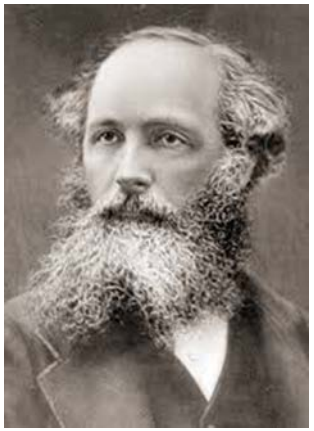
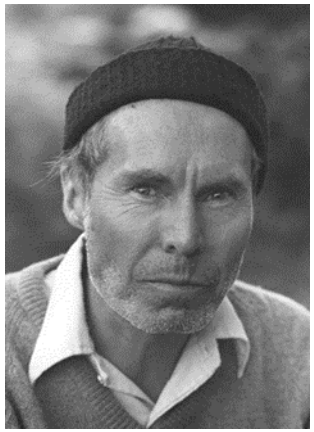
Chapter 2
VECTOR AND TENSOR ANALYSES



James Clerk Maxwell
(1831-1879)
Physics/Math
Maxwell's Equations
"EM Wave = Light"

Lecture 5

E2.2 Microscopic Maxwell's Equations
E2.3 Macroscopic Maxwell's Equations



John David Jackson
(1925-2016)
Physics (UIUC, UC Berkeley)
EM Text
"Classical Electrodynamics"

E2-2 Microscopic Maxwell's Equation

On a scale larger than 10^{-4} Å, nuclei and electrons can be approximated as point charges, and the microscopic sources are **discrete point-like moving charges in vacuum** given by

$$\zeta(\mathbf{r},t) = \sum_i q_i \delta\left[\mathbf{r} - \mathbf{r}_i(t)\right] \qquad \text{Microscopic Charge Density}$$

$$\mathbf{j}(\mathbf{r},t) = \sum_i q_i \mathbf{v}_i(t) \delta\left[\mathbf{r} - \mathbf{r}_i(t)\right] \qquad \text{Microscopic Current Density} \qquad \text{(E2.1)}$$

In the ordinary electromagnetic theory, although not essential, it is assumed that the total charge is conserved,

$$\frac{d\zeta(\mathbf{r},t)}{dt} = 0 \qquad \text{Microscopic Charge Conservation} \qquad \text{(E2.2)}$$

from which we can show

$$\frac{\partial \zeta(\mathbf{r},t)}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{r},t) = 0 \qquad \text{Microscopic Current Continuity} \qquad \text{(E2.3)}$$

[Q] What about the current continuity for electrons and holes in semiconductors?

In a nonrelativistic regime ($|\mathbf{v}_i| \ll c$), the dynamics of charged particles are described by the Newton-Lorentz (or simply Lorentz) force equation,

$$m_i \frac{d^2\mathbf{r}_i(t)}{dt^2} = q_i \left\{\mathbf{e}[\mathbf{r}_i(t),t] + \mathbf{v}_i(t) \times \mathbf{b}[\mathbf{r}_i(t),t]\right\} \quad \text{Microscopic Lorentz Force} \quad \text{(E2.4)}$$

where $\mathbf{e}$ and $\mathbf{h}$ are the **microscopic electric and magnetic fields**, respectively.

Therefore, the microscopic electromagnetic phenomena, *i.e.*, the interaction between microscopic field and sources (atomic and molecular charges) is governed by the microscopic Maxwell's equations* :

$$\nabla \times \mathbf{e}(\mathbf{r},t) = -\frac{\partial \mathbf{b}(\mathbf{r},t)}{\partial t}$$

$$\nabla \times \mathbf{b}(\mathbf{r},t) = \mu_0 \varepsilon_0 \frac{\partial \mathbf{e}(\mathbf{r},t)}{\partial t} + \mu_0 \mathbf{j}(\mathbf{r},t)$$

$$\nabla \cdot \mathbf{e}(\mathbf{r},t) = \frac{1}{\varepsilon_0}\zeta(\mathbf{r},t)$$

$$\nabla \cdot \mathbf{b}(\mathbf{r},t) = 0$$

Microscopic Maxwell's Equation (E2.5)

*The microscopic Maxwell's equations are important for molecular dynamics in physics and chemistry.

In contrast to the fields in macroscopic Maxwell's equations, **e** and **h** are the only fields defined in the macroscopic Maxwell's equations.

In real materials, the atoms or molecules are spatially arranged in a certain manner, often with some defects and irregularities, and we need to consider the **free (conduction) and bound charges**, separately. The free charges can move around the lattice, while the bound charges are **immobile**, localized to the constituent atoms or molecules. Thus we can decompose the total charge and current densities into free and bound components:

$$\zeta(\mathbf{r},t) = \zeta_f(\mathbf{r},t) + \zeta_b(\mathbf{r},t)$$
$$\mathbf{j}(\mathbf{r},t) = \mathbf{j}_f(\mathbf{r},t) + \mathbf{j}_b(\mathbf{r},t) \quad \text{(E2.6)}$$

where the subscripts *f* and *b* stand for "free" and "bound," respectively,

The free and bound charges are then given by

$$\zeta_f(\mathbf{r},t) = \sum_{i(\,free)} q_i \delta[\mathbf{r} - \mathbf{r}_i(t)]$$
$$\zeta_b(\mathbf{r},t) = \sum_{n(mol)} \zeta_n(\mathbf{r},t) \quad \text{(E2.7)}$$

where the bound sources (see FIG-E2.1) are then given by

$$\zeta_n(\mathbf{r},t) = \sum_{\alpha(n)} q_{\alpha(n)} \delta[\mathbf{r} - \mathbf{r}_n(t) - \mathbf{r}_{\alpha(n)}(t)] \quad \text{(E2.8)}$$

Similarly, for free and bound current densities, we have

$$\mathbf{j}_f(\mathbf{r},t) = \sum_{i(\,free)} q_i \mathbf{v}_i \delta[\mathbf{r} - \mathbf{r}_i(t)]$$
$$\mathbf{j}_b(\mathbf{r},t) = \sum_{n(mol)} \mathbf{j}_n(\mathbf{r},t) \qquad \text{(E2.9)}$$

The bound current density of the n-th molecule are then given by

$$\mathbf{j}_n(\mathbf{r},t) = \sum_{\alpha(n)} q_{\alpha(n)}(\mathbf{v}_n + \mathbf{v}_{\alpha(n)})\delta[\mathbf{r} - \mathbf{r}_n(t) - \mathbf{r}_{\alpha(n)}(t)] \qquad \text{(E2.10)}$$

where we use local coordinates for molecule as shown in FIG-E2.1:

$\mathbf{r}_n(t), \mathbf{v}_n(t)$: position, velocity of the n-th molecule

$q_{\alpha(n)}, \mathbf{r}_{\alpha(n)}(t), \mathbf{v}_{\alpha(n)}(t)$: charge, position, velocity of the α-th charge within the n-th molecule (local coordinate)

Note that the local (inside the molecule) and laboratory (observation) coordinates have very different scales:

$$\left|\mathbf{r}_{\alpha(n)}\right| << \left|\mathbf{r}_n\right| << \left|\mathbf{r}\right| \qquad \text{(E2.11)}$$

[Q] What about the current continuity for electrons and holes in semiconductors?

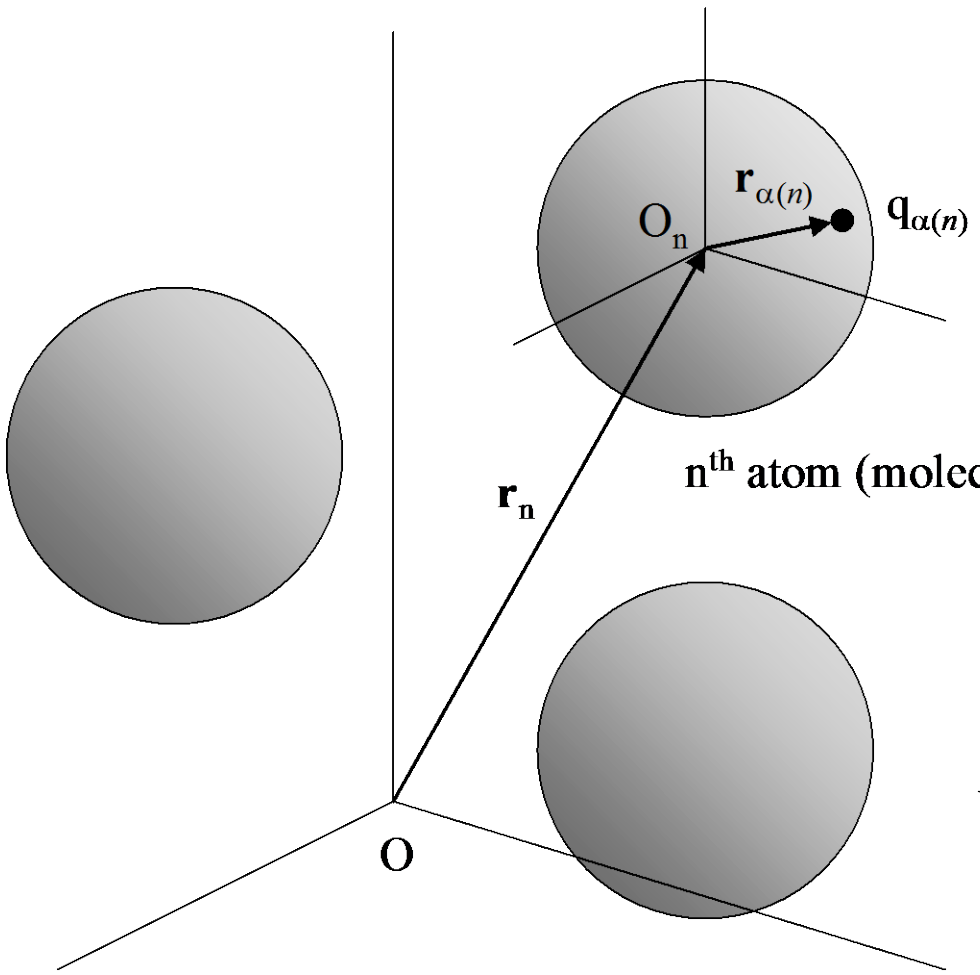


FIG-E2.1 Coordinates for bound charges in a molecular system

E2-2 Macroscopic Maxwell's Equation: Simple Spatial Average

The number of electrons and nuclei in a macroscopic amount of a material are of the order of 10^{23}. Even in the absence of external fields, there will exist **microscopic fields** due to the **thermal agitation**, **orbital motion**, and even **zero-point vibration** of the charged particles.

These microscopic fields usually vary extremely rapidly in both space and time. The spatial variation occurs in a distance shorter than 0.01 Å, and the period of the temporal fluctuation is in the range of 0.01 fs ~ 0.1 ps.

Consequently, for any macroscopic measurement in the real world, where the spatial averaging process inevitably occurs. This means that we need more **practical governing equations** than the microscopic Maxwell's equations.

Spatial Average

The spatial average of a function $f(\mathbf{r},t)$ by a macroscopic measurement can be described by using a sampling function $F_s(\mathbf{r},t)$

$$\langle f(\mathbf{r},t)\rangle = \int d^3\mathbf{r}' f(\mathbf{r},t) F_s(\mathbf{r}-\mathbf{r}') \qquad \text{(E2.12)}$$

[Q] How about $\langle f(\mathbf{r},t)\rangle = \int d^3\mathbf{r}' f(\mathbf{r},t) F_s(\mathbf{r}-\mathbf{r}')$?

The properties of $F_s(\mathbf{r},t)$ do not need to be specified in all the detail, except that it is just a "well behaved" function that is localized to a molecular dimension, with a normalization condition:

$$\int d^3\mathbf{r}'\, F_s(\mathbf{r}') = 1 \tag{E2.13}$$

After averaging (E2.5), we have the macroscopic Maxwell's equations:

$$\begin{aligned}
\nabla \times \mathbf{E}(\mathbf{r},t) &= -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t} \\
\nabla \times \mathbf{B}(\mathbf{r},t) &= \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} + \mu_0 \mathbf{J}(\mathbf{r},t) \\
\nabla \cdot \mathbf{E}(\mathbf{r},t) &= \frac{1}{\varepsilon_0}\rho(\mathbf{r},t) \\
\nabla \cdot \mathbf{B}(\mathbf{r},t) &= 0
\end{aligned} \tag{E2.14}$$

Here, we define the macroscopic fields and sources as

$$\begin{aligned}
\mathbf{E}(\mathbf{r},t) &= \langle \mathbf{e}(\mathbf{r},t) \rangle, \quad \mathbf{B}(\mathbf{r},t) = \langle \mathbf{b}(\mathbf{r},t) \rangle \\
\rho(\mathbf{r},t) &= \langle \zeta(\mathbf{r},t) \rangle, \quad \mathbf{J}(\mathbf{r},t) = \langle \mathbf{j}(\mathbf{r},t) \rangle
\end{aligned} \tag{E2.15}$$

Note that we still have only the macroscopic fields, $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$.