22.51 Problem Set 6 (due Nov. 2)

1 Spatially Averaged Maxwell Equations

Question:

a. Denote convolution,

$$\int_{-\infty}^{\infty} b(x')g(x-x')dx', \quad x, x' \in \mathbf{R},$$

as $b(x) * g(x)$. Prove that if $a(x) \equiv b(x) * g(x)$, then $[db(x)/dx] * g(x) = da(x)/dx$. In other words, differentiation commutes with convolution.

b. The Intel Pentium 4 chip is based on $.18\mu$m CMOS technology, which means that the smallest feature on the chip is $.18\mu$m. Therefore, a description of the EM field down to $.01\mu$m spatial resolution should be sufficient for chip design purposes. However, even in a tiny $.01\mu\text{m} \times .01\mu\text{m} \times .01\mu\text{m}$ Si crystallite, there are $\sim 10^6$ atoms, and even more electrons. If we account for all of them *explicitly* as charge and current sources in the Maxwell equations, the problem becomes intractable. Therefore, Maxwell equations must undergo spatial averaging before it can be used for such problems.

Spatial averaging of $a(\mathbf{x})$ is generally done by defining a smoother field $\overline{a}(\mathbf{x})$ as,

$$\overline{a}(\mathbf{x}) \equiv \int d^3\mathbf{x}' a(\mathbf{x}')g(\mathbf{x}-\mathbf{x}'), \quad \int d^3\mathbf{x} g(\mathbf{x}) = 1,$$

where $g(\mathbf{x})$ is a smearing function chosen to have the lengthscale of the necessary spatial resolution. For example, in the above case we may choose,

$$g(\mathbf{x}) = \frac{1}{(2\pi L^2)^{3/2}} \exp\left(-\frac{|\mathbf{x}|^2}{2L^2}\right),$$

with $L \sim .01\mu$m. $\overline{\mathbf{E}}(\mathbf{x})$, for example, is then $\mathbf{E}(\mathbf{x}')$ averaged around $\mathbf{x}$ over a size $\sim (.01\mu\text{m})^3$ region, which is what we want.

Prove that the form of Maxwell equations remain invariant *after averaging*. That is,

$$\nabla \cdot \overline{\mathbf{B}} = 0, \quad \nabla \times \overline{\mathbf{E}} = -\frac{1}{c}\frac{\partial \overline{\mathbf{B}}}{\partial t},$$

$$\nabla \cdot \overline{\mathbf{E}} = 4\pi\overline{\rho}, \quad \nabla \times \overline{\mathbf{B}} = \frac{4\pi}{c}\bar{\mathbf{j}} + \frac{1}{c}\frac{\partial \overline{\mathbf{E}}}{\partial t}.$$

So as far as the macroscopically averaged EM fields are concerned, material effects come in only via the macroscopically averaged $\overline{\rho}$ and $\bar{\mathbf{j}}$. We have eliminated a lot of degrees of freedom by this procedure!

2 Bound Charge Density

Question: There is no inherent difference between "free" and "bound" electrons; "free" and "bound" are descriptions of its relation to the molecule. While "bound" electrons cannot be displaced by more than $\sim 1\text{Å}$ from the molecule, thereby maintaining its total charge neutrality, free electrons can migrate by macroscopic length L (see Problem 1).

Let us label molecules by n. Within each molecule, there are multiple charges $\{q_n^i\}$, with,

$$\sum_i q_n^i \;=\; 0, \quad \forall n,$$

and whose positions are $\{\mathbf{x}_n^i\}$. Each molecule also has a center of mass $\mathbf{x}_n$. Let us define,

$$\Delta\mathbf{x}_n^i \;=\; \mathbf{x}_n^i - \mathbf{x}_n.$$

$\Delta\mathbf{x}_n^i$ is clearly microscopic, $|\Delta\mathbf{x}_n^i| \ll L$. Let us define dipole moment $\mathbf{p}_n$ for the molecule and dipole moment density $\mathbf{p}(\mathbf{x})$ for the medium as,

$$\mathbf{p}_n \;\equiv\; \sum_i q_n^i \Delta\mathbf{x}_n^i, \quad \mathbf{p}(\mathbf{x}) \;\equiv\; \sum_n \mathbf{p}_n \delta(\mathbf{x} - \mathbf{x}_n),$$

and quadruple moment $\mathbf{Q}_n$ and quadruple moment density $\mathbf{Q}(\mathbf{x})$ as,

$$(\mathbf{Q}_n)_{\alpha\beta} \;\equiv\; 3\sum_i q_n^i (\Delta\mathbf{x}_n^i)_\alpha (\Delta\mathbf{x}_n^i)_\beta, \quad \mathbf{Q}(\mathbf{x}) \;\equiv\; \sum_n \mathbf{Q}_n \delta(\mathbf{x} - \mathbf{x}_n).$$

The charge density contribution from all bound charges is,

$$\rho_{\text{bound}}(\mathbf{x}) \;\;\equiv\;\; \sum_n \sum_i q_n^i \delta(\mathbf{x} - \mathbf{x}_n^i).$$

As we see in Problem 1, $\rho_{\text{bound}}(\mathbf{x})$ is not as handy as $\overline{\rho}_{\text{bound}}(\mathbf{x})$. Prove that,

$$\overline{\rho}_{\text{bound}}(\mathbf{x}) \;\;=\;\; -\nabla\cdot\overline{\mathbf{p}}(\mathbf{x}) \;+\; \frac{1}{6}\sum_{\alpha,\beta} \frac{\partial^2 \overline{Q}_{\alpha\beta}(\mathbf{x})}{\partial x_\alpha \partial x_\beta} \;+\; \ldots$$

in the limit of $|\Delta \mathbf{x}_n^i| \ll L$ and explain why all terms except the first one should become negligible.