Kramers-Kronig relations

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There are general analytic properties that the susceptibility or the permeability must satisfy. These follow from causality. Let us assume that the electric polarization is linearly related to the applied electric field, but depends only on values of he electric fields at earlier times, but not on fields present later,

$$\mathbf{P}(t) = \int_{-\infty}^{t} dt' \chi(t-t')\mathbf{E}(t') = \int_{-\infty}^{\infty} dt\, \eta(t-t')\chi(t-t')\mathbf{E}(t'), \tag{1}$$

where the Heaviside step-function is defined by

$$\eta(t-t') = \begin{cases} 1, \; t > t', \\ 0, \; t < t'. \end{cases} \tag{2}$$

A convenient representation for the latter is

$$\eta(t-t') = \frac{i}{2\pi}\int_{-\infty}^{\infty} d\nu \frac{e^{-i\nu(t-t')}}{\nu + i\epsilon}, \tag{3}$$

where ϵ is a positive number tending to zero. This may be verified by noting that the contour may be closed in the lower half plane for $t - t' > 0$, where the residue theorem gives the value 1, while for $t - t' < 0$ the contour must be closed in the upper half plane, so the integral vanishes by Cauchy's theorem. Now define the Fourier transform of χ by

$$\chi(t-t') = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega'(t-t')}\tilde{\chi}(\omega'), \tag{4}$$

which, because $\chi(t-t')$ is real, satisfies

$$\tilde{\chi}(\omega')^* = \tilde{\chi}(-\omega'), \tag{5}$$

which says that the real part of $\tilde{\chi}(\omega)$ is even, the imaginary part odd.

Now take the Fourier transform of the polarization,

$$\begin{aligned}\mathbf{P}(t) &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t}\mathbf{P}(\omega) \\ &= \int_{-\infty}^{\infty} dt' \frac{i}{2\pi} \int_{-\infty}^{\infty} d\nu \frac{e^{-i\nu(t-t')}}{\nu + i\epsilon} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega'(t-t')} \tilde{\chi}(\omega')\mathbf{E}(t'). \qquad (6)\end{aligned}$$

Now, interchanging orders of integration, we obtain

$$\mathbf{P}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi(\omega)\mathbf{E}(\omega), \qquad (7)$$

where

$$\chi(\omega) = i \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \frac{\tilde{\chi}(\nu)}{\omega + i\epsilon - \nu}. \qquad (8)$$

Thus we conclude that

$$\mathbf{P}(\omega) = \chi(\omega)\mathbf{E}(\omega). \qquad (9)$$

Because $\chi(t-t')$ is undefined (because of the step function) for $t-t' < 0$, we can choose its definition to simplify the results. Let us choose

$$\chi(t - t') = -\chi(t' - t), \qquad (10)$$

an odd function. Then we see from Eq. (5) that $\tilde{\chi}(\omega)$ is imaginary and odd. Then using the property

$$\frac{1}{\omega + i\epsilon - \nu} = P\frac{1}{\omega - \nu} - i\pi\delta(\omega - \nu), \qquad (11)$$

where P denotes principal part, we see that

$$\mathrm{Im}\chi(\omega) = -\frac{i}{2}\tilde{\chi}(\omega), \qquad (12)$$

and hence

$$\chi(\omega) = -\int_{-\infty}^{\infty} \frac{d\nu}{\pi} \frac{\mathrm{Im}\chi(\omega)}{\omega + i\epsilon - \nu} = -\int_{-\infty}^{\infty} \frac{d\nu}{\pi} \frac{\nu\mathrm{Im}\chi(\nu)}{(\omega + i\epsilon)^2 - \nu^2}, \qquad (13)$$

and in particular

$$\mathrm{Re}\chi(\omega) = -P \int_{-\infty}^{\infty} \frac{d\nu}{\pi} \frac{\mathrm{Im}\chi(\nu)}{\omega - \nu}. \qquad (14)$$

Equation (13) is the famous Kramers-Kronig relation. It says that that the susceptibilty is zero unless dissipation is present! We can further prove (see Chapter 51) that

$$\mathrm{Im}\chi(\nu) \geq 0, \quad \text{for} \quad v > 0. \qquad (15)$$

- **Problem:** Prove explicitly that the harmonic oscillator model for the permittivity satisfies the Kramers-Kronig relation,

$$\chi(\omega) = \frac{n_b e^2/m}{\omega_0^2 - \omega^2 - i\omega\gamma}. \tag{16}$$