(w_0) = -\int_{-\infty}^{\infty} \frac{dw}{2\pi} \mathcal{P} \frac{\text{Re } \chi(w_0)}{w-w_0} \]

\[ \text{Re } \chi(w_0) = \int_{-\infty}^{\infty} \frac{dw}{2\pi} \mathcal{P} \frac{\text{Im } \chi(w_0)}{w-w_0} \]

This is the same as quoted with the subs \( w_0 \to w \) and \( w \to w' \).
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 \( \omega = \omega_1 \).

\[
\text{Im } x(\omega) \sim C \pi \delta(\omega - \omega_1) + \text{regular}
\]

\( \uparrow \)

absorption at \( \omega_1 \)

Then

\[
\text{Re } x(\omega) = - \int \frac{dw'}{\pi} \frac{P}{\omega - \omega'} \text{Im } x(\omega')
\]

\[
\sim - \frac{P}{\omega - \omega_1} + \text{regular}
\]

So, qualitatively we will always see the following structure:

\[
\text{Re } x \quad \text{Im } x
\]

This explains the success of the Lorenz Model.