7.10 Causality in the Connection Between $\underline{D}$ and $\underline{E}$. Kramers Kronig Relations.

Assuming $\epsilon = \epsilon(\omega)$ implies

$$\underline{D}(\underline{x}, \omega) = \epsilon(\omega)\, \underline{E}(\underline{x}, \omega) \qquad (7.103)$$

$\epsilon(\omega)$ contains information about the time response.

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

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\epsilon(\omega) - \epsilon_0\right] \underline{E}(\underline{x}, \omega)\, e^{-i\omega t}\, d\omega + \epsilon_0\, \underline{E}(\underline{x}, t)$$

Express $\underline{E}(\underline{x}, \omega)$ in terms of $E(\underline{x}, t)$:

$$\underline{E}(\underline{x}, \omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underline{E}(\underline{x}, t')\, e^{i\omega t'}\, dt'$$

$$\rightarrow \quad \underline{D}(\underline{x}, t) = \epsilon_0\, \underline{E}(\underline{x}, t) + \frac{\epsilon_0}{2\pi} \int_{-\infty} \underbrace{\left[\frac{\epsilon(\omega)}{\epsilon_0} - 1\right]}_{\equiv \chi_e(\omega)\ =\ \text{electric susceptibility}} \int_{-\infty} \underline{E}(\underline{x}, t')\, e^{i\omega t'}\, dt' \cdot e^{-i\omega t}\, d\omega$$

$$\underline{D}(\underline{x}, t) = \epsilon_0\, \underline{E}(\underline{x}, t) + \frac{\epsilon_0}{2\pi} \int_{-\infty}^{\infty} \chi_e(\omega) \int_{-\infty}^{\infty} \underline{E}(\underline{x}, t - \tau)\, e^{-i\omega\tau}\, d\tau\, d\omega$$

$$\tau = t - t'$$

Reversing the order of integration,

$$\underline{D}(\underline{x},t) = \epsilon_0 \underline{E}(\underline{x},t) + \frac{\epsilon_0}{2\pi}\int_{-\infty}^{\infty} \underline{E}(\underline{x},t-\tau)\int_{-\infty}^{\infty}\chi_e(\omega)e^{-i\omega\tau}\,d\omega\,d\tau$$

Let $G(\tau)$ be the Fourier transform of $\chi_e(\omega)$

$$G(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\chi_e(\omega)e^{-i\omega\tau}\,d\omega \qquad (7.106)$$

then

$$\underline{D}(\underline{x},t) = \epsilon_0\underline{E}(\underline{x},t) + \epsilon_0\int_{-\infty}^{\infty}\underline{E}(\underline{x},t-\tau)G(\tau)\,d\tau \qquad (7.105)$$

$G(\tau)$ represents the time response of the medium. The displacement at t depends on the electric field applied at $t-\tau$. The integral includes $\tau<0$, but this violates causality. Therefore, we change the lower limit from $-\infty$ to 0:

$$D(\underline{x},t) = \epsilon_0\underline{E}(\underline{x},t) + \epsilon_0\int_0^{\infty}\underline{E}(\underline{x},t-\tau)G(\tau)\,d\tau \qquad (7.111)$$

From (7.106),

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1+\chi_e(\omega) = 1+\int_0^{\infty}G(\tau)e^{i\omega\tau}\,d\tau \qquad (7.112)$$

Since $\underline{E}$ and $\underline{D}$ are real, G is real, and

$$\epsilon^*(\omega) = \epsilon(-\omega) \qquad (7.113)$$

which implies $\mathrm{Re}[\epsilon(-\omega)] = \mathrm{Re}[\epsilon(\omega)]$

Let's also assume $G(\tau) \to 0$ for $\tau \to \infty$. (The present displacement in the medium doesn't depend on the electric field in the infinite past.) Then we can integrate (7.112) by parts repeatedly:

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \int_0^\infty \frac{d}{d\tau}\left[\frac{G(\tau)e^{i\omega\tau}}{i\omega}\right] d\tau - \frac{1}{i\omega}\int_0^\infty \frac{dG}{d\tau} e^{i\omega\tau}\, d\tau$$

$$= 1 + \int_0^\infty \frac{d}{d\tau}\left[\frac{G(\tau)e^{i\omega\tau}}{i\omega}\right] d\tau$$

$$- \frac{1}{i\omega}\int_0^\infty \frac{d}{d\tau}\left[\frac{dG}{d\tau}\frac{e^{i\omega\tau}}{i\omega}\right] d\tau + \frac{1}{(i\omega)^2}\int_0^\infty \frac{d^2G}{d\tau^2} e^{i\omega\tau}\, d\tau$$

etc.

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

= asymptotic series for large ω.

Causality $\Rightarrow G(\tau) = 0$ for $\tau < 0$.
Continuity then $\Rightarrow G(0) = 0$.
$\Rightarrow$ First term vanishes $\Rightarrow$

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 - \frac{1}{\omega^2} G'(0) - \frac{i}{\omega^3} G''(0) \cdots$$

$$\mathrm{Re}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] \approx 1 - \frac{G'(0)}{\omega^2} \qquad \text{(large } \omega)$$

$$\mathrm{Im}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] \approx -\frac{1}{\omega^3} G''(0) \qquad \text{(large } \omega)$$

In general, $\epsilon(\omega)$ is complex. (e.g., (7.51)) Its real and imaginary parts are related to one another by the <u>Kramers-Kronig Relations</u>. To derive these, we need the fact that $\epsilon(\omega)$ is <u>analytic</u> in the upper half ω-plane ($\Im m\, \omega > 0$). This follows from

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \int_0^\infty G(\tau) e^{i\omega\tau} d\tau \qquad (7.112)$$

together with the facts that (1) $G(\tau)$ is real and continuous, (2) $e^{i\omega\tau}$ is an analytic function of τ in the upper half-plane of ω, and (3) the integral of an analytic function is analytic.

We also need the <u>Cauchy Integral Theorem</u>, which says that if $F(\omega)$ is analytic within a closed contour C in the complex ω-plane, and if the point $\omega = z$ is inside C, then

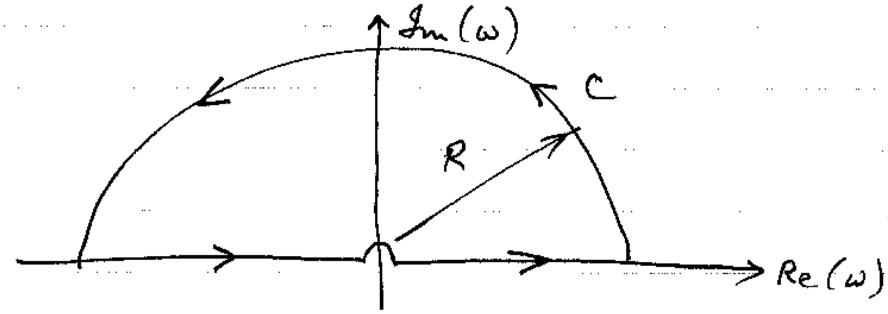
$$F(z) = \frac{1}{2\pi i} \oint_C \frac{F(\omega)\, d\omega}{\omega - z}$$

(The values of an analytic function on any closed contour determine its value at any point inside the contour. Just like a 2-D electrostatic potential.)

Setting $F(\omega) = \dfrac{\epsilon(\omega)}{\epsilon_0} - 1$ this gives

$$\frac{\epsilon(z)}{\epsilon_0} = 1 + \frac{1}{2\pi i}\oint_C \frac{\left[\frac{\epsilon(\omega)}{\epsilon_0} - 1\right]}{\omega - z}\,d\omega$$

if C is in the upper half ω-plane, where ϵ is analytic. In particular, take C as the real axis plus a great semicircle in the upper half ω plane with $R \to \infty$:



On p. 3 we showed that $\left|\dfrac{\epsilon(\omega)}{\epsilon_0} - 1\right| \to 0$ at least as fast as $\dfrac{1}{|\omega|}$ as $|\omega| \to \infty$ in the upper half plane. Thus the integral along the great semicircle is 0, and

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{\left[\frac{\epsilon(\omega')}{\epsilon_0} - 1\right]d\omega'}{\omega' - \omega} \qquad (7.115)$$

Take the limit as ω' approaches the real axis :

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{1}{2\pi i}\lim_{\eta \to 0}\left[\int_{-\infty}^{\omega-\eta} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega}\,d\omega' + \int_{\omega+\eta}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega}\,d\omega'\right]$$

$$+ \frac{1}{2\pi i}\int_{\smile} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega}\,d\omega'$$

principal part

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 + \frac{1}{2\pi i} P\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega} d\omega' + \frac{1}{2\pi i} \times 2\pi i \times \frac{1}{2} \text{ Residue at } \omega' = \omega$$

$$= 1 + \frac{1}{2\pi i} P\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega} d\omega' + \frac{1}{2}\left[\frac{\epsilon(\omega)}{\epsilon_0} - 1\right]$$

$$\frac{\epsilon(\omega)}{\epsilon_0} - 1 = \frac{1}{\pi i} P\int_{-\infty}^{\infty} \frac{\frac{\epsilon(\omega')}{\epsilon_0} - 1}{\omega' - \omega} d\omega' \qquad (7.118)$$

$$\left.\begin{aligned} \mathrm{Re}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] &= 1 + \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{\mathrm{Im}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] d\omega'}{\omega' - \omega} \\ \mathrm{Im}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] &= -\frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{\mathrm{Re}\left[\frac{\epsilon(\omega')}{\epsilon_0} - 1\right] d\omega'}{\omega' - \omega} \end{aligned}\right\} (7.119)$$

These are the <u>Kramers Kronig Relations</u>.
They say that causality requires a specific relationship between the real and imaginary parts of $\epsilon(\omega)$ (or any other analytic function). One can be calculated from the other.

Alternate form of K-K relations: Using the condition $\epsilon(-\omega) = \epsilon^*(\omega)$, we can convert (7.119) into an integral over positive ω'.

$$\mathrm{Re}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] = 1 + \frac{1}{\pi} P\left[\int_{-\infty}^{0} + \int_{0}^{\infty}\right] \frac{\mathrm{Im}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] d\omega'}{\omega' - \omega}$$

$$(\omega'' = -\omega') \qquad = 1 + \frac{1}{\pi} P\int_{0}^{\infty} \frac{\mathrm{Im}\left[\frac{\epsilon(\omega'')^*}{\epsilon_0}\right] d\omega''}{-\omega'' - \omega} + \frac{1}{\pi} P\int_{0}^{\infty} \frac{\mathrm{Im}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] d\omega'}{\omega' - \omega}$$

But $\mathrm{Im}(z^*) = -\mathrm{Im}(z)$ $\rightarrow$

$$\mathrm{Re}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] = 1 + \frac{1}{\pi} P \int_0^\infty \mathrm{Im}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] \underbrace{\left[\frac{1}{\omega'-\omega} + \frac{1}{\omega'+\omega}\right]}_{\frac{2\omega'}{\omega'^2-\omega^2}} d\omega'$$

$$\mathrm{Re}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \,\mathrm{Im}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] d\omega'}{\omega'^2 - \omega^2} \qquad (7.120\,a)$$

Same procedure with imaginary part (7.119 b) gives

$$\mathrm{Im}\left[\frac{\epsilon(\omega)}{\epsilon_0}\right] = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\mathrm{Re}\left[\frac{\epsilon(\omega')}{\epsilon_0}\right] - 1}{\omega'^2 - \omega^2} d\omega' \qquad (7.120\,b)$$