The Dielectric Constant and the Displacement Vector

30th January 2007

Let us start with what we know: If we have a set of known charges, the field due to those charges is given by

$$\nabla\cdot\vec{E}=\frac{\rho}{\varepsilon_0} \tag{1}$$

Even if the charges are not known, this equation is true, except that we would need to work further to determine ρ. Equation 1 covers all of known Electrostatics. So why do we need anything more? The reason is that we have materials with very complicated (and unknowable) structure, and we need to have some predictable equations to handle fields in the presence of these materials.

- One example is that of conductors, i.e., metals. Here we found a way to augment Eq. 1 by adding both boundary conditions and by finding an alternative equation for field within a conductor:

  $$\begin{aligned}\nabla\cdot\vec{j} &= 0\\ \vec{j} &= \sigma\left(\vec{E}+\vec{v}\times\vec{B}\right)\\ \vec{E} &= -\nabla\phi\end{aligned}$$

  This system is much more complex to solve, and once you add physics to pin down $\vec{v}$, you have the dynamo problem, plasma physics, and other interesting areas. In these systems, charges and currents are explicitly taken into account through the fluid equations and the conductivity.

- The second type of material is the insulator. Here, there are no currents flowing. There is a regular, or irregular, lattice of atoms, that tightly hold their electrons. What is the effect of the Electric Field on these materials, and what is the effect of that effect back on the Electric Field?

Insulators could either be ionic or covalent materials, and could be solids, liquids or gases. Clearly, a single theory to cover every possibility is asking for a lot. Let us see what we can do.

No Applied Field Present

When an atom is in isolation, it has electrons in various quantum levels. Depending on its atomic number, these electrons combine to form “closed shells” or have some

How strong is the field inside an atom?
Consider the Hydrogen atom. The distance between nucleus and electron is about 5×10^{-11} metres. At that distance, the Electric field of the nucleus is

$$\begin{aligned} E_r &= \frac{1}{4\pi\varepsilon_0}\frac{e}{r^2} \\ &\simeq \frac{10^{10} \times 10^{-19}}{25 \times 10^{-22}} \\ &= 4 \times 10^{11} \text{ volts/metre} \end{aligned}$$

Table 1:

asymmetry. Thus, atoms could either be spherically symmetric or could have an instantaneous dipole or quadrupole moment.

As you might remember from the lectures, I argued that the Electric force is so strong compared to the magnetic force, that any imbalance would tear materials apart. Thus, spherical symmetry is a holy grail in chemistry. That is why elements take or give up electrons to achieve closed shell configurations. Even when molecules have dipoles, the dipoles have to arrange themselves so that they tend to cancel in the bulk material. Otherwise that state of matter could not exist.

> A good example is water. H_2O is a molecule where the oxygen, being a glutton has taken too much electronic charge for its own good and the hydrogens are depleted. Thus, there is a net dipole moment in water. In liquid form, the dipoles align randomly and cancel out, and something similar to Debye shielding happens. But when water crystallizes into ice, a regular structure is required. But this regular structure requires the H_2O molecules to be stressed into a symmetric state so that all the dipoles etc will cancel. This arrangement is ok for the bulk material, but it means that the bond angles change and take up *more* room. Thus to tackle the intrinsic dipole moment of the water molecule, ice actually is less dense than water.

So your bulk material, whatever it might be, has zero charge density, zero dipole moment etc. Else, its energy of creation would tear apart the material, and it would only be seen in gas form. In gas form, these dipoles would align randomly and cancel out through a statistical process.

Applied Field Present

Now we apply a field. In the presence of this field, metals would have induced currents. That is because they have electrons in their conduction bands. But insulators don't have conduction electrons in solid or liquid states, and have high barriers to ionization in gas states. So what happens when an Electric Field is applied?

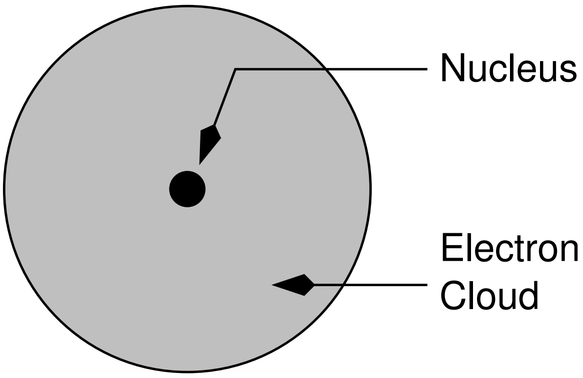
The answer to this question properly belongs to a Quantum Mechanics course. But to summarize, we have to solve a different Schrodinger's Equation, one in which we have not only the Coulomb force of the nucleus, but also the applied Electric Field. Compared to the atomic field, the applied Electric Field is quite weak. So we treat it as a “perturbation” and can solve for the new wave functions. We find that the new wave functions are slightly shifted towards higher potential (i.e., lower potential energy). Taken as a whole, the atom is now a dipole, whose dipole moment is aligned with the direction of the field.

How much is this induced dipole moment? Well it is larger for larger applied fields, but it is *not* proportional to the strength of the field. However, for weak applied fields it is well approximated as linear.

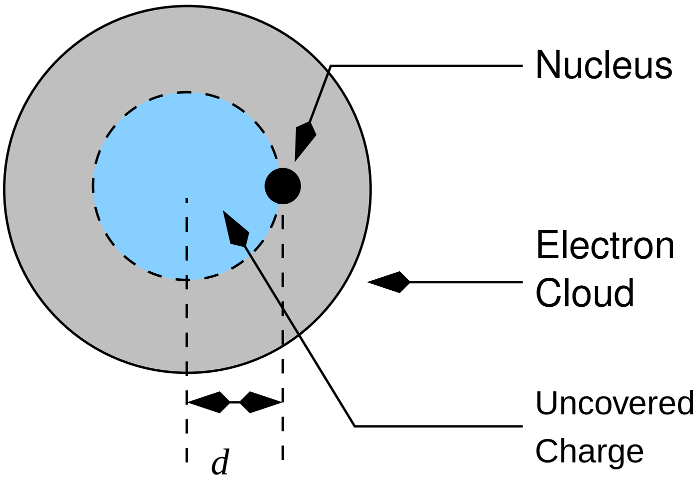
The consequence of all this is that when an external Electric Field is applied, *new charges appear, at the location of each atom or molecule. These charges consist of two equal and opposite charges separated by a tiny distance.*

If we knew what these charges were, it would be tedious but possible to compute the Electric Field. However, the charges depend on the applied field, and they also depend on the locations of the atoms in the material.

Let us make a very simplistic calculation of the displacement induced by an applied field. We start with an atom at peace with the world, with its electron wave functions symmetrically distributed about its nucleus.



When an Electric Field is applied, as argued above, the wave functions are distorted. We will *assume* that this distortion amounts to a displacement of the centre of the electron cloud, while keeping its shape fixed. This assumption is completely unwarranted. For instance, inner electron shells are more tightly held than outer shells and are displaced a smaller distance. But we will do it to get some idea of what is going on. So this is what the new situation looks like



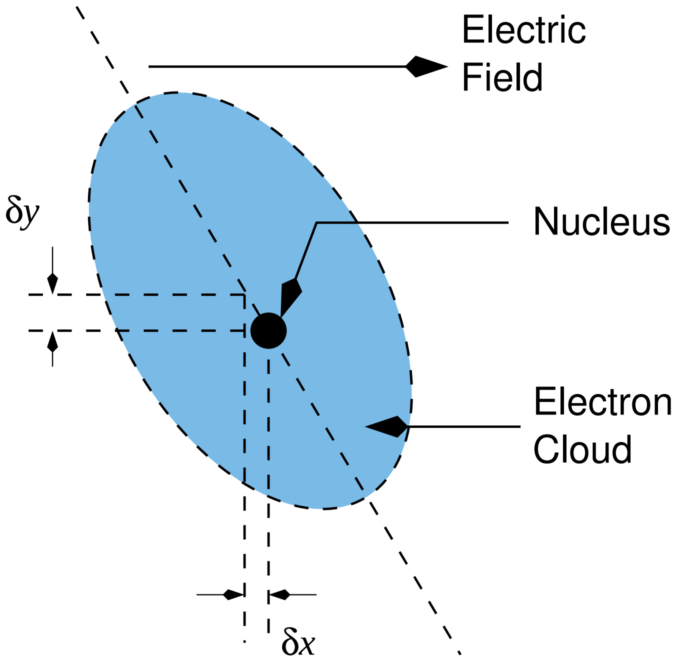
As we know from Physics 102, the Electric Field is zero inside a uniform spherical shell of charge. The gray portion of the electron cloud consists of such shells of charge, and exert no force on the nucleus. However, the blue portion exerts a force as if all the charge were concentrated at the centre of the blue sphere, i.e., at a distance d from the nucleus. Thus, the induced Electric Field is given by

$$\frac{Q}{4\pi\varepsilon_0 d^2} = \frac{-ne}{4\pi\varepsilon_0 d^2}\left(\frac{d}{a}\right)^3 \propto ned$$

where n is the atomic number of the atom. The induced Electric field is proportional to p, the induced dipole moment. The displacement that occurs for a given applied Electric field would be that displacement in which the induced Electric Field mostly cancels the applied Electric Field. Thus, we have the important result

$$\vec{p}_{\text{induced}} \propto \vec{E} \tag{2}$$

where I have also added that the direction of the induced dipole is along the direction of the applied field. In reality Eq. 2 is nonlinear, and is only a good approximation for weak fields (i.e., fields weak compared to the atomic fields). Additionally, in solids, the presence of a crystalline structure means that the atom is not equally free to deform in all directions. Thus, it tends to bulge in preferred directions



In the figure above, the Electric Field is along $\hat{x}$, but the cloud distortion is along $\left(\hat{x}+\sqrt{3}\hat{y}\right)/2$. Thus, E_x causes not only δx but also δy. In this case, $\vec{p}$ is clearly not along $\vec{E}$. However, one can still write generally

$$p_i = \alpha_{ij}E_j + \beta_{ijk}E_jE_k + \gamma_{ijkl}E_jE_kE_l + \ldots \tag{3}$$

This equation is a very good model of the material at low frequencies. Further, depending on the material, different coefficients become important. α_{ij} contributes to the dielectric constant and is often a scalar, i.e.,

$$\alpha_{ij} = \alpha_0\delta_{ij}$$

In the case of silica glass, which is widely used in optical communications, β_{ijk} is zero due to "inversion symmetry" while γ_{ijkl} has certain specific coefficients that are dominant. Equation 3 becomes for this case

$$p_i = \alpha_0E_i + \gamma_0E_iE_jE_j$$

or

$$\vec{p} = \alpha_0\vec{E} + \gamma_0\left|\vec{E}\right|^2\vec{E}$$

Material Response

Now, a dipole is induced at the location of each atom. But the atoms are in irregular positions. Even in crystalline solids, the material is often composed of microscopic crystals arranged irregular positions. How do we obtain the effect of the material on the field?

Suppose we have N atoms, each with its orientation. Thus the response of the i^{th} atom is got by rotating α_{ij} to its standard orientation, obtaining the response, and rotating back. This rotation is carried out by a “unitary” matrix (more linear algebra you ought to know) and we obtain

$$\vec{p}_i = R_i^{-1}\alpha R_i \cdot \vec{E}(\vec{r}_i)$$

The total field due to these dipoles can be obtained by using the expression for the Electric Potential far from a dipole

$$\phi_{\text{ind}}(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{N}\frac{(\vec{r}-\vec{r}_i)\cdot R_i^{-1}\alpha R_i \cdot \vec{E}(\vec{r}_i)}{|\vec{r}-\vec{r}_i|^3}$$

and it is clearly a function of the applied field at *each* $\vec{r}_i$. This is a terrible equation to deal with and totally useless for any practical application. Worse, we usually don’t even know the exact positions and orientations of the individual atoms. But it describes the *general linear response* of the material. We need a better approach, that might give up some of the detailed information (preferably the information we don’t anyway have!) but that would give us a manageable equation.

Simplified Material Response

When we give up detailed information, we necessarily make assumptions about the information we give up. For example, if by chance, all the atoms were oriented along $\hat{z}$, the material response would be quite different from the response if the atoms were randomly oriented. Here, we develop the “better equation” for a random medium (liquids, gases and amorphous solids).

Suppose we consider a ΔV that is small enough that the applied field does not vary significantly over its dimensions, but large enough that many atoms are present in the volume. We assume that the atoms have random alignments. We also assume that the volume is so small that the individual atom responses can be added vectorially assuming that they are all at the centre of the volume. What do all these assumptions imply? The rotations R_i can be parametrised by the point on the unit sphere where the new $\hat{z}$ axis points, i.e., by θ and ψ in spherical polar coordinates. So,

$$\begin{aligned}\phi_{\text{ind}}(\vec{r}) &= -\frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{N}\nabla\left(\frac{1}{\left|\vec{r}-\vec{r}_0-\vec{dr}_i\right|}\right)\cdot R^{-1}(\theta_i,\psi_i)\alpha R(\theta_i,\psi_i)\cdot\vec{E}(\vec{r}_0+\vec{dr}_i)\\ &\simeq -\frac{N}{4\pi\varepsilon_0}\nabla\left(\frac{1}{|\vec{r}-\vec{r}_0|}\right)\cdot\int_0^\pi\int_{-\pi}^{\pi}R^{-1}(\theta,\psi)\alpha R(\theta,\psi)d\Omega\cdot\vec{E}(\vec{r}_0)+O(dr,1/\sqrt{N})\\ &= -\frac{N}{4\pi\varepsilon_0}\nabla\left(\frac{1}{|\vec{r}-\vec{r}_0|}\right)\cdot\langle\alpha\rangle_{\theta,\psi}\cdot\vec{E}(\vec{r}_0)+O(dr,1/\sqrt{N}) \qquad (4)\end{aligned}$$

The assumption we have made here is that the random rotations cover the sphere uniformly in “solid angle” ($d\Omega = \sin\theta d\theta d\psi$), and that we can simply integrate over the material response for all possible orientations. For a given material, $\langle\alpha\rangle_{\theta,\psi}$ is a known quantity. We no longer need to know where each and every atom is, and how it is aligned.

This is a huge advance, but it required knowledge of the “statistics” of orientations of the atoms. One can imagine materials where orientations are locally non-random, where this assumption fails. For instance, the material properties of polymer chains could fail on two counts. It could fail because the chains line up, and it could fail because exciting one part of the polymer chain with Electric field could change the material properties over the rest of the chain, i.e., elsewhere in the material. Still this assumption has turned an intractable problem into a tractable one, so let us see where it takes us.

The Displacement Vector

We now define the "average induced dipole"

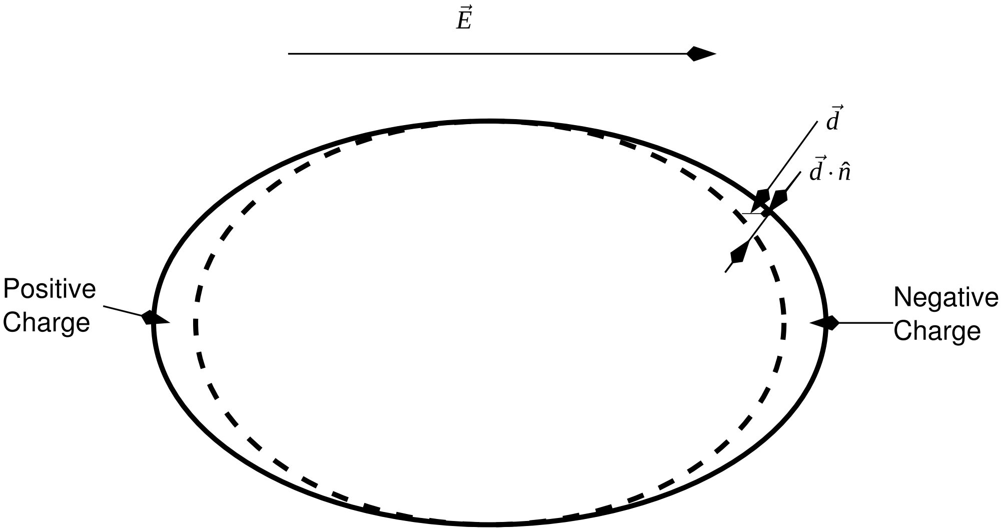
$$\vec{p}(\vec{r}) = \langle\alpha\rangle_{\theta,\psi}\vec{E}(\vec{r}) = (ne)\,\vec{d} \tag{5}$$

This dipole is due to a shift in the electron cloud by a distance $\vec{d}$. The effect of the averaging over all orientations turns the response into an isotropic one. For instance, if $E_0\hat{x}$ caused $\delta\hat{y}$, rotating the orientation in the y-z plane by π radians can yield a displacement of $-\delta\hat{y}$. So all such displacements average out, and $\vec{d}$ is along $\vec{E}$.

Now consider an arbitrary closed surface S. The divergence theorem tells us

$$\int \vec{E}\cdot\vec{dS} = \frac{Q_{\text{encl}}}{\varepsilon_0}$$

What is Q_{encl}? It clearly includes all the actual charges placed inside the volume, and it includes the induced charges that lie within the volume as well. But the Electric Field induces dipoles; i.e., with every positive charge ne, there is a negative charge $-ne$. So the dipoles cannot contribute to the enclosed charge, except at the edge, where the positive charge could lie outside the volume while the negative charge lies inside, or vice versa.



Thus, the divergence theorem becomes

$$\varepsilon_0\int \vec{E}\cdot\vec{dS} = Q_{\text{real}} + \int n_0\,(-ne)\,\vec{d}\cdot\vec{dS}$$

where n_0 is the average number of atoms per cubic metre. This can be rewritten as

$$\int \left(\varepsilon_0 \vec{E} + n_0 \vec{p}\right) \cdot \vec{dS} = Q_{\text{real}}$$

Using Eq. 5, we get our final equation

$$\int \left(\varepsilon_0 + n_0 \left\langle \alpha \right\rangle_{\theta,\psi}\right) \vec{E} \cdot \vec{dS} = Q_{\text{real}}$$

We define a new quantity, called the Displacement Vector:

$$\vec{D} = \left(\varepsilon_0 + n_0 \left\langle \alpha \right\rangle_{\theta,\psi}\right) \vec{E}$$

In terms of $\vec{D}$, the divergence theorem for Electrostatic Fields in a material become

$$\nabla \cdot \vec{D} = \rho \tag{6}$$

Defining $\vec{D}$ is not the great simplification. The great simplification is that $\vec{D}$ can be obtained from $\vec{E}$ using known, bulk properties of the material, namely n_0 and $\left\langle \alpha \right\rangle_{\theta,\psi}$.

In textbooks, the presentation of this material is similar, but uses different jargon. For example, Jackson defines the *Polarization Vector* $\vec{P}$ defined by

$$\vec{P} = n_0 \left\langle \vec{p} \right\rangle$$

which is nothing but our $n_0 \left\langle \alpha \right\rangle_{\theta,\psi} \vec{E}$. In terms of $\vec{P}$,

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P}$$

He obtains Eq. 6 via Eq. 4

$$\begin{aligned} \phi(\vec{r}) &= \frac{1}{4\pi\varepsilon_0} \int \left[\frac{\rho_{\text{real}}}{R_{12}} - \vec{P}(\vec{r}') \cdot \nabla \frac{1}{R_{12}} \right] dV' \\ &= \frac{1}{4\pi\varepsilon_0} \int \frac{1}{R_{12}} \left[\rho_{\text{real}} - \nabla' \cdot \vec{P}(\vec{r}') \right] dV' \end{aligned}$$

after some algebra. Hence,

$$\nabla \cdot \vec{E} = -\nabla^2 \phi = \frac{\rho_{\text{real}} - \nabla \cdot \vec{P}}{\varepsilon_0}$$

which gets us to Eq. 6 again. The more mathematically minded student can look at that derivation instead. In the end both approaches say the same thing.