Lecture 14

- Review
- Lorentz transformations of EM fields
- Kramers - Kronig relations, dispersion

- We return to the study of EM fields in media, but at a more advanced level

→ absorption

→ non-locality in time

→ convolution and frequency

→ analytic properties

→ Kramers – Kronig relations

→ example: resonant absorption model. →

→ very general!

- Let us remember the following effect: polarisation of dielectric media by external electric field

$$\vec{P}(\vec{x}) = \sum_n \vec{d}_n \cdot g(\vec{x}_n - \vec{x}) \rightarrow \text{smearing function}$$

↓ electric polarization of the medium.

$$\langle \eta \rangle (\vec{x}) = \rho(\vec{x}) - \vec{\nabla}_x \cdot \vec{P}(\vec{x})$$

From this we derived averaged Maxwell equations:

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\varepsilon_0} - \frac{\vec{\nabla} \cdot \vec{P}}{\varepsilon_0}$$

We also defined the Displacement vector

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P},$$

And we did a similar treatment for the magnetic phenomenon

$$\vec{H} = \frac{1}{\mu_0} \vec{B} - \vec{M} \rightarrow \text{magnetisation}$$

The Maxwell equations eventually read:

$$\vec{\nabla} \cdot \vec{D} = \rho \qquad \vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0$$

$$\vec{\nabla} \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = \vec{J} \qquad \vec{\nabla} \cdot \vec{B} = 0$$

To make use of them we need the relation between $\vec{E}$ and $\vec{D}$ and $\vec{H}$ and $\vec{B}$ which we chose as

$$\vec{D}(\vec{x},t) = \varepsilon \vec{E}(\vec{x},t)$$
$$\vec{H}(\vec{x},t) = \frac{1}{\mu} \vec{B}(\vec{x},t)$$

This result is correct for static fields, however, we also used it for our discussion of EM waves. In the case of time-dependent fields there are two new effects:

→ absorbtion (ε and μ have imaginary parts)

→ dispersion (relation between $\vec{E}$ and $\vec{D}$ ($\vec{H}$ and $\vec{B}$) is non-local in time)

The two effects turn out to be closely related.

• Let us first understand why imaginary parts of ε and μ lead to absorbtion of energy of EM fields by the medium.

Let us consider a monohromatic plane wave in a material:

$$\vec{E} = \overset{1}{\vec{E}} e^{i\omega t + i\vec{k}\cdot\vec{x}}$$

suppose $\vec{k} = (k_x, 0, 0)$

then $k_x = \sqrt{\varepsilon\mu}\, \omega \frac{1}{c}$

If ε or μ have imaginary part then k_x has imaginary part $\Rightarrow$ wave expo-nentially decays

From now on we will focus on ε, assuming μ real and constant. Then a general relation between D and E is

$$D(t) = \varepsilon_0 E(t) + \varepsilon_0 \int_0^\infty f(\tau) E(t-\tau)\, d\tau$$

Here we singled out the first term

for convenience, but most importantly, integral is over positive τ => causality!

Let us now Fourier transform this expression:

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

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

$$D(\omega) = \varepsilon_0 \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{i\omega t} E(t)\, dt +$$

$$+ \varepsilon_0 \int_0^{\infty} d\tau \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}} e^{i\omega t} f(\tau)\, E(t-\tau) =$$

$$= \varepsilon_0 E(\omega) + \varepsilon_0 E(\omega) \int_0^{\infty} d\tau\, f(\tau) e^{i\omega\tau} \equiv$$

$$\equiv \varepsilon(\omega) E(\omega)$$

$$\frac{\varepsilon(\omega)}{\varepsilon_0} = 1 + \int_0^\infty d\tau\, g(\tau)\, e^{i\omega\tau} \qquad (*)$$

$\varepsilon(\omega)$ has real and imaginary parts:

$$\varepsilon(\omega) = \varepsilon'(\omega) + i\,\varepsilon''(\omega)$$

Because $g(\tau)$ is real

$$\varepsilon(-\omega) = \varepsilon^*(\omega):$$

$$\varepsilon'(-\omega) = \varepsilon'(\omega) \text{ and } \varepsilon''(\omega) = -\varepsilon''(\omega)$$

In dielectrics when $\omega \to 0$ we get the static situation (fields do not depend on time) ε becomes equal to <u>real</u> static susceptibility.

Causality and analytic properties of $\varepsilon(\omega)$

- We will now consider ε as a function of complex variable ω, like we did for the Green's function of $\Box$ operator.

- Because integral in (*) starts at $\tau=0$ $\varepsilon(\omega)$ is an analytic function in the upper half plane: integral converges if $\operatorname{Im}\omega > 0$ $e^{i\omega\tau} \sim e^{-(\operatorname{Im}(\omega))\cdot\tau}$.

We assume that the "memory" is finite so integral also converges for real ω (it is not true for conductors for $\omega=0$)

For very large real ω we can show that $\dfrac{\varepsilon(\omega)}{\varepsilon_0} = 1 - \dfrac{\text{const}}{\omega^2} + \dots$

This is because at very high frequencies charged particles are basically free.

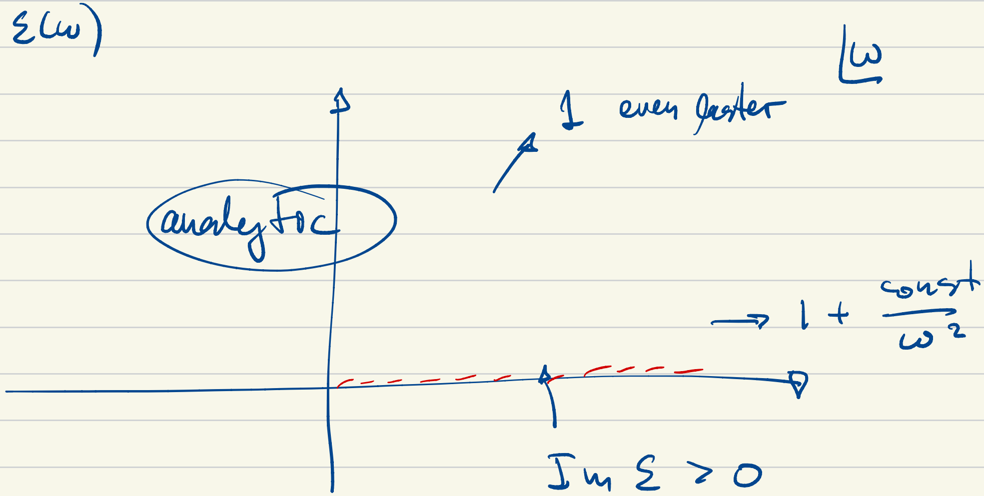
Then

$$m\ddot{r} = eE e^{i\omega t} \Rightarrow$$

$$\Rightarrow r \sim \frac{1}{\omega^2}$$

$$\vec{P} = \Sigma e\vec{r} \approx \frac{1}{\omega^2} \Rightarrow \vec{D} - \varepsilon_0\vec{E} \sim \frac{1}{\omega^2}$$

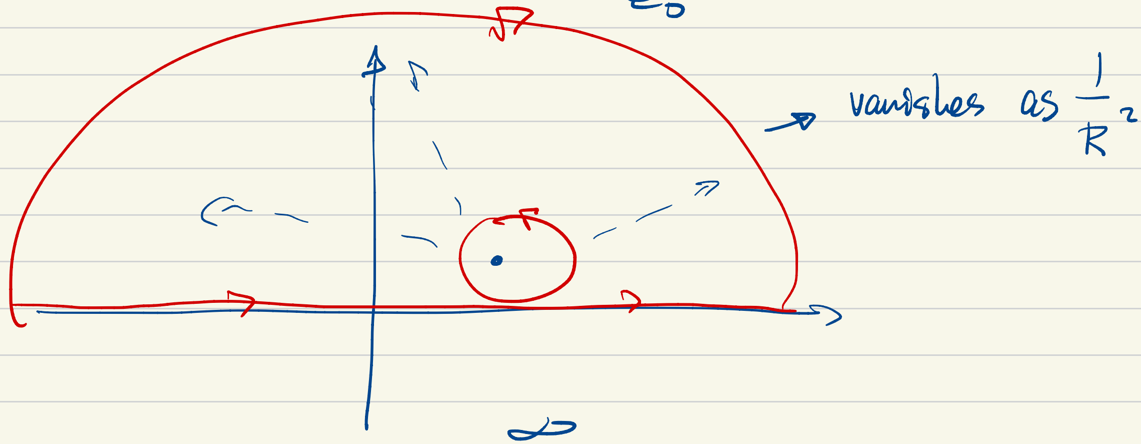
$\varepsilon(\omega)$



We will now use Cauchy's theorem to relate $\varepsilon'(\omega)$ and $\varepsilon''(\omega)$ for real ω (physical)

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

take $\quad F(z) = \dfrac{\varepsilon(z)}{\varepsilon_0} - 1$



$$\frac{\varepsilon(z)}{\varepsilon_0} - 1 = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\varepsilon(x)/\varepsilon_0 - 1}{x - z}\, dx$$

Mathematical intrelude

Next we are going to use some properties of regulated singular integrals (or distributions).

Define the "principal value" integral:

$$P\int_{-\infty}^{\infty} dx \frac{1}{x} f(x) = \lim_{\delta\to 0}\left(\int_{-\infty}^{\delta} + \int_{\delta}^{\infty}\right)\frac{1}{x} f(x)\,dx$$

The limit exists for any smooth function $f(x)$.

Define also distributions $\dfrac{1}{x+i\delta}$ and $\dfrac{1}{x-i\delta}$

so that

$$I_{+/-}[f(x)] = \lim_{\delta\to 0}\int dx \frac{1}{x\pm i\delta} f(x)$$

Again it can be shown that the limit exists.

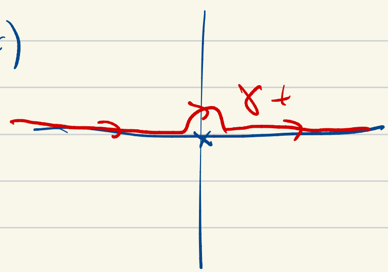
One more familiar to us distribution is Dirac δ-function:

$$\int dx\, \delta(x)\, f(x) = f(0).$$

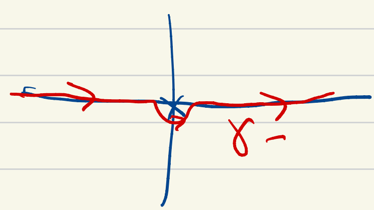
The distributions are related to each other. Let us find these relations.

$\frac{1}{x \pm i\delta}$ distributions can be equivalently thought of as small contour deformations:

$$\int_{-\infty}^{\infty} dx \frac{1}{x+i\delta} f(x) = \int_{\gamma_+} dx \frac{1}{x} f(x)$$

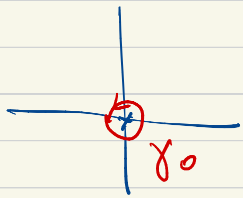


$$\int_{-\infty}^{\infty} dx \frac{1}{x-i\delta} f(x) = \int_{\gamma_-} dx \frac{1}{x} f(x)$$



Let us consider

$$I_-[f(x)] - I_+[f(x)] = \int_{\gamma_0} \frac{dx}{x} f(x) =$$



$$= 2\pi i\, f(0) = 2\pi i \int_{-\infty}^{\infty} \delta(x) f(x)$$

Here, even if $f(x)$ is not an analytic function, all what we use is that $f(x)$ is regular at zero. Since the above is true for any $f(x)$ we conclude that

$$\frac{1}{x-i\delta} - \frac{1}{x+i\delta} = 2\pi i\, \delta(x) \qquad (*)$$

Now consider

$$\int_{-\infty}^{\infty} \left(\frac{1}{x+i\delta} + \frac{1}{x-i\delta} \right) f(x)\, dx -$$

$$= \left(\int_{-\infty}^{-\Lambda} + \int_{\Lambda}^{\infty} + \int_{-\Lambda}^{\Lambda} \right) \left| \frac{1}{x+i\delta} + \frac{1}{x-i\delta} \right| \rho(x)\, dx$$

chose $1 >> \Lambda >> \delta$, then

$$\left(\int_{-\infty}^{-\Lambda} + \int_{\Lambda}^{\infty} \right) \left(\frac{1}{x+i\delta} + \frac{1}{x-i\delta} \right) \rho(x)\, dx \simeq$$

$$\simeq \left(\int_{-\infty}^{\Lambda} + \int_{\Lambda}^{\infty} \right) \frac{2}{x} \rho(x)\, dx = 2P \int_{-\infty}^{\infty} \frac{dx}{x} \rho(x)$$

At the same time,

$$\int_{-\Lambda}^{\Lambda} \left(\frac{1}{x+i\delta} + \frac{1}{x-i\delta} \right) \rho(x) dx = \overbrace{\int_{-\Lambda}^{\Lambda} dx \frac{2x}{x^2+\delta^2}}^{=0} f(0) +$$

$$+ \text{const} \cdot \int_{-\Lambda}^{\Lambda} dx \frac{2x^2}{x^2+\delta^2} \cdot \rho'(0) \leq \frac{\text{const}}{\delta^2} \cdot \Lambda^3$$

we can choose Λ and δ so that this expression is arbitrarily small. So we conclude that

$$\frac{1}{x+i\delta} + \frac{1}{x-i\delta} = 2\, P\,\frac{1}{x} \qquad (*)$$

Combining $*$ and $**$ we get

$$\frac{1}{x-i\delta} = P\,\frac{1}{x} + \pi i\, \delta(x) \,.$$

End of mathematical intrelude.

We continue with the expression

$$\frac{\varepsilon(z)}{\varepsilon_0} - 1 = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\varepsilon(x)/\varepsilon_0 - 1}{x - z}\, dx$$

now we take $z = \underset{\text{real}}{\omega} + i\underset{\text{infinitesemal}}{\delta}$.

$$\frac{1}{x-\omega-i\delta} = P\left(\frac{1}{x-\omega}\right) + \pi i\,\delta(x-\omega)$$

$$\frac{1}{2}\left(\frac{\varepsilon(\omega)}{\varepsilon_0} - 1\right) = \frac{1}{2\pi i} P\int_{-\infty}^{\infty} \frac{\varepsilon(x)/\varepsilon_0 - 1}{x-\omega}\,dx$$

Let's take real and imaginary parts:

$$\frac{\varepsilon'(\omega)}{\varepsilon_0} - 1 = \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{\varepsilon''(\omega)}{x-\omega}\,dx$$

$$\frac{\varepsilon''(\omega)}{\varepsilon_0} = -\frac{1}{\pi} P\int \frac{\varepsilon'(x)-1}{x-\omega}\,dx$$

These are the Kramers–Kronig relations

Using symmetry properties we get

$$\frac{\varepsilon'(\omega)}{\varepsilon_0} = 1 + \frac{2}{\pi} P \int_0^\infty \frac{x\,\varepsilon''(x)}{x^2-\omega^2}\,dx$$

$$\frac{\varepsilon''(\omega)}{\varepsilon_0} = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\varepsilon'(x)/\varepsilon_0 - 1}{x^2-\omega^2}\,dx$$

Importance of these relations is in the fact that measuring absorption $\varepsilon''(\omega)$ allows to reconstruct the entire dispersion of $\varepsilon(\omega)$.

Let us consider an example

$$\frac{\varepsilon}{\varepsilon_0} = 1 + \frac{\lambda}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

(resonant absorption on a line)

$$\frac{\varepsilon}{\varepsilon_0} = 1 + \frac{\text{const}}{\omega^2} \quad \text{at} \quad \omega \to \infty \quad \checkmark$$

$$\frac{\varepsilon'}{\varepsilon_0} = 1 + \lambda \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2} \simeq$$

$$\simeq 1 + \lambda \frac{1}{\omega_0^2 - \omega^2}$$, when γ is small,

and $\omega \neq \omega_0$

$$\frac{\varepsilon''}{\varepsilon_0} = \frac{\lambda \gamma \omega}{(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}$$

Let's check KK: (for $\omega \neq \omega_0$ and γ-small)

$$\int_0^\infty \frac{dx}{x^2 - \omega^2} \frac{\lambda \gamma x}{(\omega_0^2 - x^2)^2 + \gamma^2 x^2} \approx$$

$$\simeq \int_{\omega_0 - \gamma}^{\omega_0 + \gamma} \frac{1}{\omega_0^2 - \omega^2} \cdot \frac{\lambda \gamma x}{(\omega_0^2 - x^2)^2 + \gamma^2 x^2}$$

$$\int dz \frac{\lambda \gamma \omega_0}{(2\omega_0)^2 z^2 + \gamma^2 \omega_0^2} \simeq \lambda$$

- Let's come back to plane waves. $\vec{E} = \hat{E} \cdot e^{i\vec{k}\vec{x} - i\omega t}$

Since we derived all equations in frequency space, the relation between k and ω still hold:

$$i\omega \mu(\omega) \vec{H} = c \vec{\partial} \times \vec{E}$$

$$i\omega \varepsilon(\omega) \vec{E} = -c \vec{\partial} \times \vec{H} \quad \Rightarrow$$

$$k^2 = \varepsilon(\omega) \mu \frac{\omega^2}{c^2}$$

Let us first assume that ε is real. Then group velocity of light is given by $u = \frac{d\omega}{dk} = \frac{c}{d(n\omega)/d\omega}$

where $n(\omega) = \sqrt{\varepsilon(\omega)\mu}$.

If ε is imaginary k develops imaginary part. Assume $\vec{k} \sim (k_x, 0, 0)$

$$k_x = \sqrt{\varepsilon\mu}\,\frac{\omega}{c} \equiv \left[n(\omega) + i\varkappa(\omega)\right]\frac{\omega}{c}$$

extinction coefficient.

KK-like relations can be also derived for n and $\varkappa$