Kramers-Kronig Relations

In the time domain, the linear polarization:

$$\bar{P}(t) = \varepsilon_0 \int_{-\infty}^{t} \chi(t-\tau)\bar{E}(\tau)d\tau$$

Using the change of variables $\tau \to t-\tau$

$$\bar{P}(t) = \varepsilon_0 \int_{0}^{\infty} \chi(\tau)\bar{E}(t-\tau)d\tau \qquad (1)$$

This implies that the system is causal, ie $\chi(\tau) = 0$ for $\tau < 0$

Recall that the $\bar{D}$ field is given by:

$$\bar{D}(t) = \varepsilon_0 \bar{E}(t) + \bar{P}(t) = \varepsilon_0 \bar{E}(t) + \varepsilon_0 \int_0^{\infty} \chi(\tau)\bar{E}(t-\tau)d\tau \qquad (2)$$

Taking the Fourier transform, we have:

$$\bar{D}(\omega) = \varepsilon_0 \bar{E}(\omega) + \varepsilon_0 \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \int_0^{\infty} \chi(\tau)\bar{E}(t-\tau)d\tau \qquad (3)$$

$$= \varepsilon_0 \bar{E}(\omega) + \varepsilon_0 \int_0^{\infty} \chi(\tau)\left(\int_{-\infty}^{\infty} dt\, E(t-\tau)e^{-i\omega t}\right)d\tau$$

$$= \varepsilon_0 \bar{E}(\omega) + \varepsilon_0 \int_0^{\infty} \chi(\tau)\left(\int_{-\infty}^{\infty} dt\, E(t)e^{-i\omega(t+\tau)}\right)d\tau$$

$$= \varepsilon_0 \left[1 + \int_0^{\infty} \chi(\tau)e^{-i\omega\tau}\right]\bar{E}(\omega)$$

Thus the complex permitivity is:

$$\varepsilon(\omega) = \varepsilon_0\left[1 + \int_0^{\infty}\chi(\tau)e^{-i\omega\tau}d\tau\right] = \varepsilon_0\left[1 + \chi(\omega)\right] \qquad (4)$$

Note that since $\chi(\tau)$ is real (time domain!), then the permitivity must satisfy

$$\varepsilon(-\omega) = \varepsilon^*(\omega)$$

which is evident from the form of (4). If we explicitly write $\varepsilon(\omega)$ as a complex function:

$$\varepsilon(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$$

We see that the real & imaginary parts must satisfy:

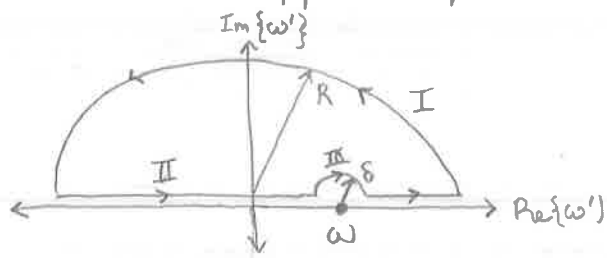
$$\varepsilon'(\omega) = \varepsilon'(-\omega) \quad \text{and} \quad \varepsilon''(-\omega) = -\varepsilon''(\omega)$$

This means that the real part of the permittivity is an even function while the imaginary part is odd. Note that, in the limit that $\omega \to \infty$, we do not expect the material to respond (if only because charge has mass and thus cannot react infinitely quickly). Thus $\varepsilon(\omega)$ must have the property that $\varepsilon(\omega\to\infty) \to \varepsilon_0$ or $\chi(\omega\to\infty) \to 0$.

It turns out to be very informative to consider the integral:

$$I = \frac{1}{2\pi i}\oint_c \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega}\,d\omega' = \frac{1}{2\pi i}\oint_c \frac{\chi(\omega')}{\omega'-\omega}\,d\omega'$$

where C is a contour in the upper complex ω'-plane:



Notice that $\chi(\tau)$ is finite and $\chi(\omega)$ is analytic. Since $\chi(\omega)$ is analytic, it follows that the whole integrand $\chi(\omega)/_{\omega'-\omega}$ is analytic everywhere except at $\omega'=\omega$. Since the closed contor C does not enclose $\omega'=\omega$, the contor integral must be zero by the Cauchy Theorem

$$I = \frac{1}{2\pi i}\oint_c \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega}\,d\omega' = 0$$

Next, as w/ a real space line integral, we can break this contour integral into integrals along the 3 connected open contours depicted above:

$$\int_{I} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' + \int_{II} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' + \int_{III} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' = 0$$

Since $\varepsilon(\omega')-\varepsilon_0$ is finite, as we take $R \to \infty$, the integral along I must go to zero. This leaves us with two integrals: II is along the real ω' axis $-\infty < \omega' < \omega - \delta$ + $\omega + \delta < \omega' < \infty$ and III is along a semi circle centered at $\omega' = \omega$ of radius δ

$$\int_{II} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' + \int_{III} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' = 0$$

let us now consider the integral around contour III. If we make the substitution $\omega' - \omega = \delta e^{i\varphi}$ then $d\omega' = i\delta e^{i\varphi} d\varphi$ and we have:

clockwise!

$$\int_{III} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' = \int_{\pi}^{0} d\varphi \frac{\varepsilon(\omega+\delta e^{i\varphi})-\varepsilon_0}{\delta e^{i\varphi}} i\delta e^{i\varphi} = i\int_{\pi}^{0} d\varphi \left[\varepsilon(\omega+\delta e^{i\varphi})-\varepsilon_0\right]$$

In the limit that $\delta \to 0$, the contour C encloses the whole upper ω' plane and we have:

$$\int_{III} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega' = \lim_{\delta\to 0} -i\int_{0}^{\pi} d\varphi \left[\varepsilon(\omega+\delta e^{i\varphi})-\varepsilon_0\right] = -i\pi\left[\varepsilon(\omega)-\varepsilon_0\right]$$

Thus it follows that

$$\varepsilon(\omega)-\varepsilon_0 = \frac{1}{i\pi}\int_{II} \frac{\varepsilon(\omega')-\varepsilon_0}{\omega'-\omega} d\omega'$$

The remaining integral over contour II is really just the <u>principle part</u> of the integral along the whole real ω' axis

That is:

$$\int_{\mathrm{II}} \frac{\varepsilon(\omega') - \varepsilon_0}{\omega' - \omega} d\omega' = \int_{-\infty}^{\omega-\delta} \frac{\varepsilon(\omega') - \varepsilon_0}{\omega' - \omega} d\omega + \int_{\omega+\delta}^{\infty} \frac{\varepsilon(\omega') - \varepsilon_0}{\omega' - \omega} d\omega'$$

$$= PP \int_{-\infty}^{\infty} \frac{\varepsilon(\omega') - \varepsilon_0}{\omega' - \omega} d\omega'$$

Thus we are left with the relationship:

$$\varepsilon(\omega) - \varepsilon_0 = \frac{1}{i\pi} PP \int_{-\infty}^{\infty} \frac{\varepsilon(\omega') - \varepsilon_0}{\omega' - \omega} d\omega'$$

We can easily separate this into real and imaginary parts given $\varepsilon(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$;

$$\boxed{\begin{aligned} \varepsilon'(\omega) - \varepsilon_0 &= \frac{1}{\pi} PP \int_{-\infty}^{\infty} \frac{\varepsilon''(\omega')}{\omega' - \omega} d\omega' \\ \varepsilon''(\omega) &= -\frac{1}{\pi} PP \int_{-\infty}^{\infty} \frac{\varepsilon'(\omega') - \varepsilon_0}{\omega' - \omega} d\omega' \end{aligned}}$$

These are the Kramers-Kronig relations.