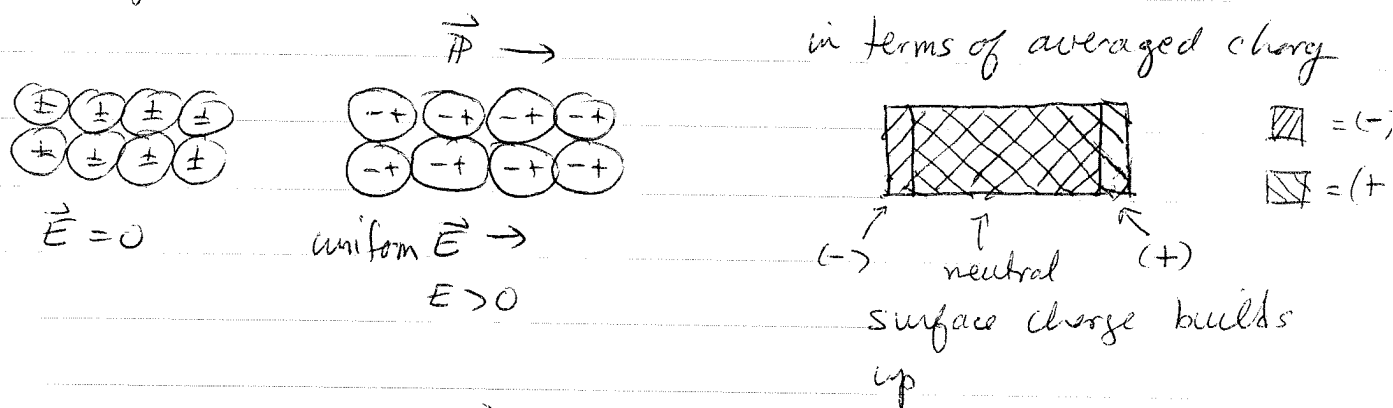


Polarization density $\vec{P}(\vec{r}) = \sum_i \vec{p}_i \delta(\vec{r} - \vec{r}_i)$

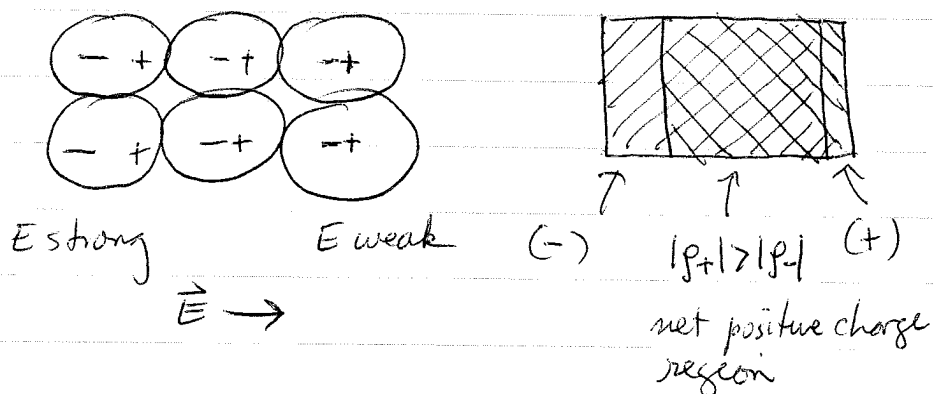
$\vec{p}_i$
dipole moment of atom i
at position $\vec{r}_i$

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)

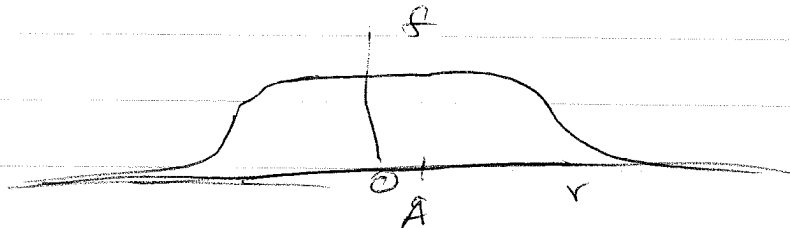
Define spatially averaged quantities by

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

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 $f \approx 1$ for $r < R$

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

where R is length scale
in between micro + macro

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

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

Define the macroscopic fields

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

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

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

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

$$\rightarrow \vec{\nabla} \cdot \vec{B} = 0$$

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

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

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

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

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

↑ charge distribution of molecule n

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

$$\begin{aligned}
 \langle \rho_n(\vec{r}, t) \rangle &= \int d^3r' f(\vec{r}') \rho_n(\vec{r} - \vec{r}', t) \\
 &= \sum_{i \in n} g_i \int d^3r' f(\vec{r}') \delta(\vec{r} - \vec{r}' - \vec{r}_i(t)) \\
 &= \sum_{i \in n} g_i f(\vec{r} - \vec{r}_i(t))
 \end{aligned}$$

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

$\uparrow$ position of center of ~~charge~~ ~~mass~~ mass of molecule n
 $\uparrow$ position of charge i of molecule n with respect to center of ~~mass~~ ~~charge~~ mass

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

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

$$\begin{aligned}
 \langle \rho_n(\vec{r}, t) \rangle &= \sum_{i \in n} g_i \left[f(\vec{r} - \vec{r}_n) - (\vec{\nabla} f(\vec{r} - \vec{r}_n)) \cdot \vec{r}_{ni} \right. \\
 &\quad \left. + \frac{1}{2} \sum_{\alpha, \beta=1}^3 \frac{\partial^2 f(\vec{r} - \vec{r}_n)}{\partial r_\alpha \partial r_\beta} (\vec{r}_{ni})_\alpha (\vec{r}_{ni})_\beta + \dots \right]
 \end{aligned}$$

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

$$- (\vec{\nabla} f(\vec{r} - \vec{r}_n)) \cdot \sum_{i \in n} g_i \vec{r}_{ni}$$

$$+ \sum_{\alpha, \beta=1}^3 \left(\frac{1}{6} \frac{\partial^2 f(\vec{r} - \vec{r}_n)}{\partial r_\alpha \partial r_\beta} \right) \sum_{i \in n} g_i (r_{ni})_\alpha (r_{ni})_\beta$$

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

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

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

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

$$\langle \rho_n(\vec{r}, t) \rangle = q_n f(\vec{r} - \vec{r}_n) - \vec{p}_n \cdot \vec{\nabla} f(\vec{r} - \vec{r}_n) + \frac{1}{6} \sum_{\alpha\beta} (Q'_n)_{\alpha\beta} \frac{\partial^2 f(\vec{r} - \vec{r}_n)}{\partial r_\alpha \partial r_\beta}$$

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

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

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

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

Now

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

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

$$+ \frac{1}{6} \sum \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \langle \dots \rangle$$

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

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

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

~~Define~~

Define the macroscopic charge density

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

Then

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

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

Define electric displacement vector

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

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 $\propto a_0$

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

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

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

quadrupole moment

$$Q \sim a_0^2$$

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

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

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 ~~by~~ by additional factors of $\left(\frac{a_0}{L}\right)$

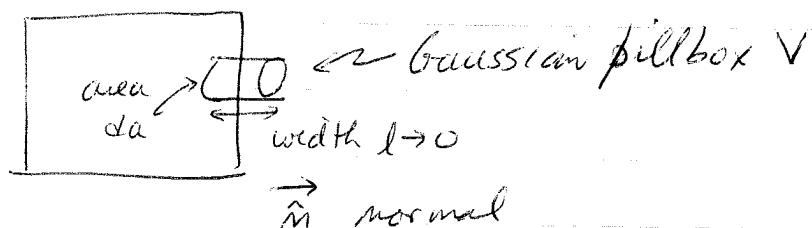
For insulators one generally has $q_n = 0$
molecules are neutral.

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

And the bound charge is just

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

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 $\vec{P} = 0$ 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)

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

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

QED