

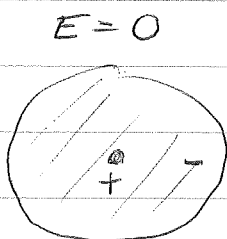
Rather than worry about the microscopic details of ρ and \vec{j} and resulting \vec{E} and \vec{B} we want to describe phenomena in terms of ~~averaged~~ ~~smoothly varying~~ ~~smoothly varying~~ ~~smoothly varying~~ averaged quantities that are smoothly varying at the atomic scale. This results in what are known as the macroscopic Maxwell equations.

Dielectric Materials

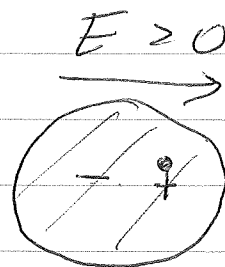
can be solid, liquid or gas

A dielectric material is an insulator. Electrons are bound to the ionic cores of the atoms.

When no electric field is present, the averaged ρ in the dielectric vanishes! One might therefore think that electrostatics in a dielectric is just due to whatever "extra" or "free" charge is added to the dielectric. However this is not true due to the phenomena of "polarization".



electron cloud centered on ionic ~~core~~ core
dipole moment vanishes



electron cloud and ionic core displaced $\vec{d} \propto \vec{E}$
atom is "polarized"
has dipole moment $\vec{p} = q\vec{d} \propto q\vec{E}$

$$\vec{p} = \alpha \vec{E}$$

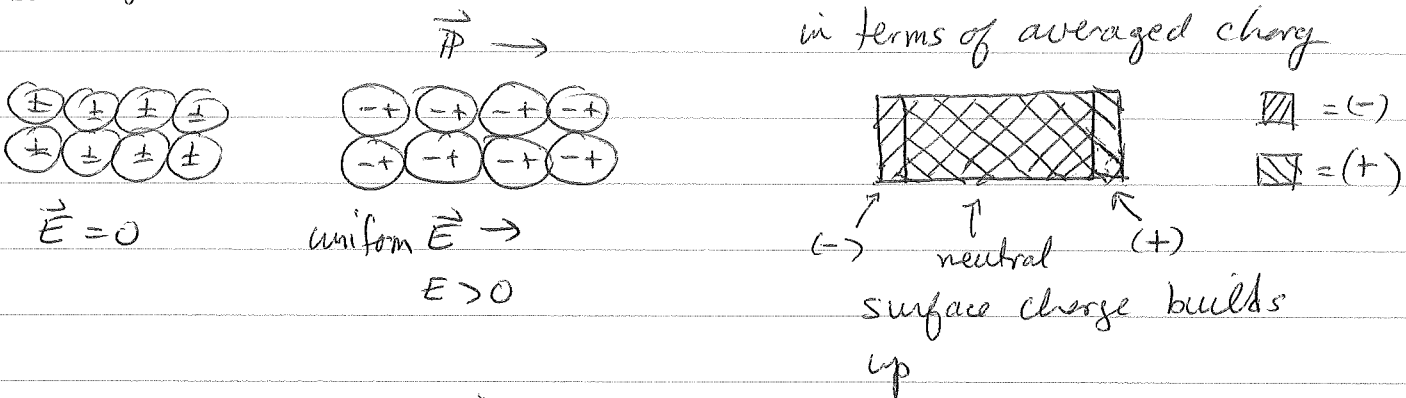
↑
atomic polarizability

Polarization density $\vec{P}(\vec{r}) = \sum_i \vec{p}_i \delta(\vec{r} - \vec{r}_i)$

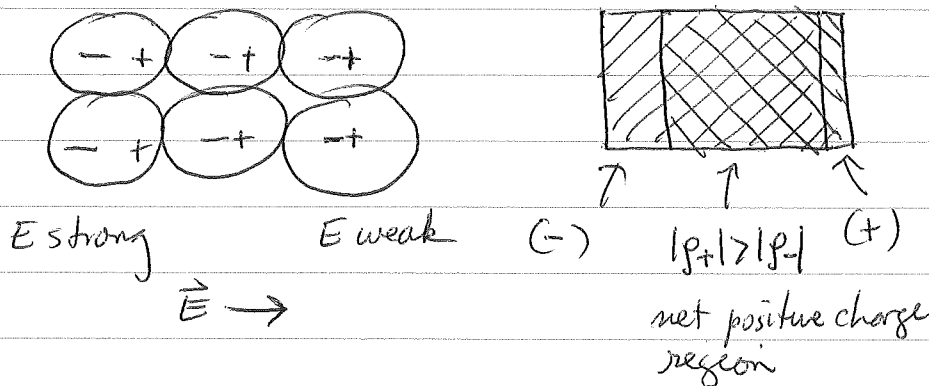
\vec{p}_i
 dipole moment of atom i
 at position \vec{r}_i

Polarization density \vec{P} can give rise to regions of net charge - sometimes called "bound charge"

Example



For a non uniform \vec{E} , atoms are more strongly polarized where E is largest



For uniform \vec{P} , build up surface charge σ_b
 For nonuniform \vec{P} , also can build up vol charge density ρ_b .

We now carry out the averaging explicitly to see how such polarization enters the macroscopic Maxwell equations

(Jackson 6.6)

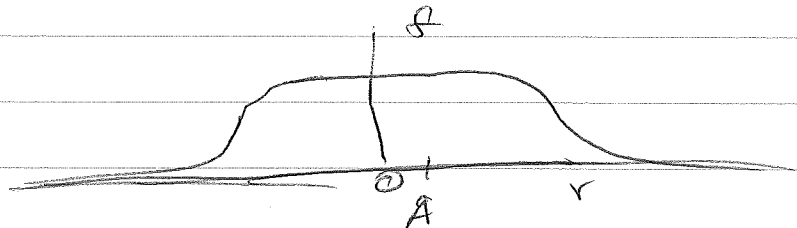
Define spatially averaged quantities by

$$\langle F(\vec{r}, t) \rangle = \int d^3r' f(\vec{r}') F(\vec{r} - \vec{r}', t)$$

where $f(\vec{r})$ vanishes for $|\vec{r}|$ large on microscopic length scales, but short on macroscopic length scales.

$f(\vec{r})$ normalized to unity, $\int d^3r f(\vec{r}) = 1$.

Other details of $f(\vec{r})$ are not too important, as long as $f(\vec{r})$ is a smooth function of \vec{r}



want $f \approx \text{const}$ for $r < R$

$f \approx 0$ for $r \gg R$

where R is length scale
in between micro + macro

$$\frac{\partial}{\partial r_i} \langle F(\vec{r}, t) \rangle = \int d^3r' f(\vec{r}') \frac{\partial F(\vec{r} - \vec{r}')}{\partial r_i} = \left\langle \frac{\partial F}{\partial r_i} \right\rangle$$

$$\frac{\partial}{\partial t} \langle F(\vec{r}, t) \rangle = \left\langle \frac{\partial F}{\partial t} \right\rangle$$

Define the macroscopic fields

$$\vec{E}(\vec{r}, t) \equiv \langle \vec{e}(\vec{r}, t) \rangle$$

$$\vec{B}(\vec{r}, t) \equiv \langle \vec{b}(\vec{r}, t) \rangle$$

$$\begin{aligned} \text{Then } \vec{\nabla} \cdot \vec{b} = 0 &\Rightarrow \langle \vec{\nabla} \cdot \vec{b} \rangle = 0 \\ &\Rightarrow \vec{\nabla} \cdot \langle \vec{b} \rangle = 0 \\ &\Rightarrow \vec{\nabla} \cdot \vec{B} = 0 \end{aligned}$$

$$\vec{\nabla} \times \vec{e} + \frac{\partial \vec{b}}{\partial t} = 0 \Rightarrow \vec{\nabla} \times \langle \vec{e} \rangle + \frac{\partial \langle \vec{b} \rangle}{\partial t} = 0$$

$$\Rightarrow \vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0$$

Remaining Maxwell eqn, upon averaging, become

$$\vec{\nabla} \cdot \vec{E} = 4\pi \langle \rho_0 \rangle$$

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c} \langle \vec{j}_0 \rangle + \frac{\partial \vec{E}}{\partial t}$$

Consider $\langle \rho_0 \rangle$

$$\rho_0 = \sum_i q_i \delta(\vec{r} - \vec{r}_i(t)) \quad \text{sum over all charges}$$

Consider dividing the charge into "free" charges and "bound" charges, where the latter are associated with the molecules that make up the dielectric

$$\rho_{\text{free}} = \sum_{i \text{ free}} q_i \delta(\vec{r} - \vec{r}_i(t)) \quad \begin{array}{l} \text{sum over only free charges} \\ \text{ie, external charges added to} \\ \text{the material} \end{array}$$

$$\rho_{\text{bound}} = \sum_n \rho_n(\vec{r}, t)$$

↑ charge distribution of molecule n

$$\rho_n(\vec{r}, t) = \sum_{i \in n} q_i \delta(\vec{r} - \vec{r}_i(t)) \quad \text{sum over charges in molecule n}$$

Define $q_n \equiv \sum_{i \in n} q_i$ total charge molecule n

$\vec{p}_n \equiv \sum_{i \in n} q_i \vec{r}_{ni}$ dipole moment about center of mass of molec n

$\overset{\leftrightarrow}{Q}'_n \equiv \sum_{i \in n} 3 q_i \vec{r}_{ni} \vec{r}_{ni}$ quadrupole moment about center of mass of molec n

(prime on $\overset{\leftrightarrow}{Q}'$ since definition here is a little different from that of multipole exp)
 $\overset{\leftrightarrow}{Q}'$ is not traceless

$$\langle \rho_n(\vec{r}, t) \rangle = q_n f(\vec{r} - \vec{r}_n) - \vec{p}_n \cdot \vec{\nabla} f(\vec{r} - \vec{r}_n)$$

$$+ \frac{1}{6} \sum_{\alpha\beta} (\overset{\leftrightarrow}{Q}'_n)_{\alpha\beta} \frac{\partial^2 f(\vec{r} - \vec{r}_n)}{\partial r_\alpha \partial r_\beta}$$

Now use $\langle \delta(\vec{r} - \vec{r}_n) \rangle = f(\vec{r} - \vec{r}_n)$ by definition of averaging

$$\Rightarrow \langle \rho_n(\vec{r}, t) \rangle = \langle q_n \delta(\vec{r} - \vec{r}_n) \rangle$$

$$- \vec{\nabla} \cdot \langle \vec{p}_n \delta(\vec{r} - \vec{r}_n) \rangle \quad \vec{\nabla} \cdot p \delta = \vec{p} \cdot \vec{\nabla} \delta$$

$$+ \frac{1}{6} \sum_{\alpha\beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \langle (\overset{\leftrightarrow}{Q}'_n)_{\alpha\beta} \delta(\vec{r} - \vec{r}_n) \rangle$$

Now

$$\langle \rho_{\text{bound}}(\vec{r}, t) \rangle = \sum_n \langle \rho_n(\vec{r}, t) \rangle$$

$$= \left\langle \sum_n q_n \delta(\vec{r} - \vec{r}_n) \right\rangle - \vec{\nabla} \cdot \left\langle \sum_n \vec{p}_n \delta(\vec{r} - \vec{r}_n) \right\rangle$$

$$+ \frac{1}{6} \sum_{\alpha\beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \left\langle \sum_n (\overset{\leftrightarrow}{Q}'_n)_{\alpha\beta} \delta(\vec{r} - \vec{r}_n) \right\rangle$$

Define $\vec{P}(\vec{r}, t) \equiv \left\langle \sum_n \vec{p}_n \delta(\vec{r} - \vec{r}_n) \right\rangle$ average polarization density

$\vec{Q}'(\vec{r}, t) \equiv \frac{1}{6} \left\langle \sum_n \vec{Q}'_n \delta(\vec{r} - \vec{r}_n) \right\rangle$ average quadrupole density

$\langle \rho_{\text{bound}} \rangle = \sum_n \langle q_n \delta(\vec{r} - \vec{r}_n) \rangle - \vec{\nabla} \cdot \vec{P} + \sum_{\alpha\beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \vec{Q}'_{\alpha\beta}$

Define the macroscopic charge density

$\rho \equiv \left\langle \sum_{i \text{ free}} q_i \delta(\vec{r} - \vec{r}_i) \right\rangle + \left\langle \sum_n q_n \delta(\vec{r} - \vec{r}_n) \right\rangle$

then

↑ vanishes if molecule is charge neutral

$\vec{\nabla} \cdot \vec{E} = 4\pi \langle \rho_0 \rangle = 4\pi \left[\rho - \vec{\nabla} \cdot \vec{P} + \sum_{\alpha\beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \vec{Q}'_{\alpha\beta} \right]$

$\sum_{\alpha} \frac{\partial}{\partial r_\alpha} \left[E_\alpha + 4\pi P_\alpha - 4\pi \sum_{\beta} \frac{\partial}{\partial r_\beta} Q'_{\alpha\beta} \right] = 4\pi \rho$

Define electric displacement vector

$D_\alpha = E_\alpha + 4\pi P_\alpha - 4\pi \sum_{\beta} \frac{\partial}{\partial r_\beta} Q'_{\alpha\beta}$

then $\boxed{\vec{\nabla} \cdot \vec{D} = 4\pi \rho}$

In most materials, the quadrupole and higher terms are negligible and we can take

$\vec{D} = \vec{E} + 4\pi \vec{P}$

Why quadrupole + higher order terms
can generally be ignored:

Let a_0 be the length scale that characterizes the size of a molecule in the dielectric

Let l be the typical spacing between molecules

Let L be the length scale of the spatial averaging function $f(\vec{r})$. $L \gg a_0$

dipole moment per a_0

$$\Rightarrow \text{polarization density } \vec{P} \sim \frac{a_0}{l^3}$$

$$\vec{\nabla} \cdot \vec{P} \sim \left(\frac{a_0}{L}\right) \frac{1}{l^3}$$

since P cannot vary on length scale shorter than the averaging length L

quadrupole moment

$$Q \sim a_0^2$$

$$\text{quadrupole density } \vec{Q} \sim \frac{a_0^2}{l^3}$$

$$\frac{\partial^2 Q}{\partial r_x \partial r_y} \sim \left(\frac{a_0}{L}\right)^2 \frac{1}{l^3}$$

each higher moment gives extra factor a_0

each higher derivative gives extra factor $\frac{1}{L}$

so quadrupole is smaller than dipole term by factor $\left(\frac{a_0}{L}\right) \ll 1$. Higher terms smaller ~~is~~ by additional factors of $\left(\frac{a_0}{L}\right)$

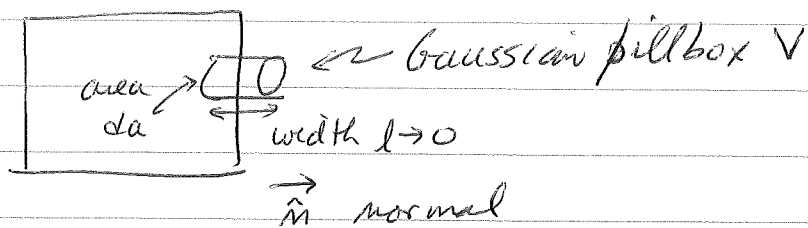
For insulators one generally has $\rho_n = 0$
 molecules are neutral.

In this case the macroscopic ρ is just the
 free charge $\rho = \langle \rho_{\text{free}} \rangle$.

And the bound charge is just

$$\langle \rho_{\text{bound}} \rangle = -\nabla \cdot \vec{P}$$

At a surface of a dielectric



$$-\int_V d^3r \nabla \cdot \vec{P} = -\int_S da \hat{n} \cdot \vec{P}$$

contrib from sides $\rightarrow 0$ as $l \rightarrow 0$

contrib from outside surface = 0
 as $P=0$ outside

$$= \hat{n} \cdot \vec{P} da$$

only contrib is from inside surface

$$= \int_V d^3r \rho_{\text{bound}}$$

(\hat{n} is outward normal)

as $l \rightarrow 0$, $\int_V d^3r \rho_{\text{bound}} \rightarrow \int da \sigma_{\text{bound}} = da \sigma_{\text{bound}}$ surface charge

$$\Rightarrow \boxed{\sigma_{\text{bound}} = \hat{n} \cdot \vec{P}} \text{ at surface of dielectric}$$

to