

Kramers-Kronig relations

①

The Kramers-Kronig relations imply that the real and imaginary parts of material parameters, such as $\epsilon(\omega)$, $\chi(\omega)$, or $\kappa(\omega)$, are not independent but are connected by integral relations. The Kramers-Kronig relations are unexpected on physical grounds. They are purely a consequence of linearity and causality.

Consider a linear functional relationship between two time-dependent functions $\vec{P}(t)$ and $\vec{E}(t)$:

$$\vec{P}(t) = \epsilon_0 \int_{-\infty}^{\infty} \tilde{\chi}(t, t') \vec{E}(t') dt' \quad (1)$$

For $\vec{E}(t') = \vec{E}_0 \delta(t-t')$: $\vec{P}(t) = \epsilon_0 \tilde{\chi}(t, t_0) \vec{E}_0$

If the properties of the medium do not change with time, \vec{P} must only depend on the the time elapsed between t_0 and t

$$\rightarrow \tilde{\chi}(t, t_0) = \tilde{\chi}(t-t_0)$$

Causality implies that the system (\vec{P}) cannot respond before it has been excited (\vec{E}). Thus: $\tilde{\chi}(t-t_0) = 0$ for $t < t_0$.

Fourier transform: $\chi(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\chi}(\tau) e^{i\omega\tau} d\tau = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} \tilde{\chi}(\tau) e^{i\omega\tau} d\tau \quad (2)$

where $\tau = t - t_0$

(2)

Generalize ω as complex variable s with $\text{Im}\{s\} \geq 0$:

$$\chi(s) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} \tilde{\chi}(\tau) e^{is\tau} d\tau \quad (\text{Laplace transform}) \quad (3)$$

On the real axis of s , $\chi(s)$ coincides with $\chi(\omega)$.

$\tilde{\chi}(\tau) e^{is\tau}$ is an analytic function of s . Because of $\text{Im}\{s\} \geq 0$, we have for times $\tau \geq 0$: $|\tilde{\chi}(\tau) e^{is\tau}| \leq |\tilde{\chi}(\tau)|$.

Therefore, if the integral

$$\int_0^{\infty} |\tilde{\chi}(\tau)| d\tau \quad (4)$$

converges, then the integral in Eq. (3) also converges in the upper half-space of the s -plane. Thus, provided Eq. (4) is true, $\chi(s)$ is an analytic function. If $\chi(s)$ is an analytic function

then also

$$f(s) = \frac{\chi(s)}{(s-\omega)}$$

is an analytic function except at the pole $s=\omega$ which is chosen on the real axis of s . Cauchy's theorem states that

$$\oint_{\Gamma} f(s) ds = 0 \quad (5)$$

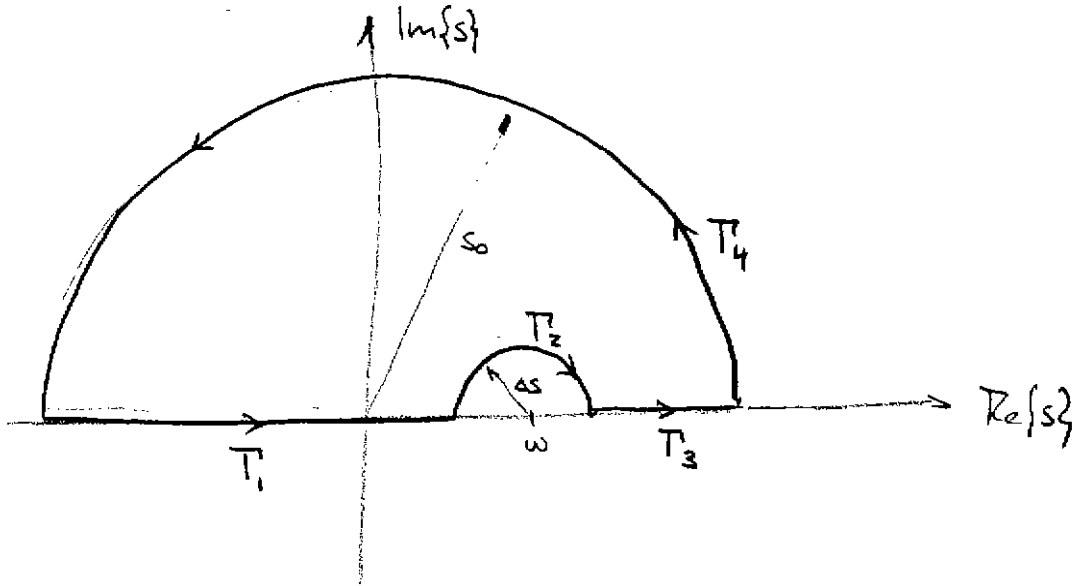
provided that the closed path Γ does not enclose any poles.

Let us evaluate the integral

$$\int_{\Gamma} \frac{\chi(s)}{(s-w)} ds$$

(6)

on the contour shown below



The contour Γ is divided into four curves. Obviously, the integral vanishes on Γ_4 if we let $s_0 \rightarrow \infty$. Therefore,

$$\int_{-\infty}^{w-\Delta s} \frac{\chi(s)}{(s-w)} ds + \int_{w+\Delta s}^{\infty} \frac{\chi(s)}{(s-w)} ds = - \int_0^{\pi} \frac{\chi(w-\Delta s e^{-i\phi})}{[w-\Delta s e^{-i\phi}] - w} (i \Delta s e^{-i\phi}) d\phi$$

$$= i \int_0^{\pi} \chi(w-\Delta s e^{-i\phi}) d\phi$$

Let $\Delta s \rightarrow 0$;

$$\lim_{\Delta s \rightarrow 0} \left[\int_{-\infty}^{w-\Delta s} \frac{\chi(s)}{(s-w)} ds + \int_{w+\Delta s}^{\infty} \frac{\chi(s)}{(s-w)} ds \right] = i\pi \chi(w)$$

(7)

or, with \mathcal{P} denoting the Cauchy principal value:

$$\boxed{X(\omega) = \frac{1}{i\pi} \mathcal{P} \left[\int_{-\infty}^{\infty} \frac{X(s)}{s-\omega} ds \right]} \tag{8}$$

Making use of $X^*(s) = X(-s)$, Eq. (8) can be written as

$$X(\omega) = \frac{1}{i\pi} \mathcal{P} \left[\int_0^{\infty} \frac{X(s)}{s-\omega} ds - \int_0^{\infty} \frac{X(s)}{s+\omega} ds \right]. \tag{9}$$

Taking the real and imaginary part of Eq. (9) gives:

$$\boxed{\begin{aligned} X'(\omega) &= \frac{2}{\pi} \mathcal{P} \left[\int_0^{\infty} \frac{s X''(s)}{s^2-\omega^2} ds \right] \\ X''(\omega) &= -\frac{2\omega}{\pi} \mathcal{P} \left[\int_0^{\infty} \frac{X'(s)}{s^2-\omega^2} ds \right] \end{aligned}} \tag{10}$$

Thus, if the real part of $X(\omega)$ is known for all ω , the imaginary part of $X(\omega)$ is uniquely determined (and vice versa) !

Notice that

$$\int_0^{\infty} |\hat{\epsilon}(\tau)| d\tau$$

does not converge. Therefore, the Kramers-Kronig relations as derived in Eq. (10) do not hold for $\epsilon(\omega)$. Instead, we have to use $\epsilon(\omega) = 1 + \chi(\omega)$ and obtain

$$\begin{aligned} \epsilon'(\omega) &= 1 + \frac{2}{\pi} \mathcal{P} \left[\int_0^{\infty} \frac{s \epsilon''(s)}{s^2 - \omega^2} ds \right] \\ \epsilon''(\omega) &= -\frac{2\omega}{\pi} \mathcal{P} \left[\int_0^{\infty} \frac{\epsilon'(s) - 1}{s^2 - \omega^2} ds \right] \end{aligned} \quad (11)$$

Are there materials with no absorption? No! If $\epsilon''(\omega) = 0$ then $\epsilon'(\omega) = 1$ which is the case for vacuum.