

6. Electrostatics in Matter

Thus far, apart from our considerations about conductors, we have studied the fields created by static charges in vacuum. We next address the fields created by charges in matter.

In order to do so, we need to take into account the charges and currents associated with the microscopic building blocks of matter: electrons and nuclei, and we have to distinguish between microscopic and macroscopic fields.

Typically, we do not have access to the electric field at any point inside matter, \vec{E} . Instead, we can only measure spatial averages of this

microscopic field over microscopically large regions:

$$\vec{E}(\vec{r}) \equiv \langle \vec{e} \rangle(\vec{r}) = \int d^3\vec{r}' W(\vec{r}-\vec{r}') \vec{e}(\vec{r}')$$

where $W(\vec{r})$ is a "window function" that determines the extent of the volume average, with $\int d^3r W(\vec{r}) = 1$.

Examples: Top-hat window function

$$W(\vec{r}) = \begin{cases} \frac{3}{4\pi R^3} & r < R \\ 0 & r > R \end{cases}$$

leads to a spatial average over a sphere of radius R . A smoother window function is

the gaussian

$$W(\vec{r}) = \frac{e^{-r^2/R^2}}{(\pi R^2)^{3/2}}$$

(convenient with Fourier transforms.)

Consider now the full Maxwell's eqs.

$$\vec{\nabla} \cdot \vec{b} = 0, \quad \vec{\nabla} \times \vec{e} + \frac{1}{c} \partial_t \vec{b} = 0 \quad \text{homogeneous}$$

$$\vec{\nabla} \cdot \vec{e} = 4\pi \rho_{\text{micro}}, \quad \vec{\nabla} \times \vec{e} - \frac{1}{c} \partial_t \vec{e} = \frac{4\pi}{c} \vec{j}_{\text{micro}} \quad \text{inhomogeneous}$$

Taking spatial averages (and using linearity)

we find

$$\vec{\nabla} \cdot \vec{B} = 0, \quad \vec{\nabla} \times \vec{E} + \frac{1}{c} \partial_t \vec{B} = 0$$

$$\vec{\nabla} \cdot \vec{E} = 4\pi \langle \rho_{\text{micro}} \rangle, \quad \vec{\nabla} \times \vec{E} - \frac{1}{c} \partial_t \vec{E} = \frac{4\pi}{c} \langle \vec{j}_{\text{micro}} \rangle$$

In electrostatic situations there is no macroscopic magnetic field \vec{B} , so

$$\vec{\nabla} \times \vec{E} = 0,$$

and we may still write $\vec{E} = -\vec{\nabla} \phi$.

Let us write the charge density as the sum of the bound charges in molecules ρ_{bound} , and the free charges that are not localized.

Then, $\rho_{\text{micro}} = \rho_{\text{bound}} + \rho_{\text{free}}$, where

$$\rho_{\text{bound}} = \sum_{\text{molecules } n} \rho_n(\vec{r}) \quad \text{and}$$

$$\rho_{\text{free}} = \sum_j q_j \delta(\vec{r} - \vec{r}_j). \quad \text{Let us assume that}$$

the charge density of molecule n is

$$\rho_n(\vec{r}) = \sum_{j(n)} q_j \delta(\vec{r} - (\vec{r}_j + \vec{r}_n)).$$

\nearrow \nwarrow CM of molecule
 charge location in CM frame.

average is

$$\begin{aligned} \langle \rho_n(\vec{r}) \rangle &= \int d^3r' W(\vec{r} - \vec{r}') \rho_n(\vec{r}') = \int d^3r' W(\vec{r}') \rho_n(\vec{r} - \vec{r}') = \\ & \quad \vec{r}' \rightarrow \vec{r} - \vec{r}' \\ &= \sum_{j(n)} q_j W(\vec{r} - \vec{r}_n - \vec{r}_{jn}) \end{aligned}$$

Since W averages over a macroscopic region, and

\vec{r}_{jn} is of microscopic length, Taylor expand

$$\begin{aligned} \langle \rho_n(\vec{r}) \rangle &= \sum_{j(n)} q_j \left[W(\vec{r} - \vec{r}_n) - \vec{r}_{jn} \cdot \vec{\nabla} W(\vec{r} - \vec{r}_n) + \right. \\ & \quad \left. + \frac{1}{2} (\vec{r}_{jn})_i (\vec{r}_{jn})_k \frac{\partial^2 W(\vec{r} - \vec{r}_n)}{\partial r_i \partial r_k} + \dots \right] \end{aligned}$$

We can thus write

$$\langle \rho_n(\vec{r}) \rangle = q_n W(\vec{r} - \vec{r}_n) - \vec{p}_n \cdot \vec{\nabla} W(\vec{r} - \vec{r}_n) + \frac{1}{6} (Q_n')_{ik} \frac{\partial^2 W(\vec{r} - \vec{r}_n)}{\partial r_i \partial r_k},$$

where $q_n = \sum_{j(n)} q_j$ is molecular charge

$\vec{p}_n = \sum_{j(n)} q_j \vec{r}_{jn}$ " dipole

$(Q_n')_{ik} = 3 \sum_{j(n)} q_j (r_{jn})_i (r_{jn})_k$ quadrupole (not traceless)

Therefore, because of the spatial average, we can regard the molecule as a collection of point multipoles.

Finally taking the average over all charges we find

$$\langle \rho(\vec{r}) \rangle = \rho_{macro}(\vec{r}) - \vec{\nabla} \cdot \vec{P}(\vec{r}) + \sum_{ik} \frac{\partial^2 Q'_{ik}}{\partial r_i \partial r_k}, \quad \text{where}$$

ρ_{macro} is the macroscopic charge density:

$$\rho_{macro}(\vec{r}) = \left\langle \sum_{j \text{ free}} q_j \delta(\vec{r} - \vec{r}_j) + \sum_{\substack{n \\ \text{molecules}}} q_n \delta(\vec{r} - \vec{r}_n) \right\rangle$$

\vec{P} is the macroscopic charge density:

$$\vec{P}(\vec{r}) = \left\langle \sum_{\substack{\text{molecules} \\ n}} \vec{p}_n \delta(\vec{r} - \vec{r}_n) \right\rangle$$

and Q'_{in} is the macroscopic quadrupole.

We thus find that the equation $\vec{\nabla} \cdot \vec{E} = 4\pi \langle \rho_{micro} \rangle$ becomes

$$\underline{\vec{\nabla} \cdot (\vec{E} + 4\pi \vec{P} - 4\pi \dots) = 4\pi \rho_{macro}}$$

Typically, the macroscopic quadrupole is negligible, so the last equation becomes

$$\vec{\nabla} \cdot \vec{D} = 4\pi \rho_{macro}, \quad \text{where}$$

$$\vec{D} \equiv \vec{E} + 4\pi \vec{P} \quad \text{is the electric displacement}$$

To close the system of equations

$$\begin{cases} \vec{\nabla} \cdot \vec{D} = 4\pi \rho & \text{(skip "macro" from now on)} \\ \vec{\nabla} \times \vec{E} = 0 \end{cases}$$

we need a "constitutive relation" between \vec{E} and \vec{D} (or \vec{E} and \vec{P})

Many molecules do not have a dipole moment in the absence of external electric fields. These materials are known as dielectrics.

For small fields, we expect that \vec{P} is linear in \vec{E} : $\vec{P} = \chi_e \cdot \vec{D}$.

χ_e is the electric susceptibility. In general χ_e is a tensor (a linear operator), which transforms appropriately under rotations.

- If the medium is isotropic, χ_e is proportional to the identity matrix.
- If the medium is homogeneous χ_e is a constant in space.

Under both assumptions we have

$$\vec{D} = \epsilon \cdot \vec{E} \quad \text{with} \quad \epsilon = 1 + 4\pi\chi_e$$

ϵ is the dielectric constant or permittivity.

6.3. Uniqueness theorem.

As for $\chi_e = 0$ (the case we studied so far), one can show that for two sols. ∇

$$\begin{cases} \nabla \cdot \vec{D} = 4\pi\rho \\ \nabla \times \vec{E} = 0 \end{cases} \quad (*)$$

and with $\vec{E} = -\nabla\phi$,

$$\oint_{\partial V} (\phi_1 - \phi_2) (\vec{D}_1 - \vec{D}_2) \cdot d\vec{A} = - \int_V (\vec{D}_1 - \vec{D}_2) \cdot (\vec{E}_1 - \vec{E}_2) dV.$$

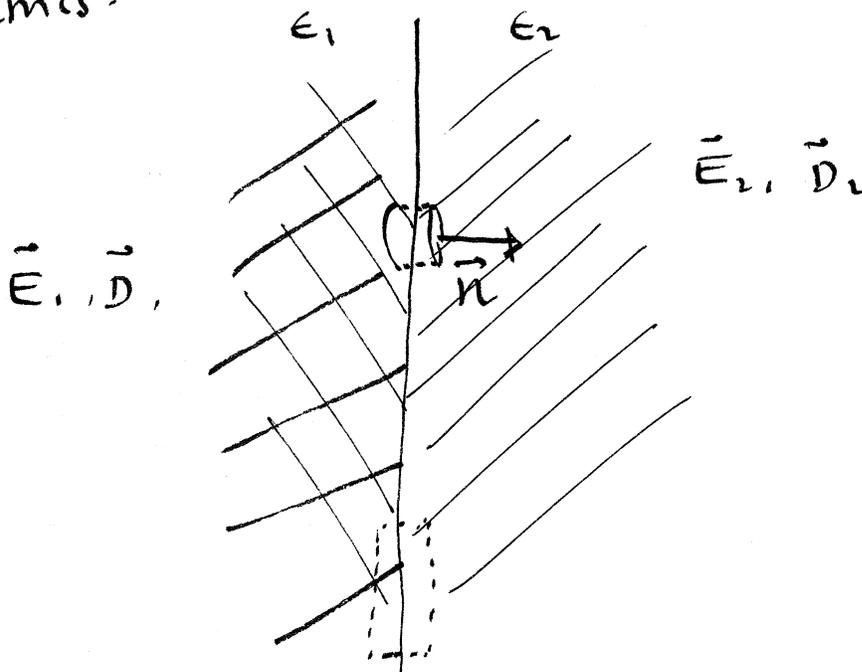
Therefore, if the tensor $\epsilon = 1 + 4\pi\chi_e$ is positive definite, the solution of (*) is unique if :

- Dirichlet problem : ϕ specified on ∂V
- Neumann problem : $\vec{n} \cdot \vec{D}$ " " "

6.4. Boundary value problems with Polarization

6.4.1. Boundary conditions on \vec{D} , \vec{E} and ϕ

Sometimes we need to solve problem in which a boundary separates two different dielectrics:



Applying $\vec{\nabla} \cdot \vec{D} = 4\pi\rho$ ($\int_V dV 4\pi\rho = \oint_{\partial V} \vec{D} \cdot d\vec{A}$)

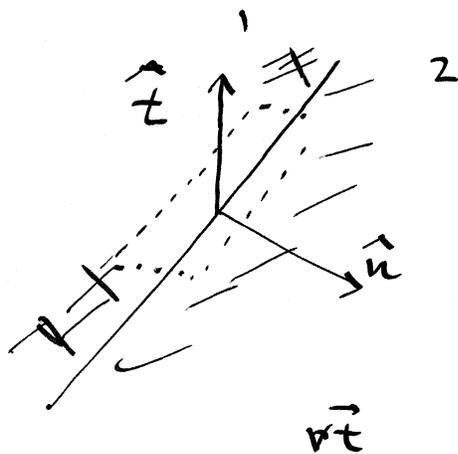
to a pillbox on the interface, we find

$$\underline{(\vec{D}_2 - \vec{D}_1) \cdot \vec{n} = 4\pi\sigma}, \text{ where}$$

σ is the macroscopic charge density.

Applying $\vec{\nabla} \times \vec{E} = 0$ ($\int_A \vec{\nabla} \times \vec{E} \cdot d\vec{A} = \oint_{\partial A} \vec{E} \cdot d\vec{l}$)

to a contour bridging the interface:



$$(\hat{t} \times \hat{n}) \cdot \vec{E} = 0. \quad \text{And since}$$

$$\vec{E} \cdot (\hat{t} \times \hat{n}) = \hat{t} \cdot (\hat{n} \times \vec{E}) \stackrel{!}{=} 0 \quad \forall \hat{t}$$

$$\underline{\hat{n} \times \vec{E} = 0.}$$