Introduction to Electromagnetic Response of Materials

(Electrodynamics of solids - 2021)

1. Macroscopic Maxwell equations
2. Response functions
3. Fourier transforms of macroscopic Maxwell equations
4. Transverse solutions
5. Longitudinal solutions
6. Alternative approach to the dielectric function
7. Refractive index
8. Properties of $\epsilon(\omega)$

1. Macroscopic Maxwell equations

Microscopic Maxwell equations:

$$\operatorname{div}\mathbf{e} = \frac{\kappa}{\varepsilon_0}\,,\ \operatorname{rot}\mathbf{e} = -\frac{\partial \mathbf{b}}{\partial t}\,,\ \operatorname{div}\mathbf{b} = 0\,,\ \frac{1}{\mu_0}\operatorname{rot}\mathbf{b} = \varepsilon_0\frac{\partial \mathbf{e}}{\partial t} + \mathbf{j}\,. \tag{1.1.1}$$

Spatial averages:

$$\{\mathbf{e}\}\ ...\ \mathbf{E}\,, \{\mathbf{b}\}\ ...\ \mathbf{B}\,, \{\kappa\} = \rho - \operatorname{div}\mathbf{P} + \rho_{ext}\,, \{\mathbf{j}\} = \mathbf{J} + \frac{\partial \mathbf{P}}{\partial t} + \operatorname{rot}\mathbf{M} + \mathbf{J}_{ext}\,. \tag{1.1.2}$$

Here
ρ ... macroscopic charge density,
$\mathbf{P}$ ... macroscopic polarization,
$\mathbf{J}$ ... macroscopic current density,
$\mathbf{M}$ ... macroscopic magnetization.
For rigorous definitions and derivations of MME, see chapter 6 of Jackson's textbook.
ρ_{ext}, $\mathbf{J}_{ext}$ ... contributions due to external charge carriers.
Macroscopic Maxwell equations:

$$\operatorname{div}\mathbf{D} = \rho + \rho_{ext}\,,\ \operatorname{rot}\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}\,,\ \operatorname{div}\mathbf{B} = 0\,,\ \operatorname{rot}\mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} + \mathbf{J}_{ext}\,. \tag{1.1.3}$$

Here $\mathbf{D} = \varepsilon_0\mathbf{E} + \mathbf{P}$ is the electric displacement and $\mathbf{H} = (\mathbf{B}/\mu_0) - \mathbf{M}$ the magnetic field ($\mathbf{B}$ will be called the magnetic induction in the following).

2. Response functions

Relations $\mathbf{D}$ ... $\mathbf{E}$, $\mathbf{J}$ ... $\mathbf{E}$, $\mathbf{H}$ ... $\mathbf{B}$:

$$\mathbf{D}(\mathbf{r},t) = \int d\mathbf{r}'\,dt'\epsilon(\mathbf{r}-\mathbf{r}',t-t')\mathbf{E}(\mathbf{r}',t')\,, \tag{1.2.1}$$

$$\mathbf{J}(\mathbf{r},t) = \int d\mathbf{r}'\,dt'\sigma_C(\mathbf{r}-\mathbf{r}',t-t')\mathbf{E}(\mathbf{r}',t')\,, \tag{1.2.2}$$

$$\mathbf{H}(\mathbf{r},t) = \int d\mathbf{r}'\,dt'\frac{1}{\mu}(\mathbf{r}-\mathbf{r}',t-t')\mathbf{B}(\mathbf{r}',t')\,. \tag{1.2.3}$$

It has been assumed that the material under consideration is - on a macroscopic scale - homogeneous ($\rightarrow$ $\mathbf{r}-\mathbf{r}'$ in the arguments) and isotropic ($\rightarrow$ in each case a single response function, independent on the polarization of $\mathbf{E}$ or $\mathbf{B}$).
Fourier transforms of these relations (FT $f(\omega)$ of $f(t)$ defined as $\int_{-\infty}^{\infty} dt f(t)e^{i\omega t}$,
FT $f(\mathbf{q})$ of $f(\mathbf{r})$ defined as $\frac{1}{\sqrt{V}}\int d\mathbf{r} f(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}$):

$$\mathbf{D}(\mathbf{q},\omega) = \epsilon(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)\,,\ \mathbf{J}(\mathbf{q},\omega) = \sigma_C(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)\,,\ \mathbf{H}(\mathbf{q},\omega) = \frac{1}{\mu}(\mathbf{q},\omega)\mathbf{B}(\mathbf{q},\omega)\,. \tag{1.2.4}$$

$\epsilon(\mathbf{q},\omega)$ ... permittivity (due to bound charge carriers),
$\sigma_C(\mathbf{q},\omega)$ ... conductivity (due to free charge carriers),
$\frac{1}{\mu}(\mathbf{q},\omega)$ ... inverse magnetic permeability.

3. Fourier transforms of macroscopic Maxwell equations

FT of M. equations:

$$i\mathbf{q}\cdot\epsilon(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)=\rho(\mathbf{q},\omega)+\rho_{ext}(\mathbf{q},\omega)\,, \tag{1.3.1}$$

$$i\mathbf{q}\times\mathbf{E}(\mathbf{q},\omega)=i\omega\mathbf{B}(\mathbf{q},\omega)\,, \tag{1.3.2}$$

$$i\mathbf{q}\cdot\mathbf{B}(\mathbf{q},\omega)=0\,, \tag{1.3.3}$$

$$i\mathbf{q}\times\frac{1}{\mu}(\mathbf{q},\omega)\mathbf{B}(\mathbf{q},\omega)=-i\omega\epsilon(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)+\sigma_C(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)+\mathbf{J}_{ext}(\mathbf{q},\omega)\,. \tag{1.3.4}$$

The equations can be understood as equations for amplitudes of a plane wave solution,

$$\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0\,e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\,,\ \mathbf{B}(\mathbf{r},t)=\mathbf{B}_0\,e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\,\text{etc.} \tag{1.3.5}$$

Next we address two important cases:
(i) purely transverse solutions with $\mathbf{E}_0\perp\mathbf{q}$, $\mathbf{q}\cdot\mathbf{E}_0=0$, $\mathbf{B}_0\perp\mathbf{q}$, $\mathbf{q}\cdot\mathbf{B}_0=0$, in the absence of external charge carriers (i.e., $\rho_{ext}=0$, $\mathbf{J}_{ext}=0$);
(ii) purely longitudinal solutions with $\mathbf{E}_0\parallel\mathbf{q}$, $\mathbf{B}_0=0$, also in the absence of external charge carriers.

4. Transverse solutions of the Maxwell equations

(i) By combining the second and the fourth M. e. we obtain

$$-\frac{i}{\omega}\frac{1}{\mu}(\mathbf{q},\omega)\mathbf{q}^2\mathbf{E}(\mathbf{q},\omega) = -i\omega\epsilon(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega) + \sigma_C(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)\,.$$

This provides the following important relation between $\mathbf{q}$ and ω:

$$\mathbf{q}^2 = \left(\frac{\omega}{c}\right)^2 \varepsilon_\perp(\mathbf{q},\omega) \tag{1.4.1}$$

with

$$\varepsilon_\perp(\mathbf{q},\omega) = \epsilon_r(\mathbf{q},\omega) + \frac{i}{\omega\epsilon_0}\sigma_C(\mathbf{q},\omega) + \frac{c^2\mathbf{q}^2}{\omega^2}\left[1 - \frac{1}{\mu_r}(\mathbf{q},\omega)\right]\,, \tag{1.4.2}$$

$\epsilon_r = \epsilon/\epsilon_0$, $1/\mu_r = \mu_0/\mu$.
$\varepsilon_\perp(\mathbf{q},\omega)$ ... transverse dielectric function or simply dielectric function.

Remarks:
- If $\varepsilon_\perp \in R, \geq 0$, in the relevant range of variables, it is possible to find real wave vectors satisfying $\mathbf{q}^2 = \frac{\omega}{c}^2\varepsilon_\perp(\mathbf{q},\omega)$ and plane wave solutions.
- If this condition is not satisfied, there are no plane wave solutions; but there are solutions with a complex wave vector $\mathbf{q} = \mathbf{q}' + i\mathbf{q}''$, $\sim e^{i[(\mathbf{q}'+i\mathbf{q}'')\mathbf{r}-\omega t]}$.

5. Longitudinal solutions of the Maxwell equations

(ii) In the longitudinal case, $\mathbf{B} = 0$. By combining the first Maxwell equation, the continuity equation,

$$\nabla \mathbf{J} = -\frac{\partial \rho}{\partial t}\,,\ \mathbf{q} \cdot \mathbf{J}(\mathbf{q}, \omega) = \omega \rho(\mathbf{q}, \omega)\,, \tag{1.5.1}$$

and $\mathbf{J}(\mathbf{q}, \omega) = \sigma_C(\mathbf{q}, \omega)\mathbf{E}(\mathbf{q}, \omega)$ we obtain

$$i\mathbf{q} \cdot \epsilon(\mathbf{q}, \omega)\mathbf{E}(\mathbf{q}, \omega) = \frac{\mathbf{q}}{\omega}\sigma_C(\mathbf{q}, \omega)\mathbf{E}(\mathbf{q}, \omega)\,.$$

It can be seen that solutions are possible only for

$$\varepsilon_{\|}(\mathbf{q}, \omega) = 0\,,\ \varepsilon_{\|}(\mathbf{q}, \omega) = \epsilon_r(\mathbf{q}, \omega) + \frac{i}{\omega \epsilon_0}\sigma_C(\mathbf{q}, \omega)\,. \tag{1.5.2}$$

$\varepsilon_{\|}(\mathbf{q}, \omega)$ ... longitudinal dielectric function, which differs from the tranverse one, $\varepsilon_{\perp}$, in that the last term of $\varepsilon_{\perp}$, corresponding to magnetization currents, is absent.

6. Alternative approach to the dielectric function

The above approach is formally complicated due to the presence of three basic response functions: $\epsilon(\mathbf{q},\omega)$, $\sigma_C(\mathbf{q},\omega)$, $\frac{1}{\mu}(\mathbf{q},\omega)$. These are connected to the three components of the current density $\{\mathbf{j}\}$: $\frac{\partial \mathbf{P}}{\partial t}$, $\mathbf{J}$, $\mathrm{rot}\,\mathbf{M}$. Instead it is possible to define a quantity $\mathbf{D}'$, involving all the three components, as the spatial average of the quantity $\mathbf{d}'$ given by

$$\frac{\partial \mathbf{d}'}{\partial t} = \varepsilon_0 \frac{\partial \mathbf{e}}{\partial t} + \mathbf{j}\,. \tag{1.6.1}$$

The corresponding macroscopic Maxwell equations read

$$\mathrm{div}\,\mathbf{D}' = \rho_{ext}\,,\ \mathrm{rot}\,\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}\,,\ \mathrm{div}\,\mathbf{B} = 0\,,\ \frac{1}{\mu_0}\mathrm{rot}\,\mathbf{B} = \frac{\partial \mathbf{D}'}{\partial t} + \mathbf{J}_{ext}\,. \tag{1.6.2}$$

The relation between $\mathbf{D}'$ and $\mathbf{E}$:

$$\mathbf{D}'(\mathbf{r},t) = \int d\mathbf{r}\,dt'\varepsilon(\mathbf{r}-\mathbf{r}',t-t')\mathbf{E}(\mathbf{r}',t')\,,\mathbf{D}'(\mathbf{q},\omega) = \varepsilon(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)\,. \tag{1.6.3}$$

Here ε is a tensor (dielectric tensor) that can be expressed as

$$\frac{\varepsilon_{\mu\nu}(\mathbf{q},\omega)}{\epsilon_0} = \varepsilon_{\parallel}(\mathbf{q},\omega)\frac{q_\mu q_\nu}{\mathbf{q}^2} + \varepsilon_{\perp}(\mathbf{q},\omega)\left(\delta_{\mu\nu} - \frac{q_\mu q_\nu}{\mathbf{q}^2}\right)\,, \tag{1.6.4}$$

where $\varepsilon_{\parallel}(\mathbf{q},\omega)$ and $\varepsilon_{\perp}(\mathbf{q},\omega)$ were already introduced. It can be seen that the total conductivity σ_{tot} connecting $\{\mathbf{j}\}$ and $\mathbf{E}$ is given by

$$\sigma_{tot}(\mathbf{q},\omega) = -i\omega[\varepsilon(\mathbf{q},\omega) - \epsilon_0]. \tag{1.6.5}$$

7. Refractive index

In the following we limit ourselves to the transverse case. The $\mathbf{q}$ vector of a plane wave solution satisfies

$$\mathbf{q}^2 = \left(\frac{\omega}{c}\right)^2 \varepsilon_\perp(\mathbf{q},\omega)\,. \tag{1.4.1}$$

It can be seen that in case of a negative or complex $\varepsilon_\perp$ - the index $\perp$ will be omitted in the following - there are no plane wave solutions, but there are solutions with a complex wave vector $\mathbf{q} = \mathbf{q}' + i\mathbf{q}''$ satisfying

$$\mathbf{q}^2 = \mathbf{q}'^2 - \mathbf{q}''^2 + 2i\mathbf{q}'\mathbf{q}'' = \left(\frac{\omega}{c}\right)^2 \varepsilon(\mathbf{q},\omega)\,. \tag{1.7.1}$$

Any such vector $\mathbf{q}$ can be expressed as

$$\mathbf{q} = \hat{N}(\mathbf{q},\omega)\frac{\omega}{c}\mathbf{n}_\mathbf{q}\,, \tag{1.7.2}$$

where

$$\hat{N} = n + ik = \sqrt{\varepsilon(\mathbf{q},\omega)} \tag{1.7.3}$$

is the so called (in general complex) refractive index and $\mathbf{n}_\mathbf{q}$ is a (in general complex) vector such that $\mathbf{n}_\mathbf{q}^2 = 1$. The sign of the square root is chosen such that k is positive.

8. Properties of $\epsilon(\omega)$

We focus on the permittivity ϵ and assume that the response is local, i.e.,

$$\epsilon(\mathbf{r}-\mathbf{r}', t-t') = \delta(\mathbf{r}-\mathbf{r}')\left[\epsilon_0\delta(t-t') + f(t-t')\right] . \tag{1.8.1}$$

Then we have

$$\epsilon(\mathbf{q},\omega) = \epsilon(\omega) = \epsilon_0 + \int_{-\infty}^{\infty} d\tau f(\tau) e^{i\omega\tau} . \tag{1.8.2}$$

The displacement $\mathbf{D}$ at a time t can be influenced by $\mathbf{E}$ at $t' \leq t$, not by $\mathbf{E}$ at $t' > t$ (causality requirement). The function $f(\tau)$ is thus nonzero only for $\tau \geq 0$ and we can write

$$\epsilon(\omega) = \epsilon_0 + \int_{0}^{\infty} d\tau f(\tau) e^{i\omega\tau} . \tag{1.8.3}$$

The above equation can be viewed as a definition of a complex function of a complex variable $\omega = \omega' + i\omega''$.

- This function nowhere becomes infinite (i.e., has no singularities) in the upper half-plane. This follows from the fact that $f(\tau)$ is finite and from the presence of the exponentially decreasing factor $e^{-\omega''\tau}$.
- The function can be assumed not to have any singularity on the real axis.
- The definition cannot be applied to the lower half-plane, since in this case the integral diverges. The function $\epsilon(\omega)$ can be defined in the lower-half plane only as the analytical continuation of $\epsilon(\omega)$ of the upper half-plane, and in general has singularities.

8. Properties of $\epsilon(\omega)$

• It is evident from the definition and from the fact that $f(\tau)$ is a real function, that $\epsilon(-\omega' + i\omega'') = \epsilon^*(\omega' + i\omega'')$. In particular, on the real axis

$$\epsilon'(-\omega) = \epsilon'(\omega)\,,\; \epsilon''(-\omega) = -\epsilon''(\omega)\,. \tag{1.8.4}$$

• The energy dissipated in a material in the presence of a plane-wave-like wave with a complex $\mathbf{q}$-vector is proportional to $\epsilon''(\omega)|\mathbf{E}_0|^2$,

$$\frac{1}{2}\omega\epsilon''(\omega)|\mathbf{E}_0|^2 \tag{1.8.5}$$

per unit volume and unit time interval. We assume here, that $\sigma_C = 0$ and $1/\mu_r = 1$, i.e., that the only nonzero component of the current density is $\frac{\partial \mathbf{P}}{\partial t}$. Note that the derivation of Eq. (1.8.5) includes the real field, i.e., the real part of the plane wave. It follows that $\epsilon''(\omega)$ is nonnegative for positive frequencies and - this follows from $\epsilon''(-\omega) = -\epsilon''(\omega)$ - nonpositive for negative frequencies.

• Regarding the asymptotic behaviour of $\epsilon(\omega)$ on the real axis: at frequencies far above the highest resonant frequency of the material,

$$\epsilon(\omega) \approx \epsilon_0 \left[1 - \frac{\omega_P^2}{\omega^2}\right]\,, \tag{1.8.6}$$

where $\omega_P = \frac{ne^2}{\epsilon_0 m}$ is the plasma frequency, n is the total number of electrons per unit volume, the contribution of lattice vibrations is neglected.

8. Properties of $\epsilon(\omega)$

• Considering the above properties of $\epsilon(\omega)$, we can derive the famous Kramers-Kronig relations. By integrating $(\epsilon(\omega_0) - \epsilon_0)/(\omega - \omega_0)$ along the contour shown in Fig. 3.1 of Dressel's textbook we obtain

$$\epsilon'(\omega_0) - \epsilon_0 = \frac{1}{\pi} P \int_{\infty}^{\infty} \frac{\epsilon''(\omega)}{\omega - \omega_0} \, d\omega \tag{1.8.7}$$

$$\epsilon''(\omega_0) = -\frac{1}{\pi} P \int_{\infty}^{\infty} \frac{\epsilon'(\omega) - \epsilon_0}{\omega - \omega_0} \, d\omega \, . \tag{1.8.8}$$

Here P means the principal value of the integral.

• The same approach can be applied to $\varepsilon_{\perp}(\omega)$.