Rather than worry about the microscopic details of $\mathbf{j}$ and $\mathbf{E}$ as resulting from processes that are smoothly varying on a given averaged time scale, we want to describe phenomena in terms of averaged electric fields $\mathbf{E}$ and $\mathbf{j}$ that are smoothly varying at the atomic scale. This results in what are known as the macroscopic Maxwell equations.

**Dielectric Materials**

A dielectric material is an insulator. Electrons are bound to the ionic cores of the atoms. When no electric field is present, the averaged $\mathbf{j}$ in the dielectric vanishes. One might therefore think that electrodynamicism 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".

\[ E_0 \quad \quad \quad \quad \quad \quad \quad \quad E > 0 \]

- **Electron Cloud**
  - Centered on ionic core
  - Dipole moment vanishes
  - $+ \quad -$

- **Electron Cloud**
  - Centered on ionic core
  - Dipole moment $\mathbf{p}$ displaced $\mathbf{j} \times \mathbf{E}$
  - Atom is "polarized"
  - Has dipole moment $\mathbf{p} = q \mathbf{d} \times q \mathbf{E}$

A dielectric material can be solid, liquid, or gas, depending on the nature of the material.
Polarization density \( \vec{P}(\vec{r}) = \sum_i \vec{P}_i \cdot S(\vec{r} - \vec{r}_i) \)

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**

\[ \vec{P} \rightarrow \]

\[ \begin{array}{cc}
  \pm \pm \pm \pm \pm \\
  \pm \pm \pm \pm \pm \\
\end{array} \rightarrow \begin{array}{cc}
  \pm \pm \pm \pm \\
  \pm \pm \pm \pm \\
\end{array} \]

\[ \vec{E} = 0 \quad \text{uniform } \vec{E} \rightarrow \quad \vec{E} > 0 \]

\[ \quad \text{in terms of averaged charge} \]

\[ \hspace{1cm} \square = (-) \quad \square = (+) \]

\[ \text{neutral} \rightarrow \text{surface charge builds up} \]

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

\[ \begin{array}{cc}
  \pm \pm \pm \pm \\
  \pm \pm \pm \pm \\
\end{array} \rightarrow \begin{array}{cc}
  \pm \pm \pm \pm \\
  \pm \pm \pm \pm \\
\end{array} \]

\[ \vec{E} \rightarrow \]

\[ \text{E strong} \quad \text{E weak} \quad \square = (-) \quad |\rho_+| > |\rho_-| \quad (+) \quad \text{net positive charge region} \]

For uniform \( \vec{P} \), build up surface charge \( \rho_b \)

For non-uniform \( \vec{P} \), also can build up vol charge density \( \rho_b \)
We now carry out the averaging explicitly to see how such polarization enters the macroscopic Maxwell equations \( (\text{Jackson 6.6}) \).

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 \( \vec{r} \).

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

\[
\frac{\partial}{\partial t} \langle F(\vec{r}, t) \rangle = \langle \frac{\partial F}{\partial t} \rangle
\]

Define the macroscopic fields

\[
\vec{E}(\vec{r}, t) = \langle \vec{e}(\vec{r}, t) \rangle
\]

\[
\vec{B}(\vec{r}, t) = \langle \vec{b}(\vec{r}, t) \rangle
\]
\[ \nabla \cdot \vec{b} = 0 \quad \Rightarrow \quad \nabla \times \vec{b} = 0 \]

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

\[ \Rightarrow \quad \nabla \cdot \vec{B} = 0 \]

\[ \nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 \quad \Rightarrow \quad \nabla \times \langle \vec{E} \rangle + \frac{\partial \langle \vec{B} \rangle}{\partial t} = 0 \]

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

Remaining Maxwell eqn. upon averaging, become

\[ \nabla \cdot \vec{E} = 4\pi \langle \rho \rangle \]

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

Consider \( \langle \rho \rangle \)

\[ \rho = \sum_i \delta (\vec{r} - \vec{r}_i (t)) \quad \text{sum over all charges} \]

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

\[ \rho_{\text{free}} = \sum_{i, \text{free}} \delta (\vec{r} - \vec{r}_i (t)) \quad \text{sum only free charges} \]

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

\[ \rho_n (\vec{r}, t) = \sum_{i, \text{molecule } n} \delta (\vec{r} - \vec{r}_i (t)) \quad \text{sum over charges in molecule } n \]
\[ \langle \rho_n(\vec{r},t) \rangle = \int d^3\vec{r}' \, f(\vec{r}') \rho_n(\vec{r}-\vec{r}',t) \]

\[ = \sum_{\text{cen}} \delta_i \int d^3\vec{r}' \, f(\vec{r}') \delta(\vec{r}-\vec{r}'-\vec{r}_i(t)) \]

\[ = \sum_{\text{cen}} \delta_i \, f(\vec{r}-\vec{r}_i(t)) \]

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

\[ \vec{r}_n(t) \text{ position of center of mass of molecule n} \]
\[ \vec{r}_i(t) \text{ position of charge i with respect to center of mass of molecule n} \]

\[ \langle \rho_n(\vec{r},t) \rangle = \sum_{\text{cen}} \delta_i \, f(\vec{r}-\vec{r}_n-\vec{r}_{ni}) \]

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

\[ \langle \rho_n(\vec{r},t) \rangle = \sum_{\text{cen}} \delta_i \left[ f(\vec{r}-\vec{r}_n) - \left( \nabla f(\vec{r}-\vec{r}_n) \right) \cdot \vec{r}_{ni} \right. \]

\[ + \frac{1}{2} \sum_{\alpha \beta = 1}^{3} \frac{\partial f(\vec{r}-\vec{r}_n)}{\partial r_\alpha \partial r_\beta} (\vec{r}_{ni})_\alpha (\vec{r}_{ni})_\beta + \ldots \]

\[ \delta_i = 1, 2, 3 \text{ or } x, y, z \]

\[ = \frac{1}{2} \sum_{\text{cen}} \delta_i \left[ f(\vec{r}-\vec{r}_n) - \left( \nabla f(\vec{r}-\vec{r}_n) \right) \cdot \vec{r}_{ni} \right. \]

\[ - \left( \nabla f(\vec{r}-\vec{r}_n) \right) \cdot \sum_{\text{cen}} \delta_i \, \vec{r}_{ni} \]

\[ + \sum_{\alpha \beta = 1}^{3} \left( \frac{1}{6} \frac{\partial f(\vec{r}-\vec{r}_n)}{\partial r_\alpha \partial r_\beta} \right) (\vec{r}_{ni})_\alpha (\vec{r}_{ni})_\beta \sum_{\text{cen}} \delta_i \]

\[ \delta_i = 1, 2, 3 \text{ or } x, y, z \]
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 molecule \( n \)

\( \vec{Q}_n = \sum_{i \in n} 3 q_i \vec{r}_{ni} \vec{r}_{ni} \) quadrupole moment about center of mass of molecule \( n \)

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

\( \vec{Q} \) is not traceless

\[
\langle \vec{f}_n (\vec{r}, t) \rangle = q_n \vec{f}(\vec{r} - \vec{r}_n) - \vec{p}_n \cdot \vec{\nabla} \vec{f}(\vec{r} - \vec{r}_n) \\
+ \frac{1}{6} \sum_{\alpha \beta} \langle \vec{Q}_n \rangle_{\alpha \beta} \frac{\partial^2 \vec{f}(\vec{r} - \vec{r}_n)}{\partial r_\alpha \partial r_\beta}
\]

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

\[
\Rightarrow \langle \vec{f}_n (\vec{r}, t) \rangle = \langle q_n \delta(\vec{r} - \vec{r}_n) \rangle \\
- \vec{\nabla} \cdot \langle \vec{p}_n \delta(\vec{r} - \vec{r}_n) \rangle \quad \vec{\nabla} \cdot \delta = \vec{0}, \forall \delta
\]

\[
+ \frac{1}{6} \sum_{\alpha \beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \langle \vec{Q}_n \rangle_{\alpha \beta} \delta(\vec{r} - \vec{r}_n) 
\]

Now

\[
\langle \vec{f}_{\text{bound}} (\vec{r}, t) \rangle = \sum_n \langle \vec{f}_n (\vec{r}, t) \rangle \\
= \langle \sum_n q_n \delta(\vec{r} - \vec{r}_n) \rangle - \vec{\nabla} \cdot \langle \sum_n \vec{p}_n \delta(\vec{r} - \vec{r}_n) \rangle \\
+ \frac{1}{6} \sum_{\alpha \beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} \langle \sum_n \langle \vec{Q}_n \rangle_{\alpha \beta} \delta(\vec{r} - \vec{r}_n) \rangle
\]
Define \( \vec{P}(r,t) = \left\langle \sum_n \overline{p}_n \delta(r - \overline{r}_n) \right\rangle \) \text{ average polarization density} \[
\begin{align*}
\vec{Q}(r,t) = \frac{1}{6} \left\langle \sum_n \overline{Q}_n \delta(r - \overline{r}_n) \right\rangle \quad \text{average quadrupole density}
\end{align*}
\]

\[
\left\langle \vec{P}_{\text{bound}} \right\rangle = \sum_n \left\langle g_n \delta(r - \overline{r}_n) \right\rangle = \vec{V} \cdot \vec{P} + \sum_{\alpha \beta \sigma \alpha \sigma} \frac{e^2}{r_{\alpha \beta} \epsilon_{\alpha \beta}} \vec{Q}_{\alpha \beta}
\]

Define the macroscopic charge density \( \rho = \left\langle \sum_{i \text{ free}} g_i \delta(r - \overline{r}_i) \right\rangle + \left\langle \sum_{m \text{ molecule}} g_n \delta(r - \overline{r}_n) \right\rangle \)

Then \[
\nabla \cdot \vec{E} = \left\langle \rho_0 \right\rangle = 4\pi \left[ \rho - \vec{V} \cdot \vec{P} + \sum_{\alpha \beta \sigma \alpha \sigma} \frac{e^2}{r_{\alpha \beta} \epsilon_{\alpha \beta}} \vec{Q}_{\alpha \beta} \right]
\]

\[
\sum_{\alpha} \frac{2}{\sigma_{\alpha}} \left[ E_{\alpha} + 4\pi P_{\alpha} - \frac{4\pi \sum_{\beta} \frac{1}{\epsilon_{\beta}} \epsilon_{\alpha \beta} \vec{Q}_{\alpha \beta}} \right] = 4\pi \rho
\]

Define electric displacement vector \( \vec{D} = \vec{E} + 4\pi \vec{P} \)

Then \( \vec{V} \cdot \vec{D} = 4\pi \rho \)

In most materials, the quadrupole and higher items are negligible and we can take \( \vec{D} = \vec{E} + 4\pi \vec{P} \)
Why quadrupole and 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 \( d \) be the typical spacing between molecules.
Let \( L \) be the length scale of the spatial averaging function \( f(R) \), \( L \gg a_0 \)

dipole moment \( p = a_0 \)
\[ \Rightarrow \text{polarization density} \quad \mathbf{P} = \frac{a_0}{L^3} \]

\[ \nabla \cdot \mathbf{P} \sim \left( \frac{a_0}{L} \right)^2 \frac{1}{L^3} \quad \text{since } \mathbf{P} \text{ cannot vary on length scale shorter than the averaging length} \]

quadrupole moment
\[ Q = a_0^2 \]
quadrupole density \( \mathbf{Q} = \frac{a_0^2}{L^3} \)
\[ \frac{\nabla^2 \mathbf{Q}}{\nabla \mathbf{Q}} \sim \left( \frac{a_0}{L} \right)^2 \frac{1}{L^3} \]

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 additional factors of \( \left( \frac{a_0}{L} \right) \).
For insulators one generally has $q_n = 0$.

In this case the macroscopic $f$ is just the free charge $f = \langle f_{\text{free}} \rangle$.
And the bound charge is just:

$$\langle f_{\text{bound}} \rangle = -\nabla \cdot \mathbf{P}$$

At a surface of a dielectric:

$$\begin{aligned}
\text{area} \rightarrow 0 & \quad \Rightarrow \text{Gaussian pillbox } V \\
\text{width } l \rightarrow 0 & \quad \Rightarrow \hat{n} \text{ normal}
\end{aligned}$$

$$- \int_V \nabla \cdot \mathbf{P} \, dV = - \int_S \hat{n} \cdot \mathbf{P} \, dS$$

- contrib from sides $\to 0$ as $l \to 0$
- contrib from outside surface $= 0$ as $P \to 0$ outside

$$= \hat{n} \cdot \mathbf{P} \, da$$

- only contrib i from inside surface
- $\hat{n}$ is outward normal

$$= \int_V \nabla \cdot \mathbf{P} \, dV \rightarrow \int_S \hat{n} \cdot \mathbf{P} \, dS = \mathbf{d} \cdot \hat{\mathbf{n}} \text{ bound surface charge}$$

$$\Rightarrow \mathbf{P}_{\text{bound}} = \hat{n} \cdot \mathbf{P} \text{ at surface of dielectric}$$