Dielectrics + Magnetic Materials - Macroscopic Maxwell Equ

Dielectrics

Maxwell's equations apply <u>exactly</u> to the true microscopic electric and magnetic fields that arise from <u>all</u> charges and currents.

$$\vec{\nabla} \cdot \vec{b} = 0 \qquad \vec{\nabla} \times \vec{e} + \frac{1}{c} \frac{\partial \vec{b}}{\partial t} = 0$$

$$\vec{\nabla} \cdot \vec{e} = 4\pi \rho_0 \qquad \vec{\nabla} \times \vec{b} = \frac{4\pi}{c} \vec{j}_0 + \frac{\partial \vec{e}}{\partial t}$$

where $\vec{e}$ and $\vec{b}$ are <u>microscopic</u> fields from <u>total</u> charge density ρ_0 and current density $\vec{j}_0$.

However, in most problems involving macroscopic objects, if we took ρ_0 and $\vec{j}_0$ to describe charge + current of each individual atom in a material, then they, and the resulting $\vec{e}$ and $\vec{b}$ would be enormously complicated functions varying rapidly over distances $\sim 10^{-8}$ cm and times $\sim 10^{-16}$ sec.

In classical E+M we are generally concerned with phenomena that vary extremely slowly compared to these length + time scales,

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~~ ~~given~~ 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

valence

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 <u>vanishes</u>! One might therefore think that electrodynamics 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".

$E = 0$

$E > 0$
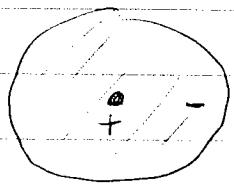
electron cloud centered on ionic ~~nucleus~~ core

dipole moment vanishes
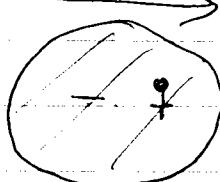
electron cloud and ionic core displaced $\vec{d} \propto \vec{E}$

atom is "polarized"

has dipole moment $\vec{p} = q\vec{d} \propto q\vec{E}$

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

atomic polarizability

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

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

$\vec{P} \rightarrow$ in terms of averaged charge
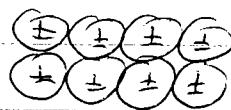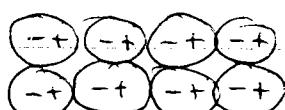
$\vec{E} = 0$ uniform $\vec{E} \rightarrow$

$E > 0$

$\boxtimes = (-)$
$\boxtimes = (+)$
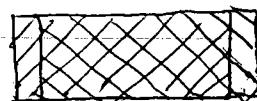
$(-)$ neutral $(+)$
surface charge builds
up

For a non uniform $\vec{E}$, atoms are more strongly polarized where E is largest
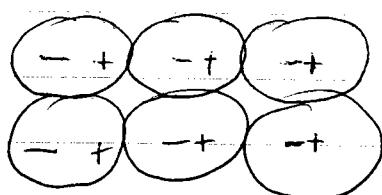
E strong   E weak $(-)$ $|\rho_+| > |\rho_-|$ $(+)$
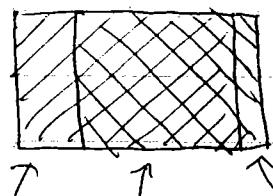
$\vec{E} \rightarrow$ net positive charge
region

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 $\vec{r}$
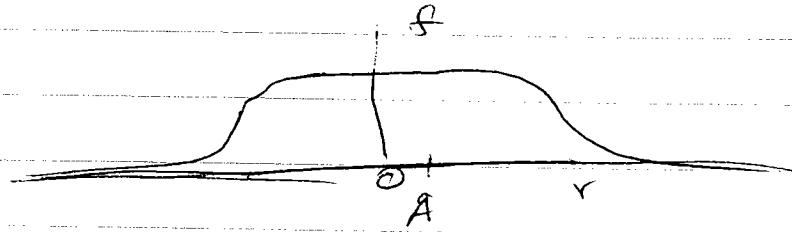
want $f \approx 1$ for $r < R$
$f \approx 0$ for $r \gg R$
where R is length scale
in between micro + macro

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

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

Define the macroscopic fields

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

Then $\quad \vec{\nabla} \cdot \vec{b} = 0 \quad \Rightarrow \quad \langle \vec{\nabla} \cdot \vec{b} \rangle = 0$

$$\Rightarrow \quad \vec{\nabla} \cdot \langle \vec{b} \rangle = 0$$

$$\Rightarrow \quad \vec{\nabla} \cdot \vec{B} = 0$$

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

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

Remaining Maxwell eqn, upon averaging, become

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

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

Consider $\langle \rho_c \rangle$

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

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

$$\rho_{free} = \sum_{i \, free} q_i \, \delta(\vec{r} - \vec{r}_i(t)) \qquad \text{sum over only free charges}$$

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

$\qquad\qquad\qquad\qquad \nwarrow$ charge distribution of molecule n

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

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

$$= \sum_{i \in n} q_i \int d^3r' \; f(\vec{r}') \, \delta(\vec{r} - \underbrace{\vec{r}' - \vec{r}_i(t)}_{})$$

$$= \sum_{i \in n} q_i \; f(\vec{r} - \vec{r}_i(t))$$

write $\quad \vec{r}_i(t) = \vec{r}_n(t) + \vec{r}_{n_i}(t)$

$$\underset{\substack{\text{position of} \\ \text{center of mass} \\ \text{of molecule } n}}{\nwarrow} \qquad \underset{\substack{\text{position of charge } i \\ \text{of molecule } n \\ \text{with respect to} \\ \text{center of mass}}}{\nearrow}$$

$$\langle \rho_n(\vec{r},t) \rangle = \sum_{i \in n} q_i \; f(\vec{r} - \vec{r}_n - \vec{r}_{n_i})$$

Since the $|\vec{r}_{n_i}|$ are all of atomic length scale, and f is slowly varying on this length scale, we can expand

$$\langle \rho_n(\vec{r},t) \rangle = \sum_{i \in n} q_i \left[f(\vec{r} - \vec{r}_n) - \left(\vec{\nabla} f(\vec{r}-\vec{r}_n) \right) \cdot \vec{r}_{n_i} \right.$$
$$\left. + \frac{1}{2} \sum_{\alpha\beta=1}^{3} \frac{\partial f(\vec{r}-\vec{r}_n)}{\partial r_\alpha \, \partial r_\beta} (\vec{r}_{n_i})_\alpha (\vec{r}_{n_i})_\beta + \cdots \right]$$

$$= f(\vec{r}-\vec{r}_n) \left[\sum_{i \in n} q_i \right]$$

$$- \left(\vec{\nabla} f(\vec{r}-\vec{r}_n) \right) \cdot \sum_{i \in n} q_i \vec{r}_{n_i}$$

$$+ \sum_{\alpha,\beta=1}^{3} \left(\frac{1}{6} \frac{\partial f(\vec{r}-\vec{r}_n)}{\partial r_\alpha \, \partial r_\beta} \right) \; 3 \sum_{i \in n} q_i (r_{n_i})_\alpha (r_{n_i})_\beta$$

Define $\quad g_n = \sum\limits_{i \in n} g_i \qquad$ total charge molecule n

$$\vec{p}_n = \sum\limits_{i \in n} g_i \vec{r}_{ni} \qquad \text{dipole moment about}$$
center of mass of molec n

$$\overleftrightarrow{Q}'_n \equiv \sum\limits_{i \in n} 3 g_i \vec{r}_{ni} \vec{r}_{ni} \qquad \text{quadrapole moment}$$
about center of mass
of molec n

(prime on $\overleftrightarrow{Q}'$ since definition
here is a little different
from that of multipole exp)

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

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

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

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

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

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

Now

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

$$= \langle \sum\limits_n g_n \, \delta(\vec{r}-\vec{r}_n) \rangle - \vec{\nabla} \cdot \langle \sum\limits_n \vec{p}_n \, \delta(\vec{r}-\vec{r}_n) \rangle$$

$$+ \frac{1}{6} \sum\limits_{\alpha\beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \langle \sum\limits_n (Q_n)'_{\alpha\beta} \, \delta(\vec{r}-\vec{r}_n) \rangle$$

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

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

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

~~Denote~~

Define the macroscopic charge density

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

then

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

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

Define <u>electric displacement vector</u>

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

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

In most materials, the quadrapole and higher terms are negligible and we can take
$$\vec{D} = \vec{E} + 4\pi \vec{P}$$

<u>Why quadrapole + higher order terms</u> ~~can~~
<u>can generally be ignored</u>:

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

$\Rightarrow$ polarization $\mathbb{P} \sim \dfrac{a_0}{l^3}$

$\vec{\nabla} \cdot \vec{\mathbb{P}} \sim \left(\dfrac{a_0}{L}\right) \dfrac{1}{l^3}$ since $\mathbb{P}$ cannot vary
on length scale shorter
than the averaging length
L

quadrapole moment

$Q \sim a_0^2$

quadrapole density $\mathbb{Q} \sim \dfrac{a_0^2}{l^3}$

$\dfrac{\partial^2}{\partial r_\alpha \partial r_\beta} \mathbb{Q} \sim \left(\dfrac{a_0}{L}\right)^2 \dfrac{1}{l^3}$

each higher moment gives extra factor a_0
each higher derivative gives extra factor $\dfrac{1}{L}$

So quadrapole is smaller than dipole
term by factor $\left(\dfrac{a_0}{L}\right) \ll 1$. Higher
terms smaller ~~$\oint$~~ by additional factors
of $\left(\dfrac{a_0}{L}\right)$

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

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

And the bound charge is just

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

"At a surface of a dielectric

Gaussian pillbox V
area da
width $l \to 0$
$\vec{n}$ normal
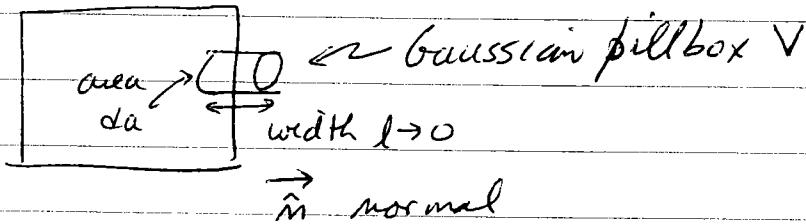
$$-\int_V d^3r \; \vec{\nabla} \cdot \vec{P} = -\oint_S da \; \hat{m} \cdot \vec{P} \qquad \text{contrib from sides} \to 0 \text{ as } l \to 0$$

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

$$= \hat{m} \cdot \vec{P} \, da \qquad \text{only contrib is from inside surface}$$

$$= \int_V d^3r \; \rho_{bound} \qquad (\hat{m} \text{ is } \underline{outward} \text{ normal}$$

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

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

the