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The Kramers-Kronig Relations

Section 7.10

“Causality and the KK relations”

$$\mathrm{Re}\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{2}{\pi\epsilon_0}\,\mathcal{P}\int_0^\infty \frac{\omega'\,\mathrm{Im}\,\epsilon(\omega')}{(\omega')^2-\omega^2}\,d\omega'$$

$$\mathrm{Im}\frac{\epsilon(\omega)}{\epsilon_0} = -\frac{2\,\omega}{\pi\epsilon_0}\,\mathcal{P}\int_0^\infty \frac{\mathrm{Re}\,\epsilon(\omega')-\epsilon_0}{(\omega')^2-\omega^2}\,d\omega'$$

Wednesday we showed that the Kramers-Kronig relations are obeyed specifically for the Lorentz model of dispersion.

Today we will show that the KK relations are general; i.e., they must be true for any theory of $\epsilon(\omega)$. And the reason is *causality*.

Causality in the connection between $\vec{D}$ and $\vec{E}$

Nonlocality in Time

Think about it physically.

We have a time-dependent field $\vec{E}(\vec{x},t)$. Then the medium will have a time-dependent polarization $\vec{P}(\vec{x},t)$.

We define $\vec{D}(\vec{x},t) = \epsilon_0\,\vec{E}(\vec{x},t) + \vec{P}(\vec{x},t)$.

Now, surely $\vec{P}(\vec{x},t) = \eta\,\vec{E}(\vec{x},t)$ cannot be true with η being a constant. That would violate ***causality.***

It must take some time for the polarization to develop as the electric field changes. But the relation $\vec{P}(\vec{x},t) = \eta\,\vec{E}(\vec{x},t)$ would imply that a change of $\vec{E}(\vec{x},t)$ produces an instantaneous response in $\vec{P}(\vec{x},t)$.

By causality the linear relationship must look something like this,

$$\vec{P}(\vec{x},t) = \int_{-\infty}^{t} \eta(t - t')\, \vec{E}(\vec{x},t')\, dt'$$

for some function $\eta(\tau)$.

For a harmonic field, we write

$$\vec{E}(\vec{x},t) = \vec{E}(\vec{x},\omega) \exp(-i\,\omega\, t)$$

$$\vec{P}(\vec{x},t) = \vec{P}(\vec{x},\omega) \exp(-i\,\omega\, t)$$

$$\vec{D}(\vec{x},t) = \vec{D}(\vec{x},\omega) \exp(-i\,\omega\, t)$$

Assume there is a linear relationship;
$\Longrightarrow$ *frequency-dependent permittivity,*

$$\vec{D}(\vec{x},\omega) = \epsilon(\omega)\, \vec{E}(\vec{x},\omega)$$

We are introducing complex functions, because

$$\exp(-i\,\omega\, t) = \cos(\omega t) - i \sin(\omega t).$$

And so, $\epsilon(\omega)$ will be complex.

The physical field is the real part of $\vec{E}(\vec{x},t)$. We introduce complex functions to make the algebra simpler; but just remember we eventually must take the real part for any physical predictions.

Why not just use real functions, like $\cos(\omega t)$ and $\sin(\omega t)$? In fact, we could do that; and it might make the physical consequences more manifest. *But the algebra would be inconvenient*.

Fourier' s Theorem

For any function we can expand in harmonic functions.

So, for example, we can write

$$\vec{D}(\vec{x},t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \vec{D}(\vec{x},\omega) \exp(-i\omega t)\, d\omega$$

and (it follows)

$$\vec{D}(\vec{x},\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \vec{D}(\vec{x},t') \exp(\, i\omega t')\, dt' \,.$$

And $\exists$ similar Fourier integrals for $\vec{E}(\vec{x},t)$ and $\vec{E}(\vec{x},\omega)$; or any function $\mathcal{F}(t)$ and $\mathcal{F}(\omega)$.

So, for a linear material,

$$\vec{D}(\vec{x},t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \epsilon(\omega)\, \vec{E}(\vec{x},\omega)\, \exp(-i\omega t)\, d\omega$$

and

$$\vec{D}(\vec{x},t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\;\; \epsilon(\omega)\, \exp(-i\omega t)\, d\omega$$

$$\int_{-\infty}^{\infty} \exp(+i\omega t')\, \vec{E}(\vec{x},t')\, dt'$$

Susceptibility

Define $\epsilon(\omega) = \epsilon_0 + \epsilon_0\, \chi_e(\omega)$

(electric susceptibility)

Then

$$\vec{D}(\vec{x},t) = \epsilon_0\, \vec{E}(\vec{x},t)$$

$$+\ \epsilon_0 \int_{-\infty}^{\infty} dt'\, \vec{E}(\vec{x},t') \square$$

$$\square \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \chi_e(\omega)\, \exp(-i\omega(t-t'))$$

Summary

$$\vec{D}(\vec{x},t) = \epsilon_0\, \vec{E}(\vec{x},t)\ +$$

$$+\ \epsilon_0 \int_{-\infty}^{\infty} G(\tau)\, \vec{E}(\vec{x},t-\tau)\, d\tau$$

where

$$G(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \chi_e(\omega)\, \exp(-i\omega\, \tau)$$

I.e., $G(\tau)$ is the inverse Fourier transform of $\chi_e(\omega)$. { $\chi_e(\omega)$ is the Fourier transform of $G(\tau)$.}

The nonlocal relation between $\vec{E}$ and $\vec{D}$

$$\vec{D}(\vec{x},t) = \epsilon_0 \left\{ \vec{E}(\vec{x},t) + \int_{-\infty}^{\infty} G(\tau)\, \vec{E}(\vec{x},t-\tau)\, d\tau \right\}$$

i.e., nonlocal in time.

In this equation, the displacement field $\vec{D}(\vec{x}, t)$ is related to the electric field $\vec{E}(\vec{x}, t')$ for all times t'.
The integral over τ is called a *convolution integral*.

Example 1: Assume $\chi_e(\tau) = \kappa\, \delta(\tau)$.

Then $\vec{D}(\vec{x},t) = \epsilon_0 \left(\vec{E}(\vec{x},t) + \kappa \vec{E}(\vec{x},t) \right)$
$\propto \vec{E}(\vec{x},t)$
and $\chi_e(\omega) = \int_{-\infty}^{\infty} G(\tau)\, e^{i\omega\tau}\, d\tau = \kappa$

If there is no frequency dependence then there is an the instantaneous connection between $\vec{D}$ and $\vec{E}$.

Example 2: Assume the Lorentz model...

$$\chi_e(\omega) = \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

Then

$$G(\tau) = \frac{\omega_p^2}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega\tau}\, d\omega}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

Evaluate by contour integration.
The integrand has 2 poles,

$$\text{at } \omega = -\frac{i\gamma}{2} \pm \sqrt{\omega_0^2 - (\gamma/2)^2} \quad ....$$

For $\tau < 0$, $G(\tau) = \oint_{UHP} (...) = 0$;

for $\tau > 0$, $G(\tau) = \oint_{LHP} (...)$

$$= \frac{\omega_p^2}{2\pi} (-2\pi i) \,(\text{ 2 residues})$$

$$= \omega_p^2\, e^{-\gamma\tau/2} \frac{\sin(\nu_0 \tau)}{\nu_0}$$

Result for the Lorentz model

$$G(\tau) = \omega_p^2 \, e^{-\gamma\tau/2} \, \frac{\sin(\nu_0 \tau)}{\nu_0} \, \Theta(\tau)$$

with these properties

- oscillates with the natural frequency;
- damped exponentially with γ
- vanishes for $\tau < 0$; that's ***causality .***

Causality and Analyticity

$$\vec{D}(\vec{x},t) = \epsilon_0 \left\{ \vec{E}(\vec{x},t) + \int_0^\infty G(\tau)\, \vec{E}(\vec{x},t-\tau)\, d\tau \right\}$$

Causality:

- $G(\tau) = 0$ for $\tau < 0$
- $\Theta(\tau)$
- Note the lower endpoint of the integral.
- **P**(**x**,t) (and ∴ **D**(**x**,t)) can only depend on **E**(**x**,t') for t' < t ; i.e., $t' = t - \tau$ with $\tau > 0$.
- "This is the most general spatially local, linear, and causal relation that can be written between ***D*** and ***E*** in a uniform isotropic medium. Its validity transcends and specific model of $\epsilon(\omega)$."

Analyticity of $\epsilon(\omega)$:

The inverse Fourier transform,

$$\epsilon(\omega)/\epsilon_0 = 1 + \int_0^\infty G(\tau)\exp(i\omega\tau)\,d\tau$$

(note the lower endpoint)

Theorem. If $G(\tau)$ is finite for all τ, then $\epsilon(\omega)/\epsilon_0$ is an analytic function of ω in the upper-half ω plane.

Proof: from the theory of Fourier integrals.

In the upper half ω plane, the factor $\exp(i\omega\tau)$ is $\propto \exp(-\omega_I\,\tau)$ which is small for $\tau > 0$; so the integral converges.

Reality: G must be a real function, so that Re{D} is related to Re{E}.

Therefore

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

$$\Rightarrow \text{Re}\,\epsilon(-z) = \text{Re}\,\epsilon(z)$$

$$\text{and Im}\,\epsilon(-z) = -\,\text{Im}\,\epsilon(z)$$

The Kramers Kronig relations

When we proved the KK relations for the Lorentz model (Wednesday) *the proof relied **only** on the analyticity and reality properties of $\epsilon(\omega)$.*

Since they are the same for any theory with complex $\epsilon(\omega)$, the KK relations are general—not limited to the Lorentz model.