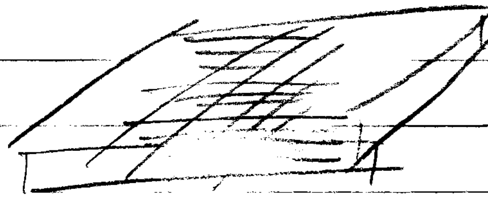
EE 692 GWMM
Whites.

Artificial Electromagnetic Materials. Local, Microscopic & Macroscopic Fields, Clausius-Mossotti / Lorenz-Lorentz Formula.

It is common to think of electromagnetic materials as naturally occurring: Materials that are homogeneous, isotropic, and formed from molecules. Examples are water, & minerals such as coal, mica, quartz, salt, etc.

But many materials are manmade and still have similar classifications in our minds as to what we commonly think is a "proper" EM material. Examples include Teflon, sheetrock (gypsum board), steel, etc.

However, many manmade materials we use in electromagnetics applications are really "composites." These are materials that are composed of two or more phases in a host material. A good example of this is Rogers RO4003C microwave substrate. It is a laminate - a fiber reinforced composite material.



Even though this is a composite, we treat it as a homogeneous material with <u>effective</u> material parameters.

Such material brings up very important questions and concepts central to applied electromagnetic materials

- The concept of an "effective" material - homogenization of the multiple phases to create an overall ϵ_r (& μ_r)

- Limits on the max. frequency (or bandwidth content in fast resitime waveforms) for which effective medium description is valid
- Anisotropy — Fibers oriented in plane of substrate, but not vertically.
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In more complicated instances of such materials, there may be magneto dielectric coupling at a microscopic level (relative to the particle sizes) leading to "chirality" or bianisotropy.

All of these topics will be discussed in the up coming lectures.

<u>Effective Medium Theories</u>

We will begin this discussion by considering the quasi-static (or simply static) response of a collection of dielectric scatterers. We will end up with a number of very famous "mixing theories" that are applicable in certain situations.

Our development here follows the work presented by D. E. Aspnes in his 1982 paper "Local-field effects and effective-medium theory: A microscopic perspective."

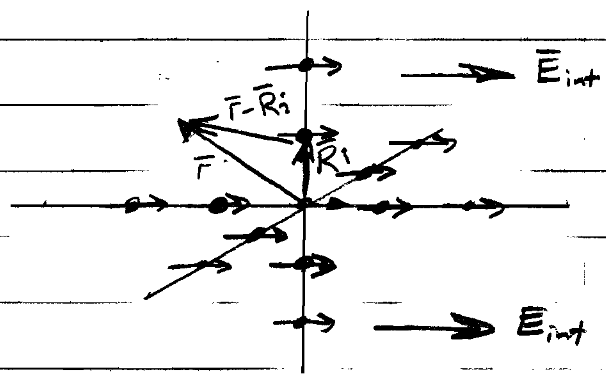
microscopic solution

We begin with a simple cubic (sc) lattice of polarizable point objects. This is an idealization of a real particle. We'll consider each pt. object as producing an electric dipole moment only according to

$$\bar{p} = \alpha \bar{E} \qquad (1)$$

$$C \cdot m \qquad \frac{V}{m}$$

where α is the polarizability.



This lattice of particles is illuminated by a uniform applied electric field $\bar{E}_{int}$. $\bar{E}_{int}$ will illuminate these particles and induce an electric dipole moment, according to (1), but not entirely directly. Every other particle in the lattice will also produce a secondary $\bar{E}$. It is this total $\bar{E}$ at each lattice site that induces the $\bar{p}$ in (1).

$$\bar{p}_i = \alpha \bar{E}(\bar{R}_i) \qquad (2)$$

our quest is to define then calculate an effective permittivity for this space.

At some arbitrary position in space $\bar{r}$ that is not at a lattice site the total electric field $\bar{E}(\bar{r})$ is the sum of the incident electric field & the scattered field. The latter is the sum of $\bar{E}$ from all the dipoles in the lattice.

$$\bar{E}(\bar{r}) = \underset{\substack{\uparrow \\ \text{applied}}}{\bar{E}_{int}} + \sum_i \underbrace{\bar{E}(\bar{p}_i, \bar{r}-\bar{R}_i)}_{E \text{ from dipoles.}} \qquad (3)$$

The electric field at any point produced by an electric dipole moment $\bar{p}$ is calculated in ~~coord.~~ free expression as

$$\bar{E}(\bar{p},\bar{r}) = \frac{3(\bar{p}\cdot\hat{a}_R)\hat{a}_R - \bar{p}}{r^3} \quad \text{(cgs units)} \qquad (4)$$

where $\hat{a}_R$ & r are defined relative to the location of $\bar{p}$. $\bar{E}(\bar{p},\bar{r})$ in (4) is used to calculate the terms in the second term in (3).

Now, at $\bar{r}=0$, we can compute the total $\bar{E}$ field illuminating the point dipole at the origin. This total field is called the <u>local field</u> and is an important concept to grasp in artificial materials work.

$$\bar{E}(0) \equiv \bar{E}_{loc} \qquad (5)$$

Using (3) in (5):

$$\bar{E}(0) = \bar{E}_{loc} = \bar{E}_{int} + \sum_i{}' \bar{E}(\bar{p}_i, -\bar{R}_i) \qquad (6)$$

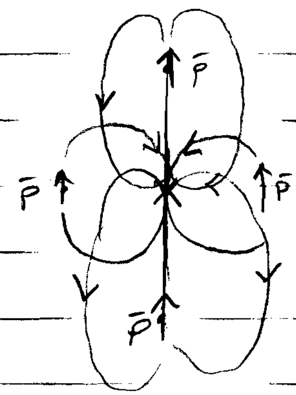
The prime indicates that we are excluding from this summation the electric field of the self particle from this summation. The particle doesn't polarize itself, in other words.

Noting that $\bar{p}_i = \alpha \bar{E}_{loc}$ (7)

in (6) is valid for every $\bar{p}_i$ in the lattice because of the symmetry of the lattice and the uniform nature of the applied E_{int}, then (4) becomes

$$\bar{E}(0) = \bar{E}_{loc} = \bar{E}_{int} + \sum_i{}' E(\alpha \bar{E}_{loc}, -\bar{R}_i) \qquad (8)$$

One important outcome of arranging the dipoles on a sc lattice is that the summation in (8) is actually **zero**! This can be shown by adding contributions to $\bar{E}$ using (4) in a layer-by-layer fashion.



The final outcome from (8) is that

$$\bar{E}_{loc} = \bar{E}_{int} \qquad (9)$$

i.e., The local field illuminating a pt. particle is simply the applied field.

Hence, the total $\bar{E}(\bar{r})$ at any position $\bar{r}$ (not at at lattice pt.) is from (3)

$$\bar{E}(\bar{r}) = \bar{E}_{int} + \sum_i \bar{E}(\alpha \bar{E}_{int}, \bar{r} - \bar{R}_i) \qquad (10)$$

This is "solved" in that we can compute $\bar{E}(\bar{r})$ everywhere in the space.

Now, our quest is to ascribe an effective permittivity to this lattice of point polarizable particles. Consider $\bar{p}(\bar{r})$ as a distributed function of space.

$$\bar{p}(\bar{r}) = \sum_i \alpha \bar{E}(\bar{R}_i)\, \delta(\bar{r} - \bar{R}_i) \qquad (11)$$

This fct. exists as a lattice of spatial delta fcts. at each lattice site.

As we've learned $\bar{E}(\bar{R}_i) = \bar{E}_{loc} \underset{(9)}{\overset{}{\underset{\uparrow}{=}}} \bar{E}_{int} \qquad (12)$

from (5), and the symmetry in the lattice and the uniform applied field E_{int}. Using (12) in (11) gives.

$$\bar{p}(\bar{r}) = \sum_i \alpha \bar{E}_{int}\, \delta(\bar{r} - \bar{R}_i) \qquad (13)$$

This also is a known quantity, provided the polarizability of the particles, α, is known.

Equations (10) & (13) constitute the solution to what we'll call the <u>microscopic problem</u>.

What is next needed is a <u>macroscopic</u> model for this space and a determination of an effective permittivity ϵ for the space.

Macroscopic Solution

For a macroscopic description of the dielectric properties of this space, we're interested in expressions relating

$$\bar{D} = \epsilon \bar{E} \qquad (\text{cgs: } \epsilon = \epsilon_r)$$
$$= \bar{E} + 4\pi \bar{P} \qquad (\text{cgs: } 4\pi \to \tfrac{1}{\epsilon_0} \text{ for mks}) \tag{14}$$

To obtain this macroscopic description, we will simply volume average $\bar{E}(\bar{r})$ and $\bar{p}(\bar{r})$, the microscopic fields. These volume averages will yield $\bar{E}$ & $\bar{P}$ as

$$\bar{E} = \frac{1}{V}\int_V \bar{E}(\bar{r})\,dv \quad ; \quad \bar{P} = \frac{1}{V}\int_V \bar{p}(\bar{r})\,dv \qquad (15),(16)$$

Starting with $\bar{P}$ we can use (13) in (16) giving

$$\bar{P} = \frac{1}{V}\int_V \left[\sum_i \alpha \bar{E}_{int}\,\delta(\bar{r}-R_i)\right] dv = \frac{1}{V_{u.c.}} \alpha \bar{E}_{int} \tag{17}$$

replace w/ volume average over 1 unit cell. Valid because of symmetry of lattice & uniform incident $\bar{E}_{int}$.

The so called number density n is the number of particles per unit volume. For one particle per unit cell, then

$$n = \frac{1}{V_{u.c.}} \tag{18}$$

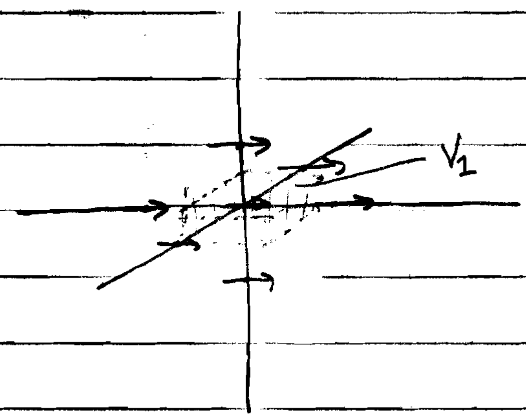
so that (17) becomes $\quad \bar{P} = n\alpha \bar{E}_{int} \qquad (19)$

For a volume average of the electric field, we can volume average over a single unit cell, say the one centered at the origin. The total $\bar{E}$ is the sum of the incident plus scattered fields as we determined in (10). The volume average of (10) gives

$$\bar{E} \equiv \frac{1}{V}\int_V \bar{E}(\bar{r})\,dv = \frac{1}{V}\int_V \bar{E}_{int}\,dv + \frac{1}{V}\int_V \left[\sum_i \bar{E}(\alpha\bar{E}_{int}, \bar{r}-\bar{R}_i)\right] dv \qquad (20)$$

just avg over cell 1.

$$\text{or} \quad \bar{E} = \bar{E}^{int} + \underbrace{\frac{1}{V_1}\int_{V_1} \bar{E}(\alpha\bar{E}_{int}, -\bar{R}_1)\,dv}_{\text{contribution from } \bar{p}_1} + \underbrace{\frac{1}{V_1}\int_{V_1}\left[\sum_{i=2}^{\infty} \bar{E}(\alpha\bar{E}_{int}, \bar{r}-\bar{R}_i)\right] dv}_{\text{contribution to } \bar{E} \text{ from all other dipoles } \bar{p}_i,\ i>1} \qquad (21)$$



We'll consider the second and third terms in the RHS of (21) separately.

- $\frac{1}{V_1}\int_{V_1} \bar{E}(\alpha\bar{E}_{int}, -\bar{R}_1)\,dv$. This is the volume average of the $\bar{E}$ produced by $\bar{p}_1$ in the u.c.

For a static $\bar{p}$, $\bar{E} = -\nabla\Phi_e$ & $\Phi_e = \frac{\bar{p}\cdot\hat{a}_R}{r^2}$ (cgs units)

$$\therefore \quad \bar{E} = -\nabla\Phi_e = -\nabla\left(\frac{\bar{p}\cdot\hat{a}_R}{r^2}\right) \qquad (22)$$

Then, $\int_{V_1} E(\alpha E_{int}, -\bar{R}_1)\, dv \underset{(22)}{=} -\int_{V_1} \nabla\left(\frac{\bar{p}_1 \cdot \hat{a}_R}{r^2}\right) dv$

$$\underset{\substack{\text{Gauss' Thm.} \\ \text{Van Bladel}}}{=} -\oint_{S_1} \frac{\bar{p}_1 \cdot \hat{a}_R}{r^2}\, d\bar{s} \underset{\substack{\text{Can show} \\ \text{For example Jackson} \\ \text{pp. 148-150 (spherical volume)}}}{=} -\frac{4\pi}{3}\bar{p} \qquad (23)$$

- $\frac{1}{V_1}\int_{V_1}\left[\sum_{i=2}^{\infty} \bar{E}(\alpha E_{int}, \bar{r}-\bar{R}_i)\right] dv$. This is the volume average throughout V_1 of the $\bar{E}$ produced by all the dipoles <u>outside</u> of V_1.

Does this integral evaluate to zero. I suspect so. From Jackson (4.19) on p. 149.

$$\int \bar{E}(x)\, d^3x = \frac{4\pi}{3} R^3 \bar{E}(0) \qquad (24)$$

if there is no charge inside a <u>sphere</u>, where $\bar{E}(0)$ is $\bar{E}$ at center of sphere. As we've shown for a s.c. lattice of dipoles, the net $\bar{E}$ at center of any u.c. = 0. But our u.c. is not spherical. I still suspect (24) is valid. Check numerically.

Collecting these results gives for (21) using (23)

$$\bar{E} = \bar{E}_{int} - \frac{1}{V_1}\frac{4\pi}{3}\bar{p} \underset{(13)}{=} \bar{E}_{int} - n\frac{4\pi}{3}\alpha E_{int} \qquad (25)$$

Finally, using the result from (19) for $\bar{P}$ gives

$$\bar{E} = \bar{E}_{int} - \frac{4\pi}{3}\bar{P} \qquad (26)$$

This result in (26) and also (19) are the final results of the macroscopic averaging of $\bar{E}$ & $\bar{P}$. From these we will derive a formula for the effective permittivity of the lattice of dipole scatterers.

Clausius-Mossotti or Lorenz-Lorentz Formula

Using this macroscopic solution for the volume averaged $\bar{E}$ & $\bar{P}$ for a SC lattice of dipole scatterers, we will derive a very famous formula for the effective permittivity of the space.

From (14) $\quad \bar{D} = \epsilon\bar{E} = \bar{E} + 4\pi\bar{P}$ (cgs units)
and using (19) gives

$$\epsilon\bar{E} = \bar{E} + 4\pi n\alpha \bar{E}_{int} \qquad (27)$$

While from (26)

$$\bar{E} = \bar{E}_{int} - \frac{4\pi}{3}\bar{P} \underset{(19)}{=} \bar{E}_{int} - \frac{4\pi}{3} n\alpha \bar{E}_{int} \qquad (28)$$

We'll solve for $\bar{E}_{int}$ in (28)

$$\bar{E} = \left(1 - \frac{4\pi}{3} n\alpha\right) \bar{E}_{int} \Rightarrow \bar{E}_{int} = \frac{\bar{E}}{1 - \frac{4\pi}{3} n\alpha} \qquad (29)$$

Substitute (29) for E_{int} in (27):

$$\epsilon \bar{E} - \bar{E} = 4\pi n\alpha \frac{\bar{E}}{1 - \frac{4\pi}{3} n\alpha}$$

$$\Rightarrow \quad \epsilon - 1 = \frac{4\pi n\alpha}{1 - \frac{4\pi}{3} n\alpha} \qquad (30)$$

With a little bit of algebra, this can be expressed as

$$\boxed{\frac{4\pi}{3} n\alpha = \frac{\epsilon - 1}{\epsilon + 2}} \quad \text{(cgs units)} \qquad (31)$$

This is the famous Clausius-Mossotti eqn, also called the Lorenz-Lorentz formula. From researchers in the middle to later 1800's. This formula allows the calculation of the effective permittivity of a lattice of dipole scatterers.

In MKS units ($4\pi \to \frac{1}{\epsilon_b}$ where ϵ_b is the background permittivity)

$$\boxed{\frac{n\alpha}{3\epsilon_b} = \frac{\epsilon_{r,eff} - 1}{\epsilon_{r,eff} + 2}} \quad \text{(MKS units)} \qquad (32)$$