1

Section 9.7
The Kramers-Kronig Relations

We have the 'simple model' for the constitutive equation for a dielectric material. It has a complex effective permittivity $\epsilon(\omega)$, which we can apply when the fields are harmonic,

$$\epsilon(\omega) = 1 + \sum \frac{4\pi e^2}{m} \; \frac{n_e}{\omega_0{}^2 - \omega^2 - i\,\omega\,\gamma}$$

For example, suppose the fields have frequency $\omega/(2\pi)$,

$\vec{E}(\vec{x},t) = \text{Re}\,\{\,\vec{E}(\,\vec{x})\,e^{-i\omega t}\}$

$\vec{D}(\vec{x},t) = \text{Re}\,\{\,\vec{D}(\,\vec{x})\,e^{-i\omega t}\}$

Then

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

For a plane wave in the material,

$\vec{E}(\vec{x}) = \vec{\mathcal{E}}\,e^{i\vec{k}\cdot\vec{x}}$.

The *dispersion relation*—the relation between k and ω—is

$k^2 = \mu\;\epsilon(\omega)\;\omega^2\;/\,c^2$.

1

$$k^2 = \mu\;\epsilon(\omega)\;\omega^2\;/\,c^2$$

- If $\vec{k}$ is real then there is a propagating wave with constant amplitude.
- If $\vec{k}$ has an imaginary part then the wave is damped; i.e., the amplitude decreases as the wave travels in the material.

So the *complex function* $\epsilon(\omega)$ describes how electromagnetic waves behave in the material.

An important question is, how are Re $\epsilon(\omega)$ and Im $\epsilon(\omega)$ related? That is the issue in Section 9.7.

2

/1/ The Electromagnetic Response Function

First, what does the *frequency dependence* of $\epsilon(\omega)$ imply about the *time dependence* of the physical fields? In frequency space,

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

For static fields ($\omega = 0$) we can write

$$\vec{D}(\vec{x}) = \epsilon(0)\, \vec{E}(\vec{x}).$$

But now consider general time-dependent fields, $\vec{D}(\vec{x},t)$ and $\vec{E}(\vec{x},t)$, not necessarily harmonic.

2

Fourier Analysis

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$$\vec{D}(\vec{x},t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \vec{D}(\vec{x},\omega) \qquad (168)$$

Out[•]=

$$\vec{E}(\vec{x},t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \vec{E}(\vec{x},\omega)$$

$$\vec{E}(\vec{x},\omega) = \int_{-\infty}^{\infty} dt'\, e^{i\omega t'}\, \vec{E}(\vec{x},t') \qquad (169)$$

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

Now relate $\vec{D}(\vec{x},t)$ and $\vec{E}(\vec{x},t)$.

3

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$$\vec{D}(\vec{x},t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \epsilon(\omega) \int_{-\infty}^{\infty} dt' \, e^{i\omega t'} \vec{E}(\vec{x},t')$$

$$= \int_{-\infty}^{\infty} dt' \, \vec{E}(\vec{x},t') \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \epsilon(\omega) \qquad (170)$$

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} [1 + \epsilon(\omega) - 1]$$

Out[•]=

$$= \delta(t-t') + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} [\epsilon(\omega) - 1]$$

$$\boxed{\tau = t - t'}$$

$$\vec{D}(\vec{x},t) = \vec{E}(\vec{x},t) + \int_{-\infty}^{\infty} d\tau \, \vec{E}(\vec{x},t-\tau) \, G(\tau) \qquad (171)$$

$$G(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} [\epsilon(\omega) - 1] \qquad (172)$$

The relation between $\vec{D}(\vec{x},t)$ and $\vec{E}(\vec{x},t)$ is non-local in time. The kernel $G(\tau)$ is called the *response function*.

4▫

The Response Function — what do we learn from it?

By causality, $G(\tau) = 0$ for $\tau < 0$.
Therefore $\epsilon(\omega)$ may have poles in the L H ω P only.
(Recall the retarded Green's function; see Section 8.6.)
Consequences:

- $G(\tau) = 0$ for $\tau < 0$. [1]
- $G(0-) = G(0+) = 0$. "continuity" [2]
- $G(\tau) \longrightarrow 0$ as $\tau \longrightarrow \infty$. [3]
- $G(\tau)$ is a finite function. [4]

Also, we will have

- $\epsilon(\omega) - 1 \sim O(1/\omega^2)$ as $\omega \longrightarrow \infty$. [5]

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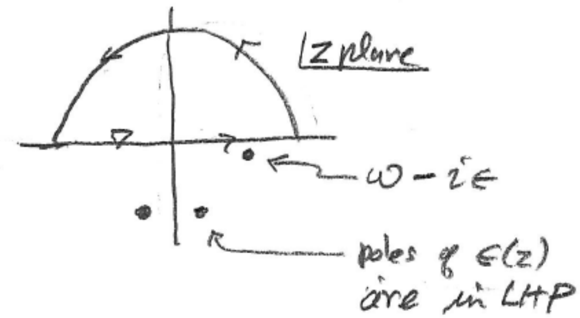
(the ϵ in the denominator → 0 +)

$$0 = \oint_C dz \, \frac{\epsilon(z) - 1}{z - \omega + i\epsilon}$$



Out[189]=

$$\epsilon(\omega) = 1 + \int_{0-}^{\infty} d\tau \, G(\tau) e^{i\omega\tau}$$

$\omega = \omega + i\epsilon$, $\epsilon \to 0$

$$G(\tau) = G(0+) + \tau G_0'(0+) + \ldots$$

$$\epsilon(\omega) = 1 + i\frac{G(0+)}{\omega} - \frac{G'(0+)}{\omega^2} + \ldots$$

$$G(0+) = 0$$

$$\therefore \; \epsilon(\omega) - 1 \sim O(1/\omega^2) \text{ as } \omega \to \infty$$

5

(You can show that Eq. 177 { $\epsilon(\omega) - 1 \sim O(1/\omega^2)$ } is true for the 'simple model'. But the previous calculation proves it in general.)

Now the contour integral becomes

$$0 = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\epsilon(\omega') - 1}{\omega' - \omega + i\epsilon} \tag{178}$$

Derivation of the Kramers-Kronig relations

First, recall the ***Plemelj formulae;***

in the limit $\epsilon \longrightarrow 0$,

$$\frac{1}{\omega' - \omega \pm i\epsilon} = P\,\frac{1}{\omega' - \omega} \mp i\,\pi\,\delta(\omega' - \omega) \tag{179}$$

So,

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$$-\frac{i}{2}\{\epsilon(\omega)-1\} + P\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\frac{\epsilon(\omega')-1}{\omega'-\omega} = 0$$

$$\epsilon(\omega) - 1 = -\frac{i}{\pi}\,P\int_{-\infty}^{\infty} d\omega'\,\frac{\epsilon(\omega')-1}{\omega'-\omega}$$

Out[•]=

Real and Imaginary Parts...

$$\mathrm{Re}\,\epsilon(\omega) = 1 + \frac{1}{\pi}\,P\int_{-\infty}^{\infty} d\omega'\,\frac{\mathrm{Im}\,\epsilon(\omega')}{\omega'-\omega} \quad (182)$$

$$\mathrm{Im}\,\epsilon(\omega) = \frac{-1}{\pi}\,P\int_{-\infty}^{\infty} d\omega'\,\frac{\mathrm{Re}\,\epsilon(\omega')-1}{\omega'-\omega} \quad (183)$$

These (182, 183) are the *Kramers-Kronig relations*.

6□

<u>A simplification</u>

G(τ) must be real. (See Eqs. 170 and 171.)

Therefore $\epsilon^*(\omega^*) = \epsilon(-\omega)$. (See Eq. 172.)

Re $\epsilon(-\omega)$ = Re $\epsilon(\omega) \Longrightarrow$ Re $\epsilon(\omega)$ is an even function of ω (ω real)

Im $\epsilon(-\omega) = -$ Im $\epsilon(\omega) \Longrightarrow$ Im $\epsilon(\omega)$ is an odd function of ω (ω real)

We can use these results to change the integrals from $-\infty$ to $+\infty$ into integrals from 0 to $+\infty$.

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Out[]=

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

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

7□

/3/ Sum Rules for the "Dielectric Constant"

Quoting Wilcox ...

" ... an important consequence of the Kramers-Kronig dispersion relations, namely *sum rules* for the dielectric constant $\epsilon(\omega)$ ..."

The Sum Rule for the imaginary part of $\epsilon(\omega)$

Define *plasma frequency* ω_p

$$\omega_p^2 = \lim_{\omega \to \infty} \omega^2 \, (\, 1 - \epsilon(\omega) \,)$$

Now you can prove

$$\omega_p^2 = \frac{2}{\pi} \int_0^\infty d\omega \; \omega \; \mathrm{Im}\, \epsilon(\omega)$$

[Exercise 9.7.2]

Wilcox verifies that the 'simple model' for $\epsilon(\omega)$ satisfies this equation, with the result

$$\omega_p^2 \; = \; \frac{4\,\pi^2\,e^2}{m} \; n_{\text{bound}}$$

□7

The Sum Rule for the real part of $\epsilon(\omega)$

From the Kramers-Kronig relations, you can show

$$\int_0^N d\omega \, [\, \mathrm{Re}\, \epsilon(\omega) - 1 \,] = \frac{\omega_p^2}{N} + O(N^{-3})$$

N is some large frequency

[Exercise 9.7.2]

Wilcox points out that the 'simple model' for $\epsilon(\omega)$ of a dielectric has

$$\int_0^\infty d\omega \, [\, \mathrm{Re}\, \epsilon(\omega) - 1 \,] = 0.$$

which is consistent with this general result.