Multipoles; Macroscopic Media; Dielectrics

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(1731 - 1810)

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Contents

In this chapter, we shall first develop the multipole expansion for the electrostatic potential and field. This is useful not only for expressing the field produced by a localized distribution of charge but is also a helpful preliminary investigation for the business of describing the electrostatics of materials containing a large number of charges and which are not conductors. These are called *dielectrics*. After developing a means of describing their electrostatic properties, we shall turn to boundary value problems in systems comprising dielectrics and conductors.

1 Multipole Expansion: An Alternate Approach

In this section we will develop the multipole expansion for a charge distribution by an alternate means to that used in Jackson (the method used in Jackson is discussed in the appendix to this chapter).

We begin by writing the general expression for the potential due to a finite charge distribution $\rho(\mathbf{x})$,

$$\Phi(\mathbf{x}) = \int d^3x'\, \rho(\mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|} \tag{1}$$

Let us consider the case where the origin is within the charge distribution and where $|\mathbf{x}| = r$ is large compared to the size of the charge distribution. Then we may expand the denominator in the integrand.

$$\frac{1}{|\mathbf{x} - \mathbf{x}'|} = \frac{1}{\sqrt{r^2 - 2\mathbf{x}\cdot\mathbf{x}' + r'^2}} = \frac{1}{r\sqrt{1 - 2\mathbf{x}\cdot\mathbf{x}'/r^2 + r'^2/r^2}}. \tag{2}$$

Using the Taylor series expansion

$$\frac{1}{\sqrt{1-x}} = 1 + \frac{1}{2}x + \frac{3}{8}x^2 + \cdots \tag{3}$$

We get

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{r}\left(1 + \frac{1}{2}\left(2\mathbf{x}\cdot\mathbf{x}'/r^2 - r'^2/r^2\right) + \frac{3}{8}\left(4(\mathbf{x}\cdot\mathbf{x}')^2/r^4\right)\right) + \text{order}\left((r'/r)^3\right) \tag{4}$$

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{r} + \frac{\mathbf{x}\cdot\mathbf{x}'}{r^3} + \frac{1}{2r^5}\left(3(\mathbf{x}\cdot\mathbf{x}')^2 - r'^2r^2\right) + \cdots \tag{5}$$

With this expansion, we can rewrite $\Phi(\mathbf{x})$ as

$$\begin{aligned}\Phi(\mathbf{x}) &= \int d^3x'\,\frac{\rho(\mathbf{x}')}{r} + \\ &\int d^3x'\,\frac{(\mathbf{x}\cdot\mathbf{x}')\rho(\mathbf{x}')}{r^3} + \\ &\int d^3x'\,\frac{\rho(\mathbf{x}')}{2r^5}\left(3(\mathbf{x}\cdot\mathbf{x}')^2 - r'^2r^2\right) + \cdots\end{aligned}$$

$$\begin{aligned}\Phi(\mathbf{x}) &= \frac{1}{r}\int d^3x'\,\rho(\mathbf{x}') \quad \text{monopole} + \\ &\frac{\mathbf{x}}{r^3}\cdot\int d^3x'\,\mathbf{x}'\rho(\mathbf{x}') \quad \text{dipole} + \\ &\frac{1}{2r^5}\int d^3x'\,\rho(\mathbf{x}')\left(3(\mathbf{x}\cdot\mathbf{x}')^2 - r'^2r^2\right) \quad \text{quadrupole} + \cdots\end{aligned}$$

or

$$\begin{aligned}\Phi(\mathbf{x}) &= \frac{1}{r}\int d^3x'\,\rho(\mathbf{x}') + \\ &\frac{\mathbf{x}}{r^3}\cdot\int d^3x'\,\mathbf{x}'\rho(\mathbf{x}') + \\ &\frac{1}{2}\sum_{i,j}\frac{x_ix_j}{2r^5}\int d^3x'\,\rho(\mathbf{x}')\left(3x'_ix'_j - r'^2\delta_{ij}\right) + \cdots\end{aligned} \tag{6}$$

where the sum is over the 3 coordinates of space. If we follow the conventional designation of these terms, then

$$\Phi(\mathbf{x}) = q/r + \frac{\mathbf{x}\cdot\mathbf{p}}{r^3} + \frac{1}{2}\sum_{ij} Q_{ij}\frac{x_i x_j}{r^5} + \cdots \tag{7}$$

where

$$q = \int d^3x'\,\rho(\mathbf{x}') \quad \text{Monopole Moment} \tag{8}$$

$$\mathbf{p} = \int d^3x'\,\rho(\mathbf{x}')\mathbf{x}' \quad \text{Dipole Moment} \tag{9}$$

$$Q_{ij} = \int d^3x'\,\rho(\mathbf{x}')\left(3x'_i x'_j - r'^2\delta_{ij}\right) \quad \text{Quadrupole Moment} \tag{10}$$

Note that the matrix Q_{ij} is real an symmetric ($Q_{ij} = Q_{ji}$). Thus only six of its elements are independent. In fact, only 5 are, since there is an additional constraint that $\mathrm{Tr}(Q) = 0$.

$$\mathrm{Tr}(Q) = \sum_i Q_{ii} = \int d^3x'\,\rho(\mathbf{x}')\sum_i 3x'_i x'_i - r'^2\delta_{ii} \tag{11}$$

then as

$$\sum_i 3x'_i x'_i = 3r'^2 \tag{12}$$

$$\sum_i r'^2\delta_{ii} = 3r'^2 \tag{13}$$

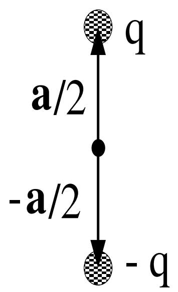
$$\mathrm{Tr}(Q) = \int d^3x'\,\rho(\mathbf{x}')\left(3r'^2 - 3r'^2\right) = 0 \tag{14}$$

Thus it must be that $Q_{33} = -Q_{11} - Q_{22}$ and only two of the diagonal components are independent. This is important, since we will relate Q to the set of five Y_2^m.

1.1 Interpretation of the Moments

What is the interpretation of these terms? The *monopole moment* is just the total charge of the distribution. Thus the monopole term gives the potential due to the charge as a whole. Since the monopole term in the potential falls off like $1/r$ at large r, it will dominate the far field potential whenever q is finite. The *dipole moment* is the first moment of the charge distribution; and refers to how the charge is distributed in space. Similarly, the quadrupole moment is a second moment of the distribution.

Let's consider the dipole in some detail, with the model shown below.



$$\Phi(\mathbf{x}) = \frac{q}{|\mathbf{x} - \mathbf{a}/2|} + \frac{-q}{|\mathbf{x} + \mathbf{a}/2|} \tag{15}$$

For $|\mathbf{x}| = r \gg a$ we can expand

$$\frac{1}{|\mathbf{x} \mp \mathbf{a}/2|} = \frac{1}{r}\left(1 \pm \frac{\mathbf{x} \cdot \mathbf{a}}{2r^2}\right) + \text{order}(a^2/r^2) \tag{16}$$

$$\Phi(\mathbf{x}) \;\approx\; \frac{q}{r}\left(1 + \frac{\mathbf{x} \cdot \mathbf{a}}{2r^2}\right) - \frac{q}{r}\left(1 - \frac{\mathbf{x} \cdot \mathbf{a}}{2r^2}\right)$$

$$\approx \frac{q}{r^3}\mathbf{x}\cdot\mathbf{a} \tag{17}$$

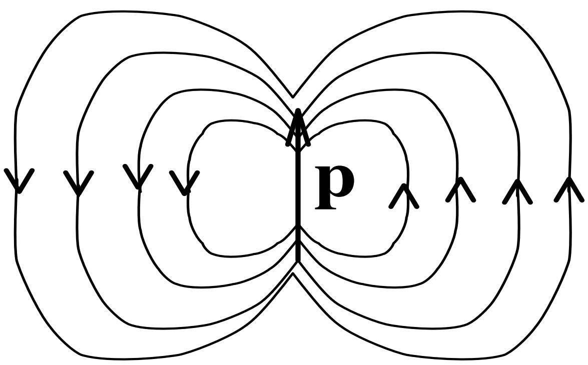
If $\mathbf{a} \to 0$ in the diagram (such that $q\mathbf{a} = \mathbf{p} =$ constant), then the higher order terms vanish, and this result becomes exact. In such a limit ($\mathbf{a} \to 0$, $q\mathbf{a} = \mathbf{p}$) we obtain a point dipole.

Now consider the field due to a dipole $\mathbf{p} = p\hat{\mathbf{z}}$

$$\Phi(\mathbf{x}) = \frac{p\cos\theta}{r^2} \tag{18}$$

$$E_r = -\frac{\partial\Phi}{\partial r} = \frac{2p\cos\theta}{r^3} \tag{19}$$

$$E_\theta = -\frac{1}{r}\frac{\partial\Phi}{\partial\theta} = \frac{p\sin\theta}{r^3}, \tag{20}$$



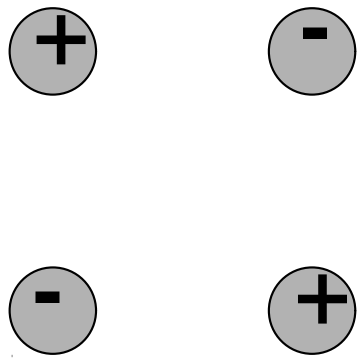
or more formally (in Cartesian coordinates).

$$\begin{aligned} E_{\mathbf{p}} &= -\nabla\left(\frac{\mathbf{p}\cdot\mathbf{x}}{r^3}\right) = -\sum_i \mathbf{e}_i \frac{\partial}{\partial x_i}\sum_j \frac{p_j x_j}{r^3} \\ &= -\sum_i \mathbf{e}_i\left(\frac{p_i}{r^3} - 3\sum_j \frac{p_j x_j}{r^4}\frac{x_i}{r}\right) \end{aligned} \tag{21}$$

where we have used the fact that $\frac{\partial r}{\partial x_i} = \frac{x_i}{r}$.

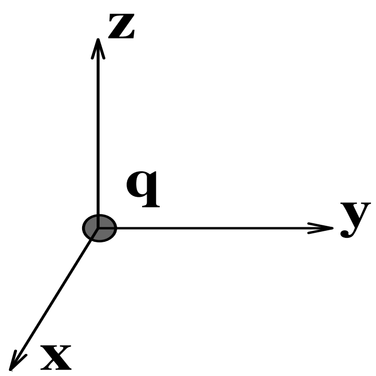
$$E_{\mathbf{p}} = \frac{3\mathbf{x}(\mathbf{p}\cdot\mathbf{x})}{r^5} - \frac{\mathbf{p}}{r^3} \tag{22}$$

In a similar fashion the potential term involving the quadrupole moment may be interpreted as due to an assembly of four charges (hence the name).



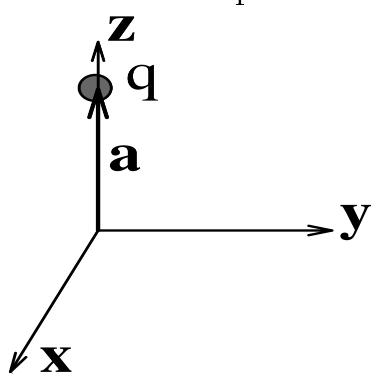
Higher-order moments (octapole, hexadecapole, etc.) may be generated in a like fashion.

It is important to note that the interpretation of the moments depends strongly upon the origin. For example consider a point charge located at the origin.



$$\Phi(\mathbf{x}) = q/r \tag{23}$$

It has only a monopole term. Now displace the charge by a vector **a**.



$$\Phi(\mathbf{x}) = \frac{q}{|\mathbf{x} - \mathbf{a}|} = q/r + q\frac{\mathbf{a}\cdot\mathbf{x}}{r^3} + \frac{q}{2}\frac{3(\mathbf{a}\cdot\mathbf{x})^2 - a^2r^2}{r^5} + \cdots \tag{24}$$

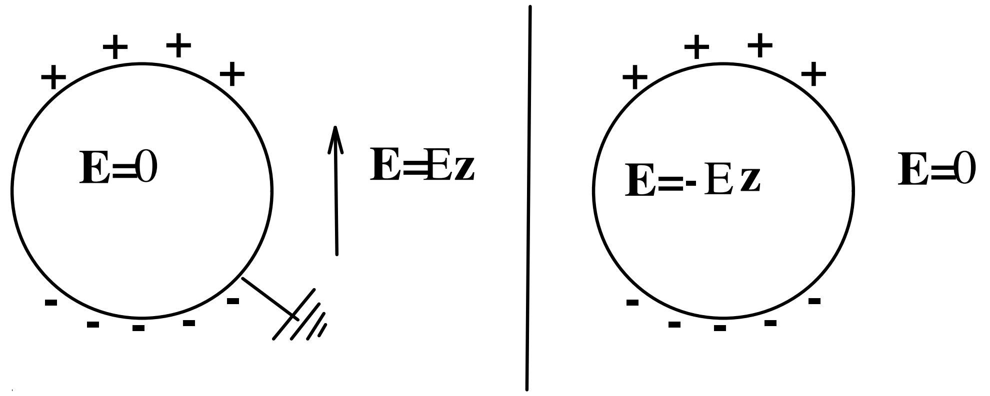
This has moments to all orders! *watch your origin*!

1.2 Dipole Field

It is interesting to ask what is going on at the origin, where our expansion fails. Let's look at the particular case of the dipole field, assuming a point dipole at $r = 0$. For any $r > 0$, we know that the potential is as given in Eq. (17). Once before we found such a potential when we solved the problem of a conducting sphere of radius a in a uniform external applied field $\mathbf{E}_0$. What we found was that the potential outside of the sphere is

$$\Phi(\mathbf{x}) = -E_0 r\cos\theta + E_0 a^3 \frac{\cos\theta}{r^2} \tag{25}$$

while inside of the sphere the potential is a constant and the field is zero.



If one removes the applied field but retains the field produced by the charges on the surface of the sphere, then the potential for $r > a$ is simply $E_0 a^3 \cos\theta / r^2$ which may also be written as $\mathbf{p} \cdot \mathbf{x}/r^3$ with $\mathbf{p} = E_0 a^3 \hat{\mathbf{z}}$. By the superposition principle, the field at $r < a$ is now $-\mathbf{E}_0 = -\mathbf{p}/a^3$. What this means is that the surface charge on the sphere has a dipole moment and, remarkably, no other multipole moments. Now let us fix $\mathbf{p}$ while letting $a \to 0$. The region $r < a$ shrinks, while the field inside gets bigger. As the region shrinks to zero, the field strength at the origin (*i.e.,* inside the sphere) diverges. The integral of the field over the spherical domain $r < a$ is, however, a constant and equal to $-(4\pi/3)\mathbf{p}$. Consequently, in the limit of vanishing a, this field may be represented by a delta function, $-(4\pi/3)\mathbf{p}\delta(\mathbf{x})$. The total field of a point dipole of moment $\mathbf{p}$ is thus the dipolar field, Eq. (21), for $r > 0$

plus a delta-function piece at the origin,

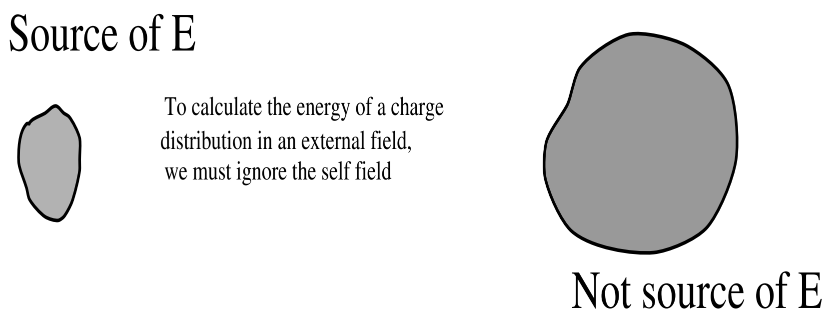
$$\mathbf{E}(\mathbf{x}) = \frac{3\mathbf{n}(\mathbf{p}\cdot\mathbf{n}) - \mathbf{p}}{r^3} - \frac{4\pi}{3}\mathbf{p}\delta(\mathbf{x}). \tag{26}$$

Our derivation of this result is not completely general since it is based on the limiting form of the solution to one particular problem involving a sphere; the result is, however, quite correct for any point dipole. See Jackson, Chapter 4, Section 1, for a more complete discussion of this point.

2 Energy of the Charge Distribution

In this section we consider the energy of a localized charge distribution $\rho(\mathbf{x})$ in an external applied electric field $\mathbf{E}(\mathbf{x})$ which may be described through its potential $\Phi(\mathbf{x})$. This energy is, as we know from Chapter 1,

$$W = \int d^3x\, \rho(\mathbf{x})\Phi(\mathbf{x}). \tag{27}$$



Notice that there is no factor of 1/2; that is because we are finding the interaction energy of a charge distribution with a field which is *not* produced by that same charge distribution and so we do not double count the energy in Eq. (24) by omitting this factor.

Now if we assume that Φ changes slowly over the region where ρ is appreciable, then we can expand the potential Φ around the origin of coordinates using a Taylor series:

$$\begin{aligned}\Phi(\mathbf{x}) &= \Phi(0) + \mathbf{x}\cdot\nabla\Phi(\mathbf{x})|_{\mathbf{x}=0} + \frac{1}{2}\sum_{i,j=1}^{3} x_i x_j \left.\frac{\partial^2\Phi(\mathbf{x})}{\partial x_i \partial x_j}\right|_{\mathbf{x}=0} + \ldots \\ &= \Phi(0) - \mathbf{x}\cdot\mathbf{E}(0) - \frac{1}{2}\sum_{i,j=1}^{3} x_i x_j \left.\frac{\partial E_j(\mathbf{x})}{\partial x_i}\right|_{\mathbf{x}=0} + \ldots \qquad (28)\end{aligned}$$

where $\mathbf{E}(\mathbf{x})$ is the external applied field. Now, this field is such that its sources are far away, or at least are zero in the region where the charge distribution $\rho(\mathbf{x})$ is located. Therefore $\nabla\cdot\mathbf{E}(\mathbf{x}) = 0$ in this region and so we can add a term proportional to $\nabla\cdot\mathbf{E}(\mathbf{x})$ to the potential $\Phi(\mathbf{x})$ without changing the result of the integral in Eq. (24). We choose this term to be

$$\frac{1}{6} r^2 \nabla\cdot\mathbf{E}(\mathbf{x})|_{\mathbf{x}=0} = \frac{1}{6}\sum_{i,j=1}^{3} r^2\delta_{ij} \left.\frac{\partial E_j(\mathbf{x})}{\partial x_i}\right|_{\mathbf{x}=0}. \qquad (29)$$

Hence we have

$$\Phi(\mathbf{x}) = \Phi(0) - \mathbf{x}\cdot\mathbf{E}(0) - \frac{1}{6}\sum_{i,j=1}^{3} (3x_i x_j - r^2\delta_{ij}) \left.\frac{\partial E_j(\mathbf{x})}{\partial x_i}\right|_{\mathbf{x}=0}, \qquad (30)$$

plus higher-order terms. If we substitute this expansion into the expression for the energy, we find

$$W = q\Phi(0) - \mathbf{p}\cdot\mathbf{E}(0) - \frac{1}{6}\sum_{i,j=1}^{3} Q_{ij} \left.\frac{\partial E_j(\mathbf{x})}{\partial x_i}\right|_{\mathbf{x}=0} + \ldots. \qquad (31)$$

2.1 Example: Dipole Energies

As an example making use of this result, suppose that we have a dipole of moment $\mathbf{p}_1$ at point $\mathbf{x}_1$ in the presence of a second dipole of moment $\mathbf{p}_2$ at $\mathbf{x}_2$. Then the energy of interaction is

$$W = -\mathbf{p}_1 \cdot \mathbf{E}_2(\mathbf{x}_1) = \frac{-3(\mathbf{p}_2 \cdot \mathbf{n})(\mathbf{p}_1 \cdot \mathbf{n}) + \mathbf{p}_1 \cdot \mathbf{p}_2}{|\mathbf{x}_1 - \mathbf{x}_2|^3} \tag{32}$$

where $\mathbf{n} = (\mathbf{x}_1 - \mathbf{x}_2)/|\mathbf{x}_1 - \mathbf{x}_2|$ is a unit vector pointing from the second dipole to the first (or vice versa).

2.2 Example: Quadrupole Energies

A second example has to do with the coupling of a nucleus' electric quadrupole moment to an external field (such as that from the electrons). By choosing the origin in an appropriate fashion, one can guarantee that any nucleus (any object with a non-zero net charge, in fact) has no dipole moment. Hence the first interesting term in the nucleus' interaction with an external field is the electric quadrupole interaction. Further, a nucleus in an angular momentum eigenstate $|J, M>$ will have a charge density which is invariant under rotation around the

z-axis,

$$\rho \propto Y_J^M Y_J^{M*} \propto e^{iM\phi} e^{-iM\phi}$$

leading to a diagonal electric quadrupole moment tensor (the matrix of Q_{lm}'s) which is such that $Q_{xx} = Q_{yy}$. Since the trace of this tensor (or matrix) is zero, this means that[1] $Q_{xx} = Q_{yy} = -Q_{zz}/2$. The upshot is that the interaction of the nuclear quadrupole with the applied field is

$$W = -\frac{1}{4} Q_{zz} \left. \frac{\partial E_z(\mathbf{x})}{\partial z} \right|_{\mathbf{x}=0} . \tag{33}$$

Bear in mind that the moment Q_{zz} is a function of the internal state of the nucleus and in particular of its angular momentum states. The quadrupolar coupling thus provides a way to lift the degeneracy associated with the different quantum numbers M for the z-component of angular momentum.

3 Dipoles in Nature: Permanent and Induced

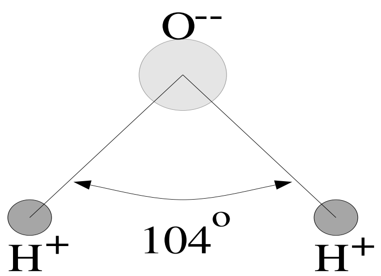
Why are dipoles so interesting?? The reason is that many atoms and molecules have dipole moments which affects their chemical and electrical properties.

[1] Or maybe that means this: $Q_{11} = Q_{22} = -Q_{33}/2$.

3.1 Permanent Dipoles

An example of a molecule with a permanent electric dipole moment is water H_2O.

$$|\mathbf{p}| = 1.86x10^{-18}\mathrm{esu-cm} = 1.86\mathrm{Debyes}$$



This dipole moment corresponds to approximately one electron charge separated across the size of the molecule. Other polar molecules have similar dipole moments (NH_3: 1.47 debyes, HCl: 1.03 debyes).

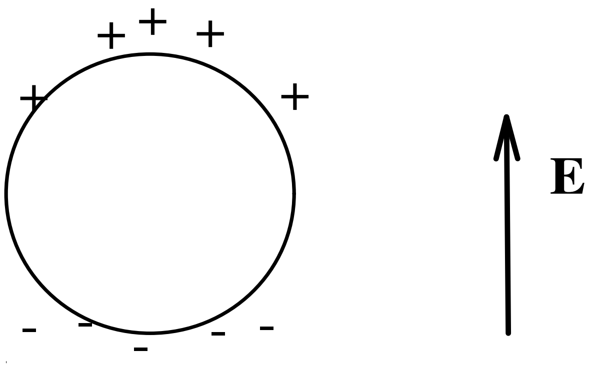
Atoms or Nuclei cannot have permanent dipole moments, since they are in states of good angular momentum l: the dipole moment of an electron in such a state vanishes. In contrast the molecules mentioned above are in sp hybrid orbitals, so that l is not a good quantum number, and thus a dipole moment is allowed.

3.2 Induced Dipoles

Atoms and molecules that lack permanent dipoles *can* have induced dipole moments when placed in an external electric field.

3.2.1 Static Models

We have already seen the effect of an external field inducing a dipole moment in a metallic sphere.



$$\Phi(\mathbf{x}) = \Phi_{external}(\mathbf{x}) + \Phi_{induced}(\mathbf{x}) \tag{34}$$

$$\Phi_{induced}(\mathbf{x}) = \frac{\mathbf{p}\cdot\mathbf{x}}{r^3} \quad \mathbf{p} = E_o a^3 \hat{\mathbf{z}} \tag{35}$$

The induced dipole moment is proportional to the external electric field. If we define α to be the polarizability of the body, then

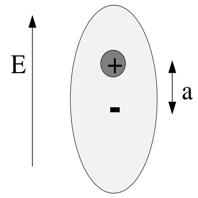
$$\mathbf{p} = \alpha\mathbf{E} \tag{36}$$

where, in this case, $\alpha = a^3$. We see that in general the polarizability of the order of magnitude of the volume of the body. Thus for an atom

$$\alpha_{atom} \approx \text{atomic volume} \approx 10^{-24}\text{cm}^3 \tag{37}$$

This is consistent with experiment.

To see what this means in realistic terms, consider an atom placed in a relatively large electric field $E = 100$ statvolts/cm.



Lets assume that the induced dipole moment is

$$\mathbf{p} = \alpha \mathbf{E} = e\mathbf{a} \tag{38}$$

where e is an electronic charge and $|\mathbf{a}|$ is the distance which separates the charge. Then

$$a = \frac{\alpha E}{e} \approx \frac{(10^{-24}\mathrm{cm}^3)(100\mathrm{statvolts/cm})}{4.8 \times 10^{-10}\mathrm{esu}} \approx 2 \times 10^{-13}\mathrm{cm} \tag{39}$$

This is of nuclear dimensions (2 fermi's). Thus the atom is quite rigid to polarization. To have a distortion of the order of and Angstrom, we need a field of order $E = 5 \times 10^6$statvolts/cm. This type of field strength is only available with a laser.

3.2.2 Dynamic Model

We may also calculate α for an atom using a simple dynamical model. Suppose that the electron is bound to the ion by a spring, so that, if displaced from equilibrium, it feels a restoring force.

$$\mathbf{F}_{restore} = -m\omega_o^2 \mathbf{x} \tag{40}$$

where m is the electronic mass, and ω_o the frequency of oscillation. If we apply an external electric field $\mathbf{E}$, the displacement $\mathbf{x}$ of the electron from equilibrium will grow until $\mathbf{F}_{restore}$ is equal and opposite to the electronic force on the electron.

$$-(-e\mathbf{E}) = -m\omega_o^2\mathbf{x} \quad \text{so} \quad \mathbf{x} = \frac{-e\mathbf{E}}{m\omega_o^2} \tag{41}$$

The induced dipole moment is then

$$\mathbf{p} = -e\mathbf{x} = \frac{e^2}{m\omega_o^2}\mathbf{E} = \alpha\mathbf{E} \tag{42}$$

So that the atomic polarizability is

$$\alpha = \frac{e^2}{m\omega_o^2} \tag{43}$$

Now, we expect that $\omega_o \approx$ angular frequency of oscillation, which is approximately the frequency of the light which is emitted by atoms. For a wavelength of 3000 Angstroms $\omega_o \approx 6 \times 10^{15} s^{-1}$, giving

$$\alpha \approx 6 \times 10^{-24}\text{cm}^3.$$

This is in accord with our previous estimate.

4 Dielectric Materials

The electrostatic properties of some insulating materials may be modeled by a collection of dipole molecules, each with a dipole moment. Higher order moments are usually neglected. Our main interest here is not in the dipole moments of individual atoms or molecules, but rather the dipole moments of atoms or molecules in a solid. In such a medium, we expect that there will be no net permanent dipole moment. This is for two reasons:

(1) If there is a permanent dipole moment in the atoms or molecules which make up the system, then the orientation of them will be random. Thus the average dipole moment $<\mathbf{p}>$ will be zero.

(2) If there is no permanent dipole moment of the component atoms or molecules, then in the absence of an external field, each will have no dipole moment, and thus the average dipole moment $<\mathbf{p}>$ will also be zero

4.1 Statistical Mechanics

Now suppose that we do apply an external electric field, what will $<\mathbf{p}>$ be then? What effect will thermal fluctuations have? We must again consider the ensemble of molecules for two different cases.

4.1.1 Induced dipoles

If each molecule has an induced dipole moment, then the Hamiltonian for each molecule is

$$U = -\mathbf{p}\cdot\mathbf{E} + \frac{1}{2}m\omega_0^2 r^2. \tag{44}$$

We can thus find the thermal average value of $\mathbf{x}$ by averaging it over the distribution $\exp(-U/kT)$, where k is Boltzmann's constant and T is the temperature:

$$< \mathbf{x} >= \frac{\int d^3x\, e^{-U/kT}\mathbf{x}}{\int d^3x\, e^{-U/kT}} \tag{45}$$

Let E define the z-direction and have

$$\begin{aligned} < \mathbf{x} >&= \frac{\int d^3x\, e^{(eEr\cos\theta - \frac{1}{2}m\omega_0^2 r^2)/kT} r\cos\theta\hat{\mathbf{z}}}{\int d^3x\, e^{(eEr\cos\theta - \frac{1}{2}m\omega_0^2 r^2)/kT}} \\ &= \frac{\int dze^{(eEz-\frac{1}{2}m\omega_0^2 z^2)/kT} z\hat{\mathbf{z}}}{\int dze^{(eEz-\frac{1}{2}m\omega_0^2 z^2)/kT}} \\ &= \frac{\int due^{-\frac{1}{2}m\omega_0^2 u^2/kT}(u + eE/m\omega_0^2)\hat{\mathbf{z}}}{\int due^{-\frac{1}{2}m\omega_0^2 u^2/kT}} \end{aligned} \tag{46}$$

where $u \equiv z - eE/m\omega_0^2$. The remaining integrals cancel nicely and we find that

$$< \mathbf{x} >= (eE/m\omega_0^2)\hat{\mathbf{z}} \quad \mathbf{p} = (e^2E/m\omega_0^2)\hat{\mathbf{z}} \quad \alpha = (e^2/m\omega_0^2) \tag{47}$$

the same as before we introduced thermal fluctuations in the separation. Thus thermal effects vanish.

4.1.2 Permanent Dipoles

For permanent dipoles (remember H_2O) we may do something similar using a Boltzmann distribution $\exp(-U/kT)$, as in the previous example but this time U is simply

$$U = -\mathbf{p} \cdot \mathbf{E} \tag{48}$$

with $\mathbf{p}$ fixed in magnitude. Thus, letting $\mathbf{E}$ define the z-direction again, we have

$$<\mathbf{p}>= \frac{\int d\Omega e^{pE\cos\theta/kT} p\cos\theta\hat{\mathbf{z}}}{\int d\Omega e^{pE\cos\theta/kT}} = kT\hat{\mathbf{z}}\frac{d}{dE}\ln\left[\int_{-1}^{1} due^{pEu/kT}\right]. \tag{49}$$

The integral is easy; upon taking the derivative and simplifying the result insofar as possible, one finds

$$<\mathbf{p}>= p\hat{\mathbf{z}}\left(\coth(Ep/kT) - kT/Ep\right). \tag{50}$$

As $T \to 0$, this becomes $p\hat{\mathbf{z}}$, meaning that the dipole is perfectly aligned with the field. For large T, $kT >> pE$, we may expand the hyperbolic cosine and find the leading term

$$<\mathbf{p}>= \frac{1}{3}\frac{p^2E}{kT}\hat{\mathbf{z}}. \tag{51}$$

This is the most frequently encountered situation at *e.g.,* room temperature; it leads to a polarizability which is

$$\alpha = \frac{1}{3}\frac{p^2}{kT}. \tag{52}$$

4.1.3 Both

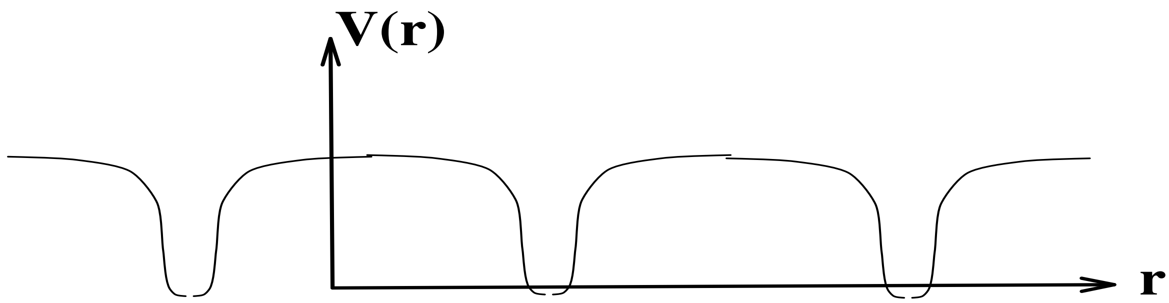
Finally, if a molecule has both a permanent moment and the possibly of being polarized, then the polarizability consists of both a temperature-independent term and one which varies inversely as the temperature,

$$\alpha = \frac{e^2}{m\omega_0^2} + \frac{p^2}{3kT}. \tag{53}$$

In each of the model calculations, where the dipoles are induced or permanent or both, the mean dipole moment induced in the material by an external field is proportional to that field. This is the basic assumption which we will use to explore the electrostatics of dielectric materials.

4.2 Macroscopic Electrostatics; Dielectrics

Before this section, we have considered only one kind of macroscopic material, conductors. Within conductors, there is no electric field, we said, because a conductor is an equipotential. If we had bothered to think a bit about that statement, we would have realized that it is a statement which applies only in some average sense. If one looks at the microscopic structure of a conductor or any other material, one finds electrons and nuclei with very strong electric fields reflecting the forces that act between these objects.



There is no electric field only in some *macroscopic* sense, that is, only if one averages over some region with a size large compared to an atomic size (which can still be much smaller than the size of a macroscopic probe whose size is at least of order 1μ).

Now we want to do the same with other materials, *i.e.,* nonconductors or insulators. Such materials are termed *dielectrics*. We concern ourselves again only with the macroscopic electric field, which is the true electric field averaged over some small domain, but it will no longer be zero, so that we must work a little harder to understand how to describe these materials.

Start by supposing that a piece of material is subjected to an externally applied electric field. This field will alter the multipole moments of the constituents of the material, which we shall call molecules (They could also be atoms or ions), yielding a net polarization of the material.

Now let's calculate the potential do to this polarization. If we regard it as a sum over the dipoles of each molecule, then

$$\Phi(\mathbf{x}) = \sum_j \frac{\mathbf{p}_j \cdot (\mathbf{x} - \mathbf{x}_j)}{|\mathbf{x} - \mathbf{x}_j|^3} \tag{54}$$

For now assume the the molecules are neutral, so that there is no monopole term. In addition, assume that quadrupole and higher terms in the series are negligible. If we define the polarization vector

$$\mathbf{P}(\mathbf{x}) = \text{ dipole moment per unit volume,} \tag{55}$$

then this becomes,

$$\begin{aligned}\Phi(\mathbf{x}) &= \int d^3x' \left[\frac{\mathbf{P}(\mathbf{x}') \cdot (\mathbf{x} - \mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|^3}\right] \\ &= \int d^3x' \left[\mathbf{P}(\mathbf{x}') \cdot \nabla' \left(\frac{1}{|\mathbf{x} - \mathbf{x}'|}\right)\right].\end{aligned} \tag{56}$$

where we have used the expression

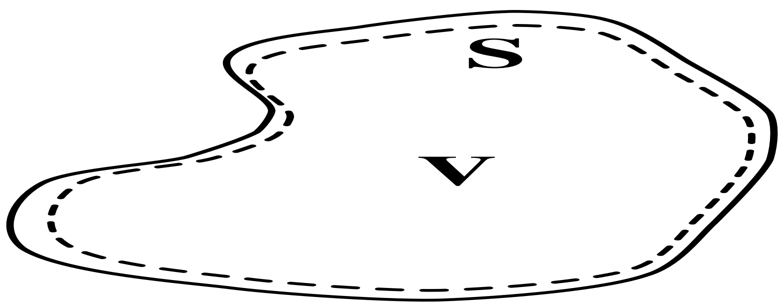
$$\frac{(\mathbf{x} - \mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|^3} = -\nabla \frac{1}{|\mathbf{x} - \mathbf{x}'|} = \nabla' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \tag{57}$$

If we integrate by parts, we get the form

$$\Phi(\mathbf{x}) = \int d^3x' \, \nabla' \cdot \left(\frac{\mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}\right) - \int d^3x' \, \frac{(\nabla' \cdot \mathbf{P}(\mathbf{x}'))}{|\mathbf{x} - \mathbf{x}'|} \tag{58}$$

There are two ways to regard this expression. Assume we have a volume V with $\mathbf{P}(\mathbf{x}')$ finite inside and zero outside.

First case. Let V be bounded by a surface S just inside the volume. Then using the divergence theorem, the equation above becomes.



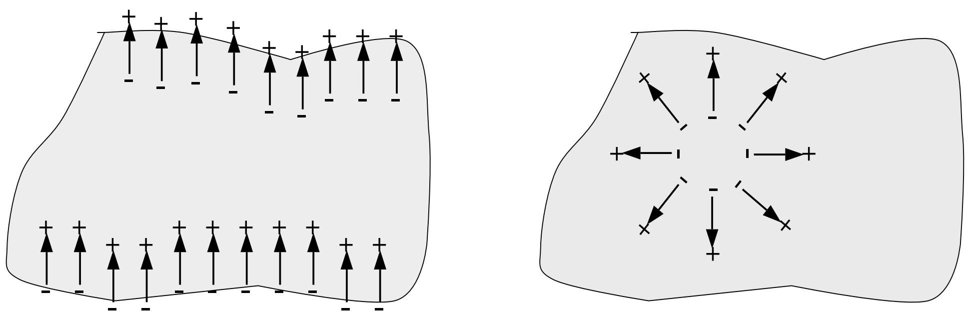
$$\Phi(\mathbf{x}) = \int_S d^2x' \, \frac{\mathbf{n}' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \int_V d^3x' \, \frac{(\nabla' \cdot \mathbf{P}(\mathbf{x}'))}{|\mathbf{x} - \mathbf{x}'|} \tag{59}$$

Thus we can define the surface and volume polarization charge densities:

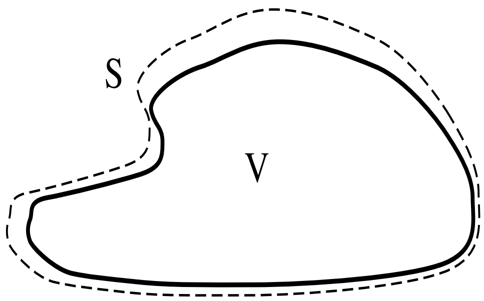
$$\sigma_p(\mathbf{x}) = \mathbf{P}_n(\mathbf{x}) \text{ or } \sigma_p(\mathbf{x}) = \mathbf{P}(\mathbf{x}) \cdot \mathbf{n} \tag{60}$$

$$\rho_p(\mathbf{x}) = -\nabla \cdot \mathbf{P}(\mathbf{x}) \tag{61}$$

These have simple physical interpretations. For example, in the figure below on the left, the material has a constant finite $\mathbf{P}$ throughout its volume, so that at the surface, charge congregates since all of the dipoles are aligned. Also, in the figure on the right a a certain location within a material the dipoles point radially outward (yielding a positive divergence). At the center of this region, where the tails of the dipoles are concentrated, there is an excess of negative charge (hence the $-$ sign in $\rho_p(\mathbf{x}) = -\nabla \cdot \mathbf{P}(\mathbf{x})$.



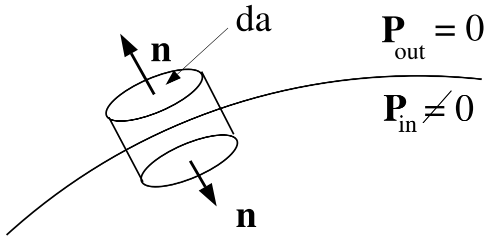
Second case. Let V be bounded by a surface S just *outside* of the region of finite polarization. Then



$$\Phi(\mathbf{x}) = \int_S d^2x' \, \frac{\mathbf{n}' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} - \int_V d^3x' \, \frac{(\nabla' \cdot \mathbf{P}(\mathbf{x}'))}{|\mathbf{x}-\mathbf{x}'|} \tag{62}$$

$$= \int_V d^3x' \, \frac{\rho_p(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \tag{63}$$

Although the surface charge does not appear explicitly, it still must be there. It may be obtained from the discontinuity in $\mathbf{P}(\mathbf{x})$ at the surface of the polarization region. To see this consider a small pill box enclosing a small section of the volume and surface of the polarized material. From the divergence theorem



$$\int_V d^3x \, \nabla \cdot \mathbf{P}(\mathbf{x}) = \int_S d^2x \, \mathbf{n} \cdot \mathbf{P}(\mathbf{x}), \tag{64}$$

or if the region is small enough

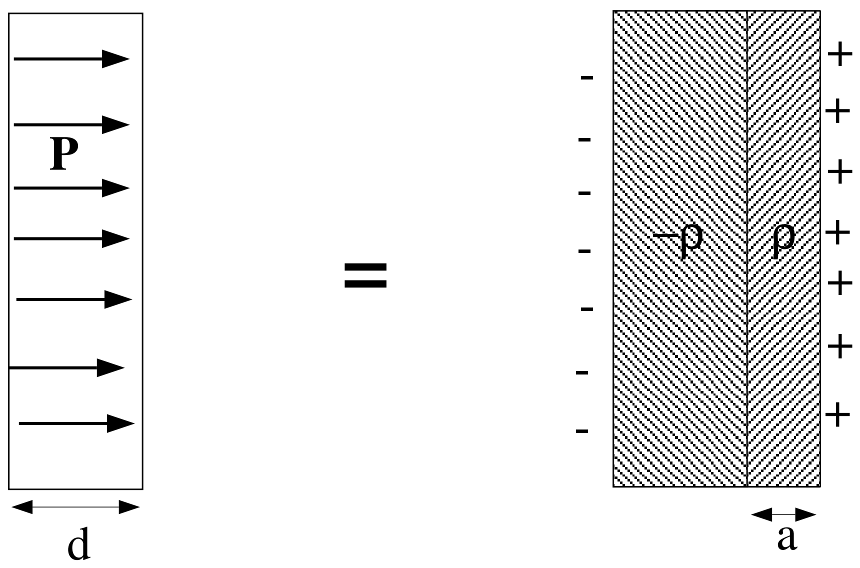
$$(-\mathbf{n} \cdot \mathbf{P}_{in} + \mathbf{n} \cdot \mathbf{P}_{out}) \, da = \nabla \cdot \mathbf{P} d^3x \tag{65}$$

so that

$$\mathbf{n} \cdot \mathbf{P}\, da = -\nabla \cdot \mathbf{P}\, d^3x, \tag{66}$$

Thus $-\nabla \cdot \mathbf{P}$ must have a delta-function at the surface, and we still have the surface polarization charge.

To understand the surface polarization charge, consider a uniformly polarized slab of dielectric.



$$\mathbf{p} = \begin{cases} \text{constant} & \text{inside} \\ 0 & \text{outside} \end{cases} \tag{67}$$

We may actually regard this as two overlapping slabs, one of uniform positive charge $+\rho$, and one of uniform negative charge $-\rho$, separated by a small distance distance $\mathbf{a}$. The whole is then electrically neutral, with uniform polarization

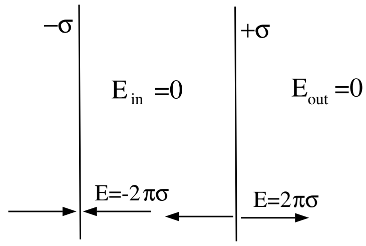
$$\mathbf{P} = \rho\mathbf{a} = \text{ dipole moment per unit volume.} \tag{68}$$

The charge density is then

$$\rho_p = -\nabla \cdot \mathbf{P} = 0 \text{ Inside the slab} \tag{69}$$

$$\sigma_p = \mathbf{P} \cdot \mathbf{n} = \begin{cases} P > 0 & \text{on rhs} \\ -P < 0 & \text{on lhs} \end{cases} \tag{70}$$

The potential due to the slab is just that of two oppositely charged sheets separated by a distance d. The corresponding electric field is just obtained by summing that due to each sheet



$$\mathbf{E} = \begin{cases} 0 & \text{outside the slab} \\ -4\pi\mathbf{P} & \text{inside the slab} \end{cases} \tag{71}$$

(We used $E_{in} = 2\pi\sigma + 2\pi\sigma = 4\pi\sigma$ and $\sigma = P$)

4.2.1 Electric Displacement

Thus far we have assumed that the dielectric is neutral. If there are free charges present as well, then the total charge density is

$$\rho_{tot} = \rho_{free} - \nabla \cdot \mathbf{P} \tag{72}$$

Then as $\mathbf{E}$ is generated by *all* charges, we have

$$\nabla \cdot \mathbf{E} = 4\pi\rho_{tot} = 4\pi \left(\rho_{free} - \nabla \cdot \mathbf{P}\right) \tag{73}$$

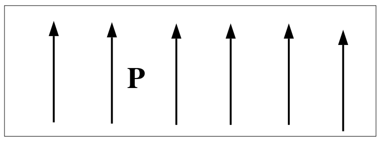
or,

$$\nabla \cdot (\mathbf{E} + 4\pi \mathbf{P}) = 4\pi \rho_{free} \qquad (74)$$

The vector $(\mathbf{E} + 4\pi \mathbf{P})$ is generated by free charges only. We will define the *electric displacement* $\mathbf{D}$ as this field

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P} \quad \nabla \cdot \mathbf{D} = 4\pi \rho_{free} \qquad (75)$$

As an example, consider the uniformly polarized slab



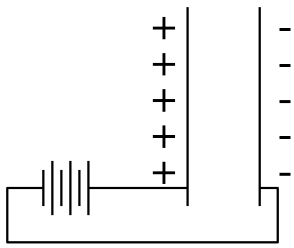
, here

$$\rho_{free} = 0 \quad \text{everywhere} \qquad (76)$$

Thus $\mathbf{E} + 4\pi \mathbf{P} = 0$, and

$$\mathbf{E} = \begin{cases} 0 & \text{where } \mathbf{P} = 0 \\ -4\pi \mathbf{P} & \text{where } \mathbf{P} \neq 0 \end{cases} \qquad (77)$$

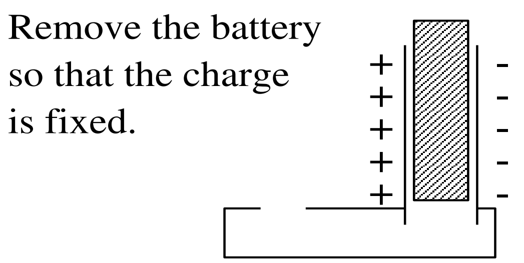
Another simple example using $\mathbf{D}$ with the same slab geometry is the parallel plate capacitor.



If we have two charged plates in a vacuum, then $\mathbf{P} = 0$ everywhere, and

$$\mathbf{D} = \mathbf{E} = \begin{cases} 0 & \text{outside} \\ -4\pi\sigma_{free} & \text{between the plates} \end{cases}$$

If we now slide a dielectric slab between the plates, then we expect it to obtain a uniform polarization, giving rise to surface charges.



However, $\mathbf{D}$ responds to only free charges, thus it is unchanged by the introduction of the dielectric slab. $\mathbf{E}$ responds to all charges, so it *is* changed. Since $\mathbf{E} = \mathbf{D} - 4\pi\mathbf{P}$, we see that $\mathbf{E}$ decreases in magnitude inside the dielectric, and since $\mathbf{D}$, $\mathbf{P}$, and $\mathbf{E}$ are parallel:

$$\frac{E_{\text{dielectric}}}{E_{\text{vacuum}}} = \frac{E_{\text{dielectric}}}{D} = \frac{E_{\text{dielectric}}}{E_{\text{dielectric}} + 4\pi P}$$

4.2.2 Summary and Discussion

At this point a summary of the dielectric equations will be useful.

$$\mathbf{P}(\mathbf{x}) = \text{ dipole moment per unit volume,}$$

$$\Phi(\mathbf{x}) = \int d^3x' \, \frac{\rho_{total}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$\rho_{total} = \rho_{free} - \nabla \cdot \mathbf{P}$$

$$\mathbf{E}(\mathbf{x}) = -\nabla\Phi(\mathbf{x}) \Longrightarrow \nabla \times \mathbf{E}(\mathbf{x}) = 0$$

$$\mathbf{D}(\mathbf{x}) = \mathbf{E}(\mathbf{x}) + 4\pi\mathbf{P}(\mathbf{x})$$

$$\nabla \cdot \mathbf{D} = 4\pi\rho_{free}$$

Several points must be made in relation to these. The first is that they do not form a sufficient set from which we can solve for $\mathbf{E}(\mathbf{x})$ as we have no way of writing $\mathbf{E}$ in terms of $\mathbf{D}$ or vice versa. The defining relation does not help as we don't know $\mathbf{P}$. What is needed is a *constitutive relation* which can be of the form $\mathbf{D} = \mathbf{D}(\mathbf{E})$ or $\mathbf{P} = \mathbf{P}(\mathbf{E})$. If there is no nonalalytic behavior entering this relation, then one can expand components of $\mathbf{P}$ as a power series in components of $\mathbf{E}$. If $\mathbf{E}$ is not too large, then only the linear term in these expansions need be kept,

$$P_i = \sum_{j=1}^{3} \chi_{ij} E_j. \tag{78}$$

where the nine numbers χ_{ij} are the components of the *electric susceptibility tensor*. When this is a good approximation, one says that the dielectric is *linear* .In disordered materials as well as highly ordered ones with a high degree of symmetry (cubic crystals, for example), this tensor reduces to a single non-zero number,

$$\chi_{ij} = \chi_e \delta_{ij}; \tag{79}$$

χ_e is called simply the electric susceptibiliity and such materials are said to be *isotropic*. Finally, if a material is uniform in its electrical properties, χ_e will be a constant, independent of position; then the material is said to be *homogeneous*. If all of these things are true, the dielectric material is as simple as it can be.

For a linear, isotropic, homogeneous dielectric, the connection between $\mathbf{E}$ and $\mathbf{D}$ is

$$\mathbf{D}(\mathbf{x}) = \mathbf{E}(\mathbf{x}) + 4\pi\chi_e\mathbf{E}(\mathbf{x}) \equiv \epsilon\mathbf{E}(\mathbf{x}) \tag{80}$$

where

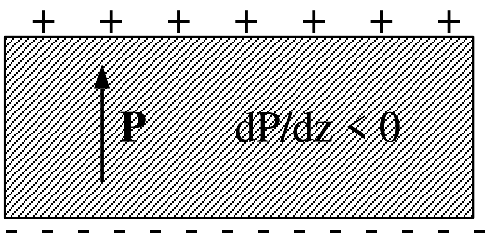
$$\epsilon = 1 + 4\pi\chi_e \tag{81}$$

is the *dielectric constant* of the material.

A second point is that the electric displacement is neither fish nor fowl, that is, neither field (force on a test charge) nor source. Look again at the integral expression for $\Phi(\mathbf{x})$; from it we see that the negative of the divergence of $\mathbf{P}(\mathbf{x})$ must be a (macroscopic) charge density; it is called the *polarization charge density*,

$$\rho_p(\mathbf{x}) = -\nabla \cdot \mathbf{P}(\mathbf{x}). \tag{82}$$

To see how this can be so, imagine a polarization which points in the z-direction and decreases in this direction so that its divergence is negative. Because of the variation of $\mathbf{P}(\mathbf{x})$, the molecules at smaller z are more polarized than those at slightly larger z, meaning that less positive charge "sticks out" on the larger-z side of the former than negative charge sticks out on the smaller-z side of the latter.



Hence there is a net positive charge density in the region between the two sets of molecules, and this is the polarization charge density. This argument leads one to believe that the total polarization charge must be zero. One can easily show by an application of the divergence theorem that it is indeed zero.

Having understood that the polarization leads to a charge density, how then may we understand the electric displacement? It is a linear combination of a macroscopic field (representing the force on a test charge) and of the polarization, whose divergence is a charge density. The polarization is itself source, being the dipole moment density of the constituent molecules of the material. Hence the displacement is neither field ($\mathbf{E}$) nor source ($\mathbf{P}$). Its usefulness lies in the fact that problems involving macroscopic electrostatics, and especially boundary value problems, are conveniently approached by making use of both the electric field and the electric displacement.

Another point that should be mentioned has to do with the higher multipole moments. We have seen how it is essential to keep the sources associated with the electric dipole moments of the molecules. What of the higher multipole moments? One may show that they contribute negligibly at the macroscopic level.

Finally, there is the question of solving for the macroscopic electric field. Given a medium such that Eq. (40) is valid, we may use $\mathbf{D} = \epsilon\mathbf{E}$ and have the field equations

$$\nabla \times \mathbf{E}(\mathbf{x}) = 0 \text{ and } \nabla \cdot \mathbf{E}(\mathbf{x}) = 4\pi(\rho(\mathbf{x})/\epsilon); \tag{83}$$

these are the same as we have been working with right along except that the charge density is rescaled by a factor of $1/\epsilon$; hence all of the lore that we have learned may be applied to solve for the macroscopic field.

5 Boundary-Value Problems in Dielectrics

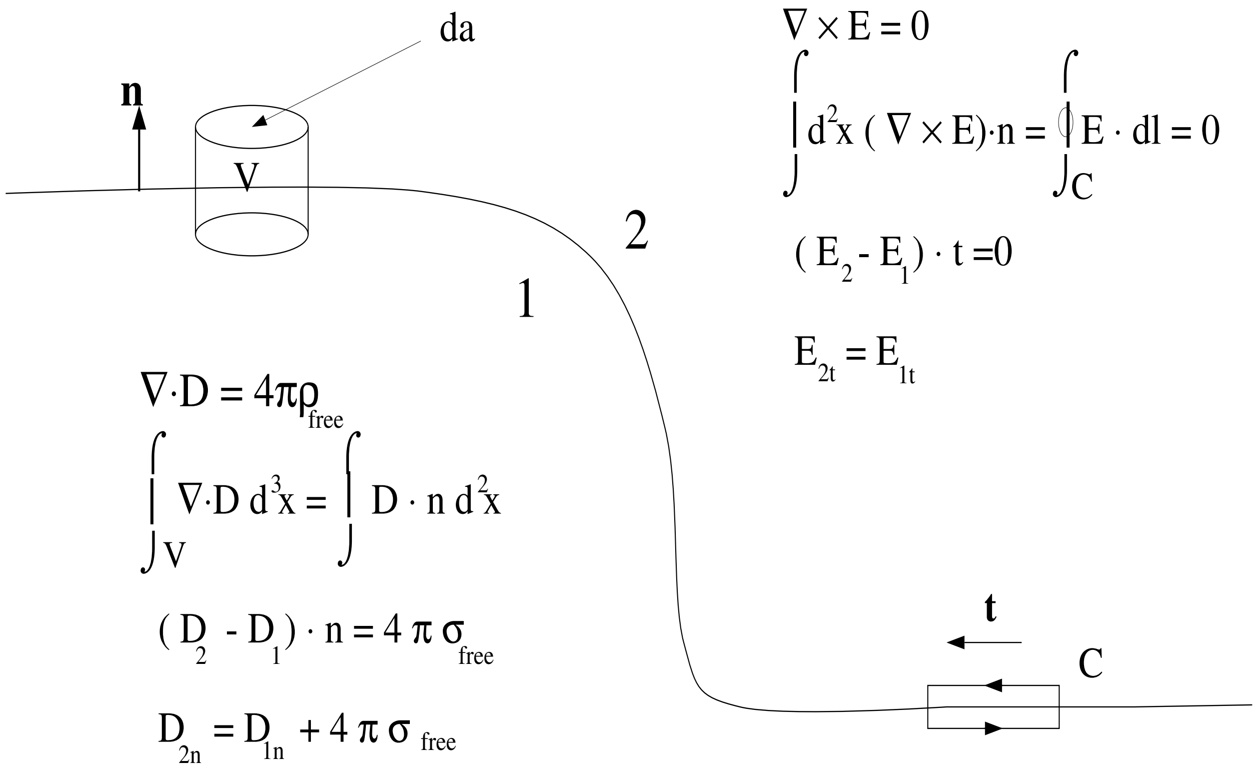
In this section we shall solve a few representative boundary-value problems involving dielectrics. Since $\nabla \times \mathbf{E} = 0$, $\mathbf{E} = -\nabla\Phi(\mathbf{x})$, $\mathbf{D} = \epsilon\mathbf{E}$, and $\nabla \cdot \mathbf{D} = 4\pi\rho$ in a dielectric, we may write

$$\nabla^2\Phi(\mathbf{x}) = 4\pi\rho/\epsilon\,.$$

Thus, all the methods we have learned (images, greens functions, series expansion etc.) will all work if properly modified.

There is of course the question of **boundary conditions**. At an interface between two materials (dielectric-vacuum, dielectric-dielectric, dielectric-conductor, etc.), we have a choice. We can either learn how to solve for the field in a system with non-homogeneous properties, or we can split the system up into pieces in each of which the material properties are uniform and then solve a boundary value problem. The latter course is the simpler if the interfaces may be treated as abrupt.

The appropriate boundary or continuity conditions may be found from the basic differential equations for **D** and**E**. Applying the divergence theorem and Stokes' theorem as we did once before, one can show that the appropriate boundary conditions are



$$[\mathbf{D}_2(\mathbf{x}) - \mathbf{D}_1(\mathbf{x})] \cdot \mathbf{n} = 4\pi\sigma \text{ and } [\mathbf{E}_2(\mathbf{x}) - \mathbf{E}_1(\mathbf{x})] \times \mathbf{n} = 0 \qquad (84)$$

which say that the discontinuity in the normal component of **D** is equal to 4π times the surface charge density (*not* including the surface charge density arising from the polarization) and that the tangential component of $\mathbf{E}$ is continuous. The unit normal in the equation for $\mathbf{D}$ points into medium 2 from medium 1.

5.1 Example: Point Charge Near a Boundary

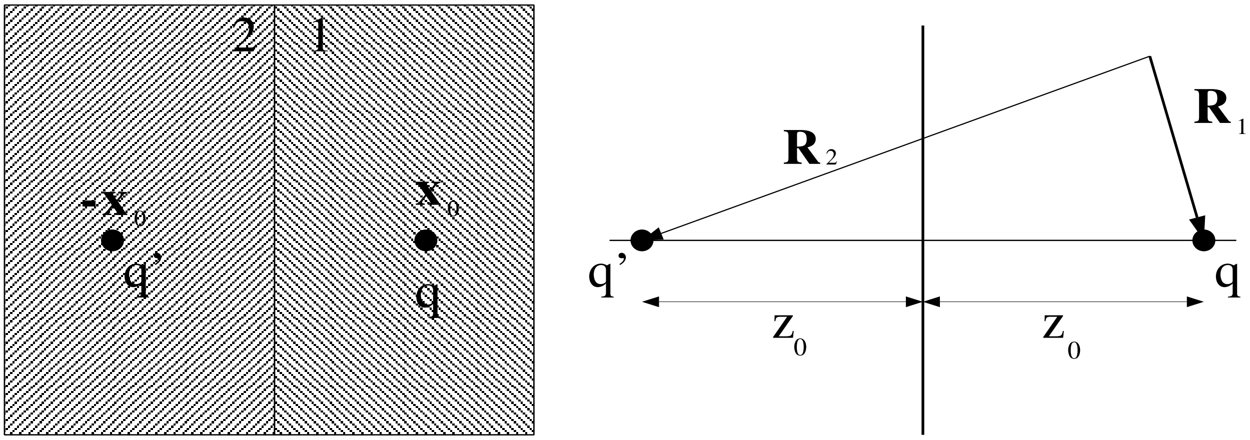
Consider that we have two dielectric materials; the first, with dielectric constant ϵ_1, occupies the half-space $z > 0$, and the second, with ϵ_2, occupies the half-space $z < 0$. Let there be a point charge q inside of the first dielectric at point $\mathbf{x}_0 = (0, 0, z_0)$.

Without a boundary, we can solve the problem easily. Since $\mathbf{D}$ is unchanged by the dielectric,

$$\mathbf{D} = -\nabla\left(\frac{q}{R}\right) = \epsilon\mathbf{E} \quad \text{thus } \mathbf{E} = -\frac{1}{\epsilon}\nabla\left(\frac{q}{R}\right) \quad \text{and } \Phi = \frac{q}{\epsilon R} \tag{85}$$

where R is the distance between the charge and where the electric displacement is evaluated

We will try to solve for the electric field using the method of images. For the region $z > 0$, following our earlier success with this approach, let us locate an image charge q' at the image position $\mathbf{x}_i = (0, 0, -z_0)$.



The potential produced by these two charges, embedded in a medium which **everywhere** has the properties of the first medium, is

$$\Phi_1(\mathbf{x}) = \frac{1}{\epsilon_1}\left(\frac{q}{R_1} + \frac{q'}{R_2}\right), \tag{86}$$

where R_1 and R_2 are, respectively, the distances of the field point from x_0 and x_i; this becomes our potential in the region $z > 0$ for the real system.

For the region $z < 0$, we imagine in the fictitious system that there is a charge q'' at the location of the real charge, embedded in a medium whose dielectric constant is everywhere ϵ_2. The potential of such a system is

$$\Phi_2(\mathbf{x}) = \frac{1}{\epsilon_2}\frac{q''}{R_1}. \tag{87}$$

This becomes our potential in the region $z < 0$.

Now we try to pick the image charges in such a way that the boundary conditions are satisfied. these conditions involve the following derivatives:

$$\frac{\partial}{\partial z}\left(\frac{1}{R_1}\right)\Big|_{z=0} = -\frac{\partial}{\partial z}\left(\frac{1}{R_2}\right)\Big|_{z=0} = \frac{z_0}{(\rho^2+z_0^2)^{3/2}} \tag{88}$$

and

$$\frac{\partial}{\partial \rho}\left(\frac{1}{R_1}\right)\Big|_{z=0} = \frac{\partial}{\partial \rho}\left(\frac{1}{R_2}\right)\Big|_{z=0} = -\frac{\rho}{(\rho^2+z_0^2)^{3/2}}. \tag{89}$$

Using these one finds that the condition of continuous normal component of $\mathbf{D}$ or, $D_{1z} = D_{2z}$ leads to (since $\sigma_{free} = 0$)

$$q - q' = q'' \tag{90}$$

and that the condition of continuous tangential component of $\mathbf{E}$ or $E_{1\rho} = E_{2\rho}$ leads to

$$\frac{1}{\epsilon_1}(q + q') = \frac{1}{\epsilon_2}q''. \tag{91}$$

The solution of these two linear equations is

$$\begin{aligned} q' &= \left(\frac{\epsilon_1-\epsilon_2}{\epsilon_1+\epsilon_2}\right) q \\ q'' &= \left(\frac{2\epsilon_2}{\epsilon_1+\epsilon_2}\right) q. \end{aligned} \tag{92}$$

Hence the potential on the right side, $z > 0$, is

$$\Phi_1(\rho, z) = \frac{q}{\sqrt{\rho^2+(z-z_0)^2}} + \frac{q(\epsilon_1-\epsilon_2)/(\epsilon_1+\epsilon_2)}{\sqrt{\rho^2+(z+z_0)^2}} \tag{93}$$

while that on the left, $z < 0$, is

$$\Phi_2(\mathbf{x}) = \frac{2q\epsilon_2/(\epsilon_1+\epsilon_2)}{\sqrt{\rho^2+(z-z_0)^2}}. \tag{94}$$

consequences The constitutive relations yield several interesting results for this problem. Since $\nabla \mathbf{D} = 4\pi\rho$, where ρ is the free charge density, it must be that

$$\nabla \cdot \mathbf{D} = 0 \quad \text{except at the real charge}$$

Then as $\mathbf{D} = \epsilon \mathbf{E}$,

$$\nabla \cdot \mathbf{E} = 0 \quad \text{except at the real charge}$$

Then since $\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}$, it must be that

$$\nabla \cdot \mathbf{P} = 0 \quad \text{except at the real charge}$$

Thus the polarization charge density is zero except at the real charge! (this is consistent with the potential for a point charge retaining $1/r$ behavior).

This line of reasoning breaks down at the surface between the two dielectrics, since there $\nabla\epsilon \neq 0$ corresponding to the polarization surface charge $\mathbf{P}\cdot\mathbf{n}$ discussed earlier. Thus

$$\sigma_p = (\mathbf{P}_2 - \mathbf{P}_1)\cdot\mathbf{n} \tag{95}$$

where $\mathbf{n}$ is the unit normal outward from medium 2 into medium 1. If we apply this to our present example, we first need to find the polarizations. These are given by, for $i = 1, 2$,

$$\mathbf{P}_i = \chi_i \mathbf{E}_i = \frac{\epsilon_i - 1}{4\pi}\mathbf{E}_i. \tag{96}$$

and so

$$\sigma_p = \frac{\epsilon_2 - 1}{4\pi}\mathbf{E}_{2z} - \frac{\epsilon_1 - 1}{4\pi}\mathbf{E}_{1z}, \tag{97}$$

evaluated at $z = 0$. Here,

$$\mathbf{E}_{1z} = -\frac{1}{\epsilon_1}\frac{(q - q')z_0}{(\rho^2 + z_0^2)^{3/2}} \tag{98}$$

and

$$\mathbf{E}_{2z} = -\frac{1}{\epsilon_2}\frac{q'' d_0}{(\rho^2 + z_0^2)^{3/2}}. \tag{99}$$

The polarization surface-charge density is then

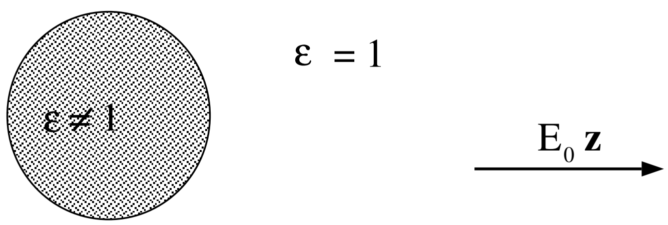
$$\begin{aligned}\sigma_p = -P_{1z} + P_{2z} &= \frac{z_0}{(\rho^2 + z_0^2)^{3/2}4\pi}\left\{\frac{\epsilon_1 - 1}{\epsilon 12}(-q + q') - \frac{\epsilon_2 - 1}{\epsilon_2}q''\right\} \\ &= \frac{q z_0}{4\pi(\rho^2 + z_0^2)^{3/2}}\left\{\frac{\epsilon_1 - 1}{\epsilon_1}\frac{2\epsilon_2}{\epsilon_1 + \epsilon_2} - \frac{\epsilon_2 - 1}{\epsilon_1}\frac{2\epsilon_1}{\epsilon_1 + \epsilon_2}\right\} \\ &= \frac{q z_0(\epsilon_1 - \epsilon_2)}{2\pi\epsilon_1(\epsilon_1 + \epsilon_2)(\rho^2 + z_0^2)^{3/2}}.\end{aligned} \tag{100}$$

An important limiting case is given by $\epsilon_1 = 1$ and $\epsilon_2 \to \infty$, in which case the material at $z < 0$ cannot support an electric field and behaves like a conductor. Then our system reduces to a point charge outside of a conductor, for which we already know that the answer is

$$\sigma_p = -\frac{qz_0}{2\pi(\rho^2 + z_0^2)^{3/2}}. \tag{101}$$

5.2 Example: Dielectric Sphere in a Uniform Field

Our second example is a dielectric sphere placed in a uniform externally applied field.



Rather than use the image charge method, this time we shall make use of an orthogonal function expansion. Because $\nabla \times \mathbf{E}(\mathbf{x}) = 0$ everywhere, we can write the electric field as the gradient of a scalar potential. Further, for a uniform medium $\mathbf{D}(\mathbf{x}) = \epsilon \mathbf{E}(\mathbf{x})$ with constant ϵ, so, from $\nabla \cdot \mathbf{D}(\mathbf{x}) = 4\pi\rho(\mathbf{x})$, we know that $\nabla \cdot \mathbf{E}(\mathbf{x}) = 0$ where there is no macroscopic charge density $\rho(\mathbf{x})$. Given that the radius of the sphere is a, we have such conditions for $r < a$ and for $r > a$. Hence the scalar potential satisfies the Laplace equation in these two regimes, and we can expand it in the usual way in spherical coordinates. The symmetries in the problem imply that the solution is independent of ϕ, so we need to use a Legendre polynomial expansion. Thus, for $r < a$, we have

$$\Phi_<(r,\theta) = E_0 a \sum_{l=0}^{\infty} A_l \left(\frac{r}{a}\right)^l P_l(\cos\theta) \tag{102}$$

and, for $r > a$,

$$\Phi_>(r,\theta) = -E_0 r\cos\theta + E_0 a \sum_{l=0}^{\infty} B_l \left(\frac{a}{r}\right)^{l+1} P_l(\cos\theta). \tag{103}$$

The first term in the second of these expansions is the potential associated with the applied field; the others come from the sources induced on the dielectric sphere (polarization charge). The boundary conditions that must be applied are (i) tangential E and (ii) normal D continuous; these are

$$\left.\frac{\partial\Phi_<}{\partial\theta}\right|_{r=a} = \left.\frac{\partial\Phi_>}{\partial\theta}\right|_{r=a} \tag{104}$$

and

$$\epsilon\left.\frac{\partial\Phi_<}{\partial r}\right|_{r=a} = \left.\frac{\partial\phi_>}{\partial r}\right|_{r=a}, \tag{105}$$

where ϵ is the dielectric constant of the sphere. By proceeding with the solution in the by now familiar way for orthogonal function expansions, one finds that all A_l and B_l are zero except for $l = 1$. For $l = 1$ the conditions are

$$A_1 = -1 + B_1 \text{ and } \epsilon A_1 = -1 - 2B_1. \tag{106}$$

These are easily solved to yield

$$A_1 = -3/(2+\epsilon) \text{ and } B_1 = (\epsilon-1)/(\epsilon+2). \tag{107}$$

Hence, the potential is

$$\Phi_<(r,\theta) = -\frac{3}{\epsilon+2}E_0 r\cos\theta \tag{108}$$

and

$$\Phi_>(r,\theta) = -E_0 r\cos\theta + E_0 a\left(\frac{\epsilon-1}{\epsilon+2}\right)\left(\frac{a}{r}\right)^2\cos\theta. \tag{109}$$

Notice that if $\epsilon\to\infty$, we recover the result for the conducting sphere.

From this result, and since $\Phi(\mathbf{x})_{dipole} = \mathbf{p}\cdot\mathbf{x}/r^3$, we can see that the sphere has a dipole moment which is

$$\mathbf{p} = E_0 a^3\left(\frac{\epsilon-1}{\epsilon+2}\right)\hat{\mathbf{z}}. \tag{110}$$

The electric field inside of the sphere is a constant, and so is $\mathbf{D}$,

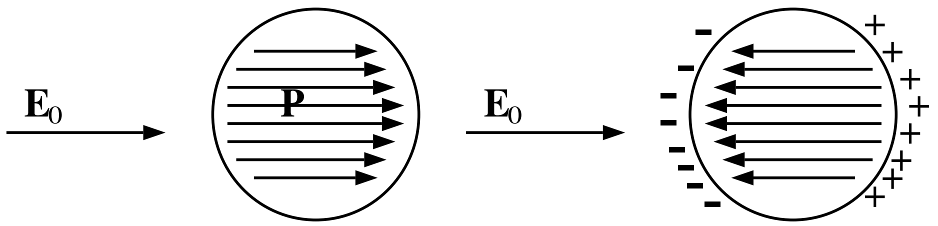
$$\mathbf{D} = \epsilon\mathbf{E} = \epsilon\left(\frac{3}{\epsilon+2}\right)E_0\hat{\mathbf{z}} \equiv \mathbf{E} + 4\pi\mathbf{P}, \tag{111}$$

so

$$4\pi\mathbf{P} = \mathbf{D} - \mathbf{E} = 3\left(\frac{\epsilon-1}{\epsilon+2}\right)E_0\hat{\mathbf{z}}, \tag{112}$$

or

$$\mathbf{P} = \frac{3}{4\pi}\left(\frac{\epsilon-1}{\epsilon+2}\right)E_0\hat{\mathbf{z}}. \tag{113}$$



Dielectric sphere in a uniform field, showing the polarization on the left and the polarization charge with its associated, apposing, electric field on the right.

Although there is no macroscopic charge density anywhere in the system, there is polarization charge density. There is no volume polarization charge density because $\mathbf{P}$ has zero divergence. However, there is a surface charge density; it is given by

$$\sigma_p = \mathbf{P} \cdot \hat{\mathbf{r}} = P_r = \frac{3}{4\pi} E_0 \left(\frac{\epsilon - 1}{\epsilon + 2} \right) \cos\theta. \tag{114}$$

As an application of the polariazble sphere problem, consider a water drop in air. For this system, roughly

$$\epsilon_{rmair} \approx 1 \quad \epsilon_{rmwater} \approx 81\,. \tag{115}$$

Water is a dielectric composed of permanent dipoles. The polarizability α ($\mathbf{p} = \alpha\mathbf{E}$) of the water drop is then

$$\alpha_{H_2O} = \frac{81 - 1}{81 + 2} a^3 \approx a^3 \tag{116}$$

Water drops look like metallic spheres to a static E-field.

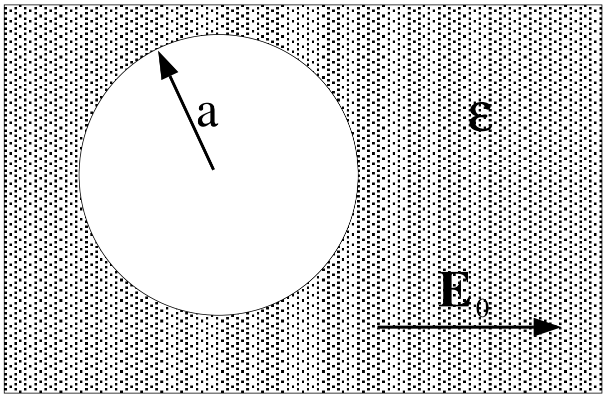
5.2.1 The Inverse Problem

The inverse problem of a dielectric with a spherical cavity is easy to solve because one has only to change ϵ into $1/\epsilon$ in the results found here. The reason is that the relative dielectric constant of the cavity to that of the surrounding medium is $1/\epsilon$. In this way we find

$$\Phi_<(r, \theta) = -\frac{3\epsilon}{2\epsilon + 1} r E_0 \cos\theta \tag{117}$$

and

$$\Phi_>(r,\theta) = -E_0 r\cos\theta - E_0 a\frac{\epsilon-1}{2\epsilon+1}\left(\frac{a}{r}\right)^2\cos\theta. \tag{118}$$



5.3 Clausius-Mossotti equation

In writing α above note that the electric field in

$$\mathbf{p} = \alpha\mathbf{E}$$

is the external field *not including the field of the induced dipole itself.* However, in

$$\mathbf{P} = \chi_e\mathbf{E}$$

the field $\mathbf{E}$ *does* include the the field due to the dipoles in $\mathbf{P}$. If we can relate these two, we can calculate the relation between α (a microscopic quantity), and the macroscopic quantities χ_e and ϵ. If we define two different $\mathbf{E}$s

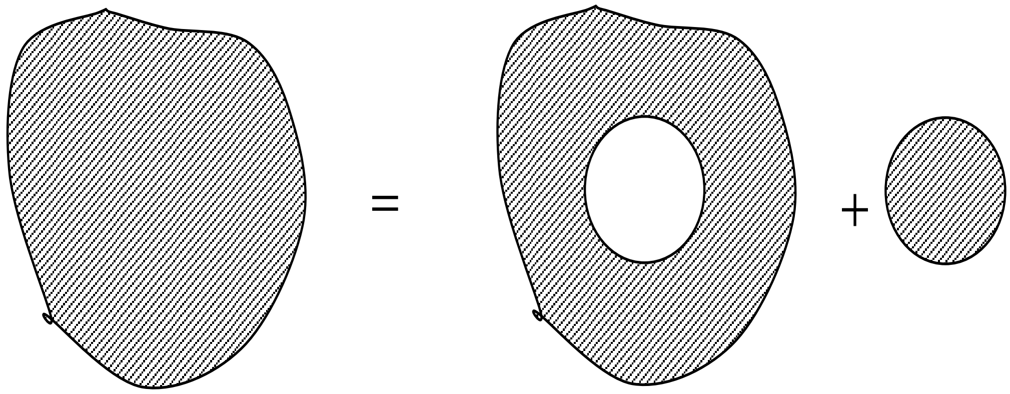
$$\mathbf{p} = \alpha\mathbf{E}_{loc} = \alpha(\text{electric field at the site of the molecule})$$

$$\mathbf{P} = \chi_e\mathbf{E}_{med} = \chi_e(\text{electric field in the medium})$$

If n is the number of molecules per unit volume, then $\mathbf{P} = n\mathbf{p}$ and

$$\mathbf{P} = n\alpha\mathbf{E}_{loc}.$$

With these equations we can find a relation between α and χ_e if we can relate $\mathbf{E}_{loc}$ and $\mathbf{E}_{med}$. We note that $\mathbf{E}_{loc}$ is the field at the site of a molecule if the molecule is removed. To calculate this, we will consider a spherical cavity in a dielectric medium. If the cavity were filled with dielectric, then the field at the center would be $\mathbf{E}_{med}$, so



$$\mathbf{E}_{med} = \mathbf{E}_{loc} + \mathbf{E}_{sphere}$$

where $\mathbf{E}_{sphere}$ is the field at the center of a uniformly polarized dielectric sphere due *only* to the polarization. From Eq. (111) it is clear that the field inside the sphere (due to *both* the polarization and the external field) is

$$\mathbf{E}_{inside\ sphere} = \frac{3}{2+\epsilon}\mathbf{E}_0 = \mathbf{E}_0 + \frac{1-\epsilon}{2+\epsilon}\mathbf{E}_0$$

Thus that due only to the polarization is

$$\mathbf{E}_{sphere} = \frac{1-\epsilon}{2+\epsilon}\mathbf{E}_0$$

Comparing this to Eq. (113) we see that

$$\mathbf{E}_{sphere} = -\frac{4\pi}{3}\mathbf{P}$$

Thus

$$\mathbf{E}_{loc} = \mathbf{E}_{med} - \mathbf{E}_{sphere} = \mathbf{E}_{med} + \frac{4\pi}{3}\mathbf{P}.$$

Now, if we multiply by $n\alpha$ and solve for $\mathbf{P}$, we get

$$\mathbf{P} = \frac{n\alpha}{1 - \frac{4\pi}{3}n\alpha}\mathbf{E}_{med}$$

Then since $\mathbf{P} = \chi_e \mathbf{E}_{med}$ and $\epsilon = 1 + 4\pi\chi_e$ we get

$$\frac{4\pi}{3}n\alpha = \frac{\epsilon - 1}{\epsilon + 2} \quad \text{Clasius} - \text{Mossotti Equation} \tag{119}$$

6 Electrostatic Energy in Dielectrics

In free space we derived the energy of a distribution of charge $\rho(\mathbf{x})$ by assembling the distribution little by little, bringing infinitesimal pieces of charge in from infinity. Following this reasoning we found that

$$W = \frac{1}{2}\int d^3x\, \rho(\mathbf{x})\Phi(\mathbf{x})$$

This is in general *not* true in the presence of dielectrics (however, as we will see, it may be true in some cases). In the presence of dielectrics work must also be done to induce polarization in the dielectric, and it is not clear if this work is included in the equation above.

When dielectrics are present we shall use a somewhat different argument (which still corresponds to the same procedure). Suppose that there is initially some macroscopic charge density $\rho(\mathbf{x})$, potential $\Phi(\mathbf{x})$, and fields $\mathbf{E}(\mathbf{x})$ and $\mathbf{D}(\mathbf{x})$. The imagine that some infinitesimal change in the charge density, $\delta\rho(\mathbf{x})$, is made. To first order in $\delta\rho$, the change in energy of the system is

$$\delta W = \int_V d^3x\, \Phi(\mathbf{x})\delta\rho(\mathbf{x}) \tag{120}$$

where the integration is done over that region of space where the integrand is non-zero. The point is that this is the interaction energy of $\delta\rho(\mathbf{x})$ with the sources already present (and which produce $\Phi(\mathbf{x})$); the interaction energy of $\delta\rho$ with itself is second-order in small (infinitesimal) quantities. (this form is consistent with the fact that W is a natural thermodynamic function of the charges, not the potential).

The change in $\mathbf{D}$ which arises as a consequence of the change $\delta\rho$ in the charge density is related to the latter by the equation $\nabla\cdot(\mathbf{D}+\delta\mathbf{D}) = 4\pi(\rho+\delta\rho)$, or

$$\nabla\cdot(\delta\mathbf{D}(\mathbf{x})) = 4\pi\delta\rho(\mathbf{x}), \tag{121}$$

so we may write the change in the energy as

$$\delta W = \int_V d^3x\, \Phi(\mathbf{x})\frac{1}{4\pi}(\nabla\cdot\delta\mathbf{D}(\mathbf{x})). \tag{122}$$

We next do an integration by parts in the by now familiar way.

$$\begin{aligned}\delta W &= \frac{1}{4\pi}\int_V d^3x\, \nabla\cdot(\Phi(\mathbf{x})\delta\mathbf{D}(\mathbf{x})) - \frac{1}{4\pi}\int_V d^3x\, \nabla\Phi(\mathbf{x})\cdot\delta\mathbf{D}(\mathbf{x}) \\ &= \frac{1}{4\pi}\int_S d^2x\, \Phi(\mathbf{x})\delta\mathbf{D}(\mathbf{x})\cdot\mathbf{n} + \frac{1}{4\pi}\int_V d^3x\, \mathbf{E}(\mathbf{x})\cdot\delta\mathbf{D}(\mathbf{x}).\end{aligned} \tag{123}$$

The surface integral is zero for a localized charge distribution if V includes all space. Thus we have simply

$$\delta W = \frac{1}{4\pi}\int d^3x\, \mathbf{E}(\mathbf{x}) \cdot \delta\mathbf{D}(\mathbf{x}). \tag{124}$$

Now we must introduce some statement about the properties of the medium. If it is **linear** ($\mathbf{D} = \epsilon\mathbf{E}$), then

$$\mathbf{E} \cdot \delta\mathbf{D} = \mathbf{E} \cdot (\epsilon\delta\mathbf{E}) = \frac{1}{2}\epsilon\delta(\mathbf{E} \cdot \mathbf{E}) = \frac{1}{2}\delta(\mathbf{E} \cdot \mathbf{D})$$

so that

$$[\mathbf{E}(\mathbf{x}) \cdot \delta\mathbf{D}(\mathbf{x})] = \frac{1}{2}\delta[\mathbf{E}(\mathbf{x}) \cdot \mathbf{D}(\mathbf{x})]. \tag{125}$$

and so

$$\delta W = \frac{1}{8\pi}\int d^3x\, \delta[\mathbf{E}(\mathbf{x}) \cdot \mathbf{D}(\mathbf{x})]. \tag{126}$$

If we now integrate from zero field up to the final fields (a *functional integration*),

$$W = \frac{1}{8\pi}\int d^3x \int_0^{\mathbf{D}} \delta[\mathbf{E}(\mathbf{x}) \cdot \mathbf{D}(\mathbf{x})]$$

we find

$$W = \frac{1}{8\pi}\int d^3x\, \mathbf{E}(\mathbf{x}) \cdot \mathbf{D}(\mathbf{x}). \tag{127}$$

This result is valid **only** for linear media.

There are several amusing consequences obtainable from this relation. First, by writing $\mathbf{E}(\mathbf{x}) = -\nabla\Phi(\mathbf{x})$ and integrating by parts, we obtain

$$W = \frac{-1}{8\pi}\int d^3x\, \nabla \cdot (\Phi(\mathbf{x})\mathbf{D}(\mathbf{x})) + \frac{1}{8\pi}\int d^3x\, \Phi(\mathbf{x})\nabla \cdot \mathbf{D}(\mathbf{x})$$

Through the divergence theorem, the first term yields a surface term which vanishes at infinity. The second term becomes

$$W = \frac{1}{2}\int d^3x\, \rho(\mathbf{x})\Phi(\mathbf{x}); \tag{128}$$

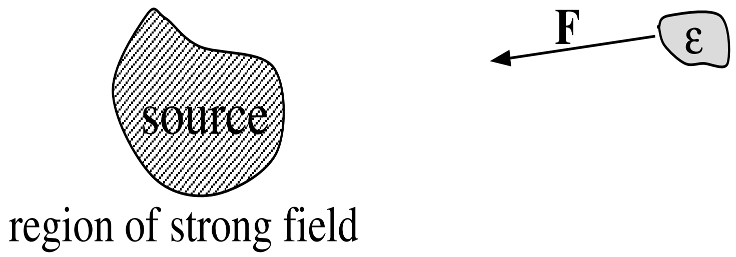
Thus for a **linear** dielectric, the original formula is valid.

6.1 Force on a Dielectric

From the above, it is clear that W, as written, is a function of the free charges, their positions, and of the positions of the dielectrics through $\epsilon(\mathbf{x})$ (which may vary from point to point). Thus we may write

$$W(\mathbf{x}, \rho) = \frac{1}{8\pi}\int d^3x\, \frac{|\mathbf{D}(\mathbf{x})|^2}{\epsilon(\mathbf{x})} \quad \text{linear only} \tag{129}$$

From this, it is clear that if the free charges (which produce $\mathbf{D}$) are fixed, and we move one of the dielectrics, then the energy is *reduced* if the change makes ϵ increase in the region where $\mathbf{D}(\mathbf{x})$ is finite. In particular, *the energy is reduced by having a dielectric move from a region of low field to one of high field. Thus the force on such a linear dielectric must always be such as to draw it into a region of greater fields.*



If the free charges are held fixed, then since W depends on the positions and magnitude of the charges and dielectrics, it follows that the force on a dielectric is

$$F_\eta = -\left(\frac{\partial W}{\partial \eta}\right)_Q \tag{130}$$

where F_η is the η-component of the force on the dielectric. This is because the most stable state of the system is that with the minimum W.

In this calculation, it is important that the energy was a natural function of the charges and positions of the charges and dielectrics. Then we could evaluate the total differential

$$dW = \left(\frac{\partial W}{\partial \eta}\right)_Q d\eta + \left(\frac{\partial W}{\partial Q}\right)_\eta dQ$$

to obtain the force. This is analogous to the situation in elementary thermodynamics where the energy U is a natural function of the volume and temperature $U(V, T)$. If we wanted to obtain a potential which was a function of the entropy S and V (suppose for example S is change in such a way as to keep T fixed, i.e. a system in a heat bath), then we made a Legendre transformation $F = U - TS$, and the most stable state of the system is that with the minimum F (For an elegant discussion of elementary thermodynamics see *Thermodynamics* by Enrico Fermi, about 77pp.)

Thus, since W is a natural function of the positions and charges, it is not appropriate for the case where the potentials are held fixed. We need the potential which is a natural function of the positions and potentials. As in the paragraph above, the way to remedy this is a Legendre transformation to a new function W', defined by

$$W' = W - \frac{1}{4\pi}\int d^3x\, \mathbf{E}(\mathbf{x}) \cdot \mathbf{D}(\mathbf{x}) \tag{131}$$

This is a general expression (not just for the linear case) where $\mathbf{E} = -\nabla\Phi(\mathbf{x})$ is a natural function of the potentials, and $\mathbf{D}$ is a function of the charges (since $\nabla \cdot \mathbf{D} = 4\pi\rho$). A differential change in W' is given by

$$\delta W' = \delta W - \frac{1}{4\pi}\int d^3x\, \mathbf{E}(\mathbf{x}) \cdot \delta\mathbf{D}(\mathbf{x}) - \frac{1}{4\pi}\int d^3x\, \mathbf{D}(\mathbf{x}) \cdot \delta\mathbf{E}(\mathbf{x}). \tag{132}$$

Then, since

$$\delta W = \frac{1}{4\pi}\int d^3x\, \mathbf{E}(\mathbf{x}) \cdot \delta\mathbf{D}(\mathbf{x})$$

$$\delta W' = -\frac{1}{4\pi}\int d^3x\, \mathbf{D}(\mathbf{x}) \cdot \delta\mathbf{E}(\mathbf{x}) \tag{133}$$

Then since $\mathbf{E}(\mathbf{x})$ is a natural function of the potential, W' is a natural function of potentials and positions, as desired.

Thus the force on a dielectric in the presence of fixed potentials (i.e. conductors connected to a battery) is

$$F_\eta = -\left(\frac{\partial W'}{\partial \eta}\right)_\Phi \tag{134}$$

In the linear case, we can evaluate this in terms of W, since

$$W' = W - \frac{1}{4\pi}\int d^3x\, \mathbf{E}(\mathbf{x})\cdot\mathbf{D}(\mathbf{x}) = -\frac{1}{8\pi}\int d^3x\, \mathbf{E}(\mathbf{x})\cdot\mathbf{D}(\mathbf{x}) = -W \tag{135}$$

Thus in **the linear case only**,

$$F_\eta = +\left(\frac{\partial W}{\partial \eta}\right)_\Phi \tag{136}$$

6.2 Forces on a Dielectric Revisited

These force formulae may also be derived in a more pedestrian manner.

We can derive one for the change in a system's energy when a piece of dielectric is moved from one place to another under conditions of constant macroscopic charge density. Consider that initially the macroscopic fields, charge density, potential, and polarization are $\mathbf{E}_0$, W_0, $\mathbf{D}_0$, ρ_0, Φ_0, and $\mathbf{P}_0$. Let the final ones have subscript 1 instead of 0. Then

$$W_1 = \frac{1}{8\pi}\int d^3x\, \mathbf{E}_1(\mathbf{x})\cdot\mathbf{D}_1(\mathbf{x}) \text{ and } W_0 = \frac{1}{8\pi}\int d^3x\, \mathbf{E}_0(\mathbf{x})\cdot\mathbf{D}_0(\mathbf{x}), \tag{137}$$

so

$$\Delta W \equiv W_1 - W_0 = \frac{1}{8\pi}\int d^3x\, [\mathbf{E}_1\cdot\mathbf{D}_1 - \mathbf{E}_0\cdot\mathbf{D}_0]. \tag{138}$$

By adding and subtracting identical terms, we can turn this expression into

$$\Delta W = \frac{1}{8\pi}\int d^3x\, [\mathbf{E}_0+\mathbf{E}_1]\cdot[\mathbf{D}_1-\mathbf{D}_0] + \frac{1}{8\pi}\int d^3x\, [\mathbf{E}_1\cdot\mathbf{D}_0-\mathbf{E}_0\cdot\mathbf{D}_1]. \tag{139}$$

By doing an integration by parts (in the usual way), one can show that the first term is zero if $\rho_1 = \rho_0$, so we have

$$\Delta W = \frac{1}{8\pi} \int d^3x\,[\mathbf{E}_1 \cdot \mathbf{D}_0 - \mathbf{E}_0 \cdot \mathbf{D}_1]. \tag{140}$$

As an example of the use of this formula, imagine that a dielectric having $\epsilon = \epsilon_1$ is moved in from infinity to occupy some domain V where formerly there was empty space. Everywhere else there is vacuum. Then $\mathbf{D}_1 = \epsilon_1 \mathbf{E}_1$ in V, and $\mathbf{D}_1 = \mathbf{E}_1$ elsewhere. Also, $\mathbf{E}_0 = \mathbf{D}_0$ everywhere. Our formula for the change in energy gives

$$\Delta W = -\frac{1}{8\pi} \int_V d^3x (\epsilon_1 - 1) \mathbf{E}_1 \cdot \mathbf{E}_0 = -\frac{1}{2} \int d^3x\, \mathbf{P}_1 \cdot \mathbf{E}_0. \tag{141}$$

This is the energy of the dielectric object placed in an external field $\mathbf{E}_0$. The factor of 1/2 distinguishes it from the energy of a permanent dipole placed in an external field which we derived earlier. It has to do with the fact that in the present case the field has to do work to polarize the dielectric in the first place.

We may also devise a formula for the force on a piece of dielectric. In the case that the (macroscopic) charge is fixed, no work is done moving any charge and so we have a conservative system in the sense that the change in the field energy must be equal to the work that an external agent does on the dielectric when the latter is moved. This force (recall our earlier arguments of this kind) is equal and opposite to the electric field force on the dielectric so we wind up concluding that

$$F_\eta = -\left(\frac{\partial W}{\partial \eta}\right)_Q \tag{142}$$

where the "Q" means that the derivative with respect to displacement in the η direction is taken at constant sources (constant $\rho(\mathbf{x})$). The result is the force in the direction of η, and this is the usual expression for a conservative system.

A more difficult case is one in which there is an external source of energy. A very common case of this kind which frequently arises in electrostatics involves a set of conducting objects or surfaces on which the macroscopic charge ρ resides, and keeping these surfaces at fixed potentials when the dielectric is moved. The latter is easily achieved by connecting the conductors to fixed voltage sources (batteries). To see what happens, imagine making a small displacement of the dielectric in two steps. First, move it by $d\eta$ while maintaining $\rho(\mathbf{x})$ fixed. Then restore $\Phi(\mathbf{x})$ to its original value at those points where there is non-zero macroscopic charge density by adjusting this charge density as necessary. We can calculate the change in field energy during either of these steps by applying the general formula for a linear system

$$W = \frac{1}{2}\int d^3x\, \rho(\mathbf{x})\Phi(\mathbf{x}), \tag{143}$$

which gives, for small changes in ρ and Φ,

$$\delta W = \frac{1}{2}\int d^3x\, [\delta\rho(\mathbf{x})\Phi(\mathbf{x}) + \rho(\mathbf{x})\delta\Phi(\mathbf{x})]. \tag{144}$$

In the first step described above, there is no change in ρ, so

$$\delta W_1 = \frac{1}{2}\int d^3x\, \rho(\mathbf{x})\delta\Phi_1(\mathbf{x}). \tag{145}$$

This is the same as δW_Q since charges are fixed in this step:

$$\delta W_1 = \delta W_Q. \tag{146}$$

In step 2, $\rho(\mathbf{x})$ is adjusted so that $\Phi(\mathbf{x})$ returns to its initial value everywhere where the charge density does not vanish. In this step

$$\delta W_2 = \frac{1}{2}\int d^3x\,\rho(\mathbf{x})\delta\Phi_2(\mathbf{x}) + \frac{1}{2}\int d^3x\,\delta\rho(\mathbf{x})\Phi(\mathbf{x}). \tag{147}$$

However, at points where $\rho(\mathbf{x})$ in non-zero, $\delta\Phi_2(\mathbf{x}) = -\delta\Phi_1(\mathbf{x})$ because in the second step we restore the potential to its original value at these points. Hence we can rewrite δW_2 as

$$\delta W_2 = -\frac{1}{2}\int d^3x\,\rho(\mathbf{x})\delta\Phi_1(\mathbf{x}) + \frac{1}{2}\int d^3x\,\delta\rho(\mathbf{x})\Phi(\mathbf{x}). \tag{148}$$

There is a second way to see what δW_2 is; in this step we make an infinitesimal change in the charge density, $\delta\rho(\mathbf{x})$, and the change in energy accompanying this adjustment is, to first order in infinitesimals,

$$\delta W_2 = \int d^3x\,\Phi(\mathbf{x})\delta\rho(\mathbf{x}). \tag{149}$$

By comparing the two equations we have for δW_2, we learn that

$$\frac{1}{2}\int d^3x\,\Phi(\mathbf{x})\delta\rho(\mathbf{x}) = -\frac{1}{2}\int d^3x\,\rho(\mathbf{x})\delta\Phi_1(\mathbf{x}). \tag{150}$$

Using this relation in Eq. (113), we find that

$$\delta W_2 = -\int d^3x\,\rho(\mathbf{x})\delta\Phi_1(\mathbf{x}) \tag{151}$$

and this is the same as $-2\delta W_1$. Consequently we can say that the total change in energy, which we shall call δW_V (the "V" signifies constant potentials at points where $\delta\rho(\mathbf{x})$ is non-zero), is

$$\delta W_V = \delta W_1 + \delta W_2 = -\delta W_1 = -\delta W_Q. \tag{152}$$

Consequently,

$$F_\eta = -\left(\frac{\partial W}{\partial \eta}\right)_Q = +\left(\frac{\partial W}{\partial \eta}\right)_V. \tag{153}$$

In other words, if we can calculate the energy as a function of η, the position of the dielectric, at constant potentials where $\rho(\mathbf{x}) \neq 0$, we can find the force on the dielectric by taking the **positive** derivative of this energy with respect to the dielectric's position.

7 Example: Dielectrophoresis

A spherical dielectric particle of radius a and $\epsilon = \epsilon_1$ is placed in a dielectric fluid ($\epsilon_2 \neq \epsilon_1$) contained within an annulus with conducting walls.

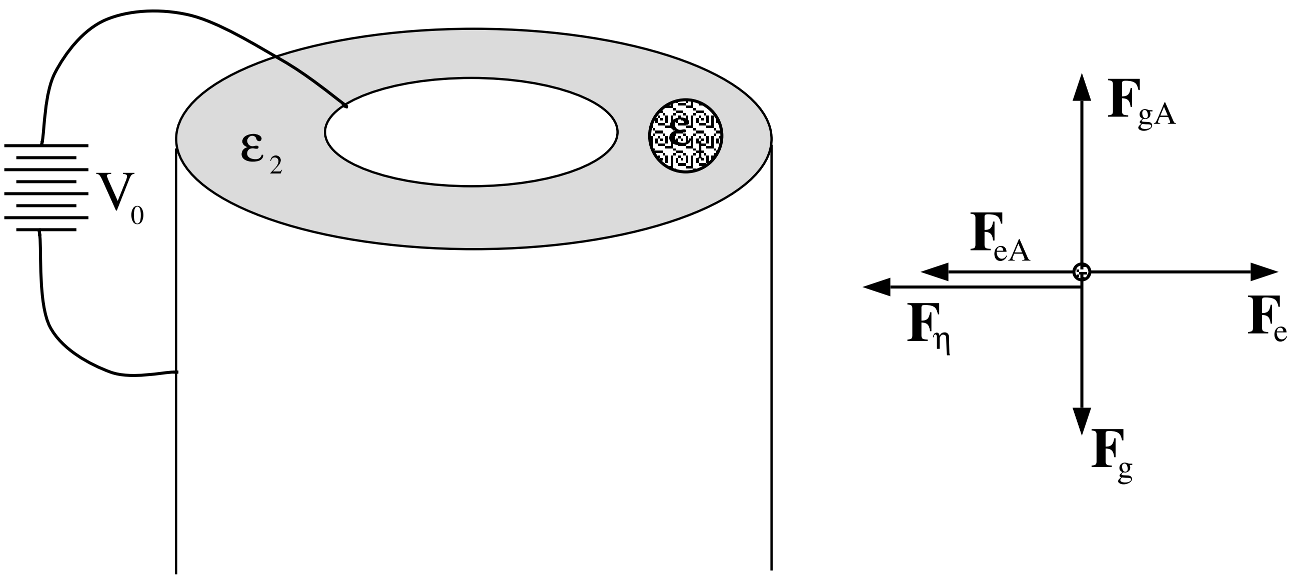


Fig.1. Dielectric fluid and particle between two conducting cylinders

The annulus is maintained at a relative potential V_0. Assuming that $a \ll$ any other dimension in the problem, and that the densities of the particle and fluid are the same:

- Show that the **net** force on the particle is

$$\mathbf{F}_{net} = -\frac{1}{3}a^3 A V_0^2 r^{-3}\left[\ln\left(R_{out}/R_{in}\right)\right]^{-2}\hat{\mathbf{r}}\,,$$

  where

$$A = \frac{\epsilon_2(4\epsilon_2+5)-\epsilon_1(\epsilon_2-1)}{(2\epsilon_2+\epsilon_1)^2}(\epsilon_1-\epsilon_2)\,.$$

- Discuss how $\mathbf{F}_{net}$ depends upon (1) ϵ_2 relative to ϵ_1 and (2) ϵ_1 for fixed ϵ_2.

- The drift velocity $\mathbf{v}$ of the particle is given by

$$\mathbf{F}_{net} = 6\pi\eta a\mathbf{v}\,,$$

(1) Discuss the dependence of $\mathbf{v}$ on a and ϵ_1 for fixed ϵ_2, and (2) Suggest possible uses for this setup (dielectrophoresis).

Solution. To solve this we must first find the field between the cylinders in the absence of the particle. To accomplish this, we use Gauss' law, the constitutive relations, and the fact that $\mathbf{D}$ and $\mathbf{E}$ are purely radial.

$$\nabla \cdot \mathbf{D} = 4\pi\rho \;\; ; \;\; \mathbf{D} = \epsilon_2 \mathbf{E}$$

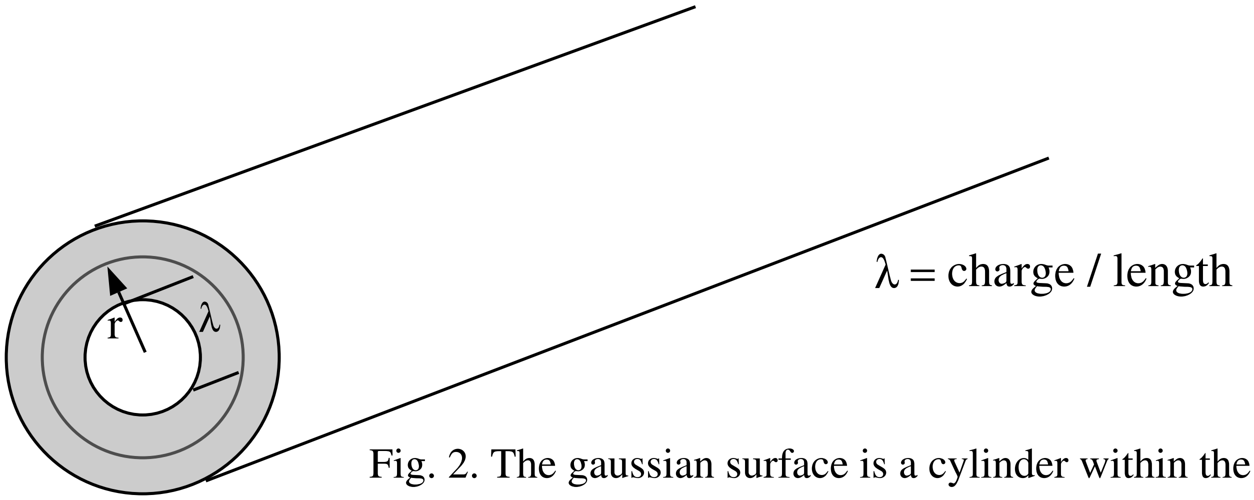


Fig. 2. The gaussian surface is a cylinder within the annulus

$$l 2\pi r \epsilon_2 E_r = 4\pi\lambda l \;\; ; \;\; E_r = \frac{2\lambda}{\epsilon_2 r}$$

$$V_0 = \int_{R_{in}}^{R_{out}} dr \frac{\partial \Phi}{\partial r} = -\frac{2\lambda}{\epsilon_2} \ln\left(R_{out}/R_{in}\right)$$

When we solve for $\lambda(V_0)$, we find that

$$\mathbf{E}_{cyl} = -\frac{V_0}{r \ln\left(R_{out}/R_{in}\right)} \hat{\mathbf{r}}$$

Now we must solve for the field within the volume of the particle. Since $a \ll R$, we will assume that $\mathbf{E}_{cyl}$ is essentially uniform over the diameter of the particle. This problem then becomes very similar to one we solved in class, that of a dielectric sphere in a uniform external field $\mathbf{E}_0$.

Fig. 3. A dielectric sphere in a uniform external field.

Recall that for this problem,

$$\mathbf{E}_{sphere} = \frac{3}{\epsilon + 2}\mathbf{E}_0$$

where $\mathbf{E}_{sphere}$ is the electric field within the sphere. However, since the dielectric constant only enters through the boundary condition in a relative way

$$D_{1n} = D_{2n} \;\Rightarrow\; \epsilon_1 E_{1n} = \epsilon_2 E_{2n} \;\Rightarrow\; \frac{\epsilon_1}{\epsilon_2}E_{1n} = E_{2n},$$

it must be that

$$\mathbf{E}_{sphere} = \frac{3\epsilon_2}{2\epsilon_2 + \epsilon_1}\mathbf{E}_{cyl}.$$

The polarization of the sphere is then

$$\mathbf{P} = \frac{\epsilon_1 - 1}{4\pi}\mathbf{E}_{sphere} = \frac{1}{4\pi}\frac{3\epsilon_2(\epsilon_1 - 1)}{2\epsilon_2 + \epsilon_1}\mathbf{E}_{cyl},$$

which corresponds to a dipole moment of the sphere

$$\mathbf{p} = \frac{4\pi}{3}a^3\mathbf{P} = a^3\frac{\epsilon_2(\epsilon_1 - 1)}{2\epsilon_2 + \epsilon_1}\mathbf{E}_{cyl}$$

Thus the electrostatic force on the sphere is given by

$$\mathbf{F}_{elec} = (\mathbf{p}\cdot\nabla)\,\mathbf{E}_{sphere} = a^3\frac{3\epsilon_2^2(\epsilon_1-1)}{(2\epsilon_2+\epsilon_1)^2}\,(\mathbf{E}_{cyl}\cdot\nabla)\,\mathbf{E}_{cyl}$$

$$\mathbf{F}_{elec} = (\mathbf{p}\cdot\nabla)\,\mathbf{E}_{sphere} = \frac{a^3}{2}\frac{3\epsilon_2^2(\epsilon_1-1)}{(2\epsilon_2+\epsilon_1)^2}\nabla\left|\mathbf{E}_{cyl}\right|^2$$

In addition to this force, there is an electric Archimedes force. This force is due to the fact that the particle displaces some of the dielectric fluid. We can calculate it by applying Archimedes principle just like we do for gravitational forces. The electric Archimedes force is minus the force that the sphere of displaced fluid experiences.

$$\mathbf{F}_{elec-Arch} = -\mathbf{F}_{elec}(\epsilon_1 \to \epsilon_2)$$

As indicated, we can get this force by replacing ϵ_1 by ϵ_2 in the force equation above.

$$\mathbf{F}_{elec-Arch} = -\frac{a^3}{6}\,(\epsilon_2-1)\,\nabla\left|\mathbf{E}_{cyl}\right|^2$$

Thus the net electric force on the sphere is

$$\mathbf{F}_{net} = \frac{a^3}{2}\left[\frac{3\epsilon_2^2(\epsilon_1-1)}{(2\epsilon_2+\epsilon_1)^2} - \frac{\epsilon_2-1}{3}\right]\nabla\left|\mathbf{E}_{cyl}\right|^2.$$

Now evaluating the gradient, we get

$$\mathbf{F}_{net} = -\frac{a^3V_0^3}{r^3\left(\ln(R_{out}/R_{in})\right)^2}\left[\frac{3\epsilon_2^2(\epsilon_1-1)}{(2\epsilon_2+\epsilon_1)^2} - \frac{\epsilon_2-1}{3}\right],$$

or, after a bit of algebra,

$$\mathbf{F}_{net} = -\frac{a^3AV_0^3}{3r^3\left(\ln(R_{out}/R_{in})\right)^2}$$

where

$$A = \frac{\epsilon_2(4\epsilon_2+5) - \epsilon_1(\epsilon_2 - 1)}{(2\epsilon_2+\epsilon_1)^2}(\epsilon_1 - \epsilon_2)$$

Interpretation. This setup has practical applications for sorting bits of dielectric particles with different ϵ_1. Thus we should consider A for fixed ϵ_2 and different ϵ_1 of the different particles. If $A > 0$, then the force is inward, toward stronger fields, and if $A < 0$, then the force is outward, toward weaker fields. The zeroes of A occur when

$$\epsilon_2 = \epsilon_1 \quad ; \quad \epsilon_1 = \frac{\epsilon_2(4\epsilon_2+5)}{\epsilon_2 - 1},$$

and the maximum for fixed ϵ_2

$$\frac{\partial A}{\partial \epsilon_1} = 0 \Rightarrow \epsilon_1 = 2(\epsilon_2+1).$$

Now lets consider a numerical example. Let $\epsilon_2 = 2.0$ and vary ϵ_1.

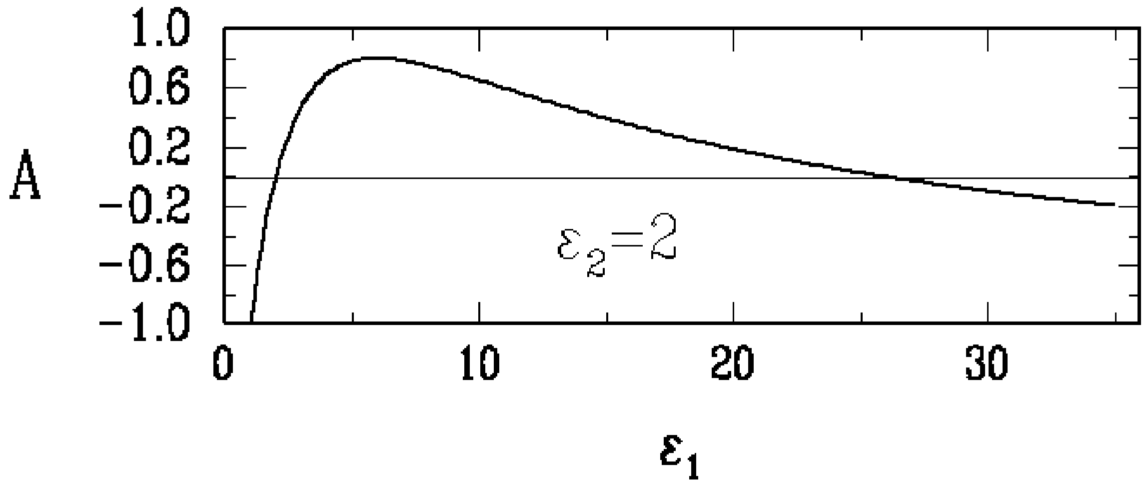


Fig. 4. Sketch of A

As shown in the figure, A is not a monotonic function of ϵ_1 In fact there are three regions

$\epsilon_1 < \epsilon_2$	force is outward
$\epsilon_2 < \epsilon_1 < \epsilon_2(4\epsilon_2 + 5)/(\epsilon_2 - 1)$	force is inward
$\epsilon_1 > \epsilon_2(4\epsilon_2 + 5)/(\epsilon_2 - 1)$	force is outward

Thus, mildly and highly polar particles move out, while particles of intermediate polarizability more in. At first it seems that this makes no sense; however, consider the following explanation:

Since the potential within the annulus is held fixed by an external source, the appropriate thermodynamic potential for this system is

$$W'(r, \Phi) = -\frac{1}{8\pi} \int_V d^3x \, \epsilon(\mathbf{x}) \, |\mathbf{E}(\mathbf{x})|^2$$

The most stable state of the system is the one which minimizes this potential. Thus the most stable state of the system is obtained by having the largest field where $\epsilon(\mathbf{x})$ is largest. Reconsider the three regions.

(1)	$\epsilon_1 < \epsilon_2$	The particle has a lower ϵ than that of the fluid, thus it is expelled to regions of low filed. Thus, $\epsilon(\mathbf{x})$ is maximized where $\mathbf{E}$ is large.
(2)	$\epsilon_2 < \epsilon_1 < \epsilon_2(4\epsilon_2 + 5)/(\epsilon_2 - 1)$	Now the particle has a higher ϵ than the fluid

thus it moves to regions of large field

(3) $\epsilon_1 > \epsilon_2(4\epsilon_2 + 5)/(\epsilon_2 - 1)$ The field inside the particle goes to zero as $\epsilon \to \infty$ (the sphere approaches a metal), and the potential is minimized by having the sphere go to regions of low field.

Now consider the motion of the particle. The drift velocity of the particle is given by

$$\mathbf{F}_{net} = 6\pi\eta\mathbf{v}.$$

If we use the following reasonable parameters

parameter	value	cgs value
a	0.1 mm	0.01 cm
ϵ_1	4.6	4.6
ϵ_2	2.3	2.3
η	6.5×10^{-4} (MKSA)	6.5×10^{-3} cgs
R_{in}	0.5 mm	0.05 cm
R_{out}	1 cm	1 cm
V_0	4.0×10^3 volts	13.34 statvolts
r	0.5 cm	0.5 cm

The value of ϵ_2 corresponds to that of organic solvents, in this case Benzene. Solving with these parameters, we find that $v = 0.031$ cm./sec.

Slow.

We could use this setup to separate living cells from dead ones due to the very different water content (since $\epsilon_{water} \approx 81$).

A Multipole Expansion: with Spherical Harmonics

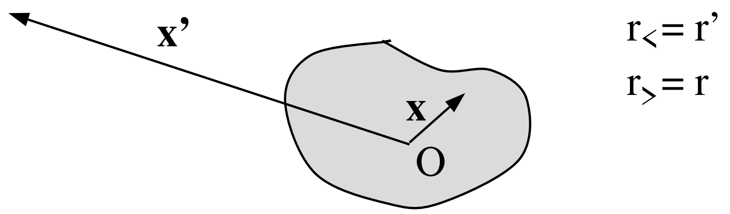
In this appendix, we will discuss the multipole expansion as it is done in Jackson.

Consider the potential $\Phi(\mathbf{x})$ produced by some localized charged distribution $\rho(\mathbf{x})$,

$$\Phi(\mathbf{x}) = \int d^3x' \, \rho(\mathbf{x}') \frac{1}{|\mathbf{x} - \mathbf{x}'|}. \tag{154}$$

Substitute the spherical harmonic expansion for $\frac{1}{|\mathbf{x}-\mathbf{x}'|}$ to have

$$\Phi(\mathbf{x}) = \sum_{l,m} \frac{4\pi}{2l+1} \left[\int d^3x' \, \rho(\mathbf{x}') Y^*_{l,m}(\theta', \phi') \frac{r^l_<}{r^{l+1}_>} \right] Y_{l,m}(\theta, \phi). \tag{155}$$



Now, if the origin of coordinates is chosen to be around the center of the charge distribution, and if the field point $\mathbf{x}$ is such that r is larger than the distance of any source point (where $\rho(\mathbf{x}') \neq 0$) $\mathbf{x}'$ from the origin, then it is true that for all $\mathbf{x}'$ of importance in the integral, $r > r'$ and so $r_< = r'$ and $r_> = r$. Thus,

$$\Phi(\mathbf{x}) = \sum_{l,m} \frac{4\pi}{2l+1} \left[\int d^3x' \, r'^l Y^*_{l,m}(\theta', \phi') \rho(\mathbf{x}') \right] \frac{Y_{l,m}(\theta, \phi)}{r^{l+1}}. \qquad (156)$$

This result may be written in the form

$$\Phi(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} q_{lm} \frac{Y_{l,m}(\theta, \phi)}{r^{l+1}} \equiv \sum_{l,m} \Phi_{lm}(\mathbf{x}), \qquad (157)$$

where

$$q_{lm} \equiv \int d^3x \, r^l Y^*_{l,m}(\theta, \phi) \rho(\mathbf{x}) \qquad (158)$$

is known as a *multipole moment* of the charge distribution. These moments, which satisfy the identity

$$q_{l,m} = (-1)^m q^*_{l,-m} \qquad (159)$$

by virtue of the same property of the spherical harmonics, completely determine the field outside of the domain where the charge is located. Note, however, that they do not contain enough information to tell us what the actual charge distribution is. The moments of greatest interest are the ones with small values of l. We can understand this statement from the fact that the moment q_{lm} is proportional to, as seen from Eq. (5), a^l, where a is the size of the charge distribution. Hence the potential produced by this moment is proportional to $(q'/r)(a/r)^l$ where q' is a characteristic charge in the distribution (The actual total charge may vanish). This contribution to the potential becomes very small for large l given that r is significantly larger than a.

The components of the electric field associated with the l, m multipole are

$$\begin{aligned} E_r &= -\frac{\partial \Phi_{lm}}{\partial r} = \frac{4\pi(l+1)}{2l+1} q_{lm} \frac{Y_{l,m}(\theta,\phi)}{r^{l+2}} \\ E_\theta &= -\frac{1}{r}\frac{\partial \Phi_{lm}}{\partial \theta} = -\frac{4\pi}{2l+1} q_{lm} \frac{1}{r^{l+2}} \frac{\partial Y_{l,m}(\theta,\phi)}{\partial \theta} \\ E_\phi &= -\frac{1}{r\sin\theta}\frac{\partial \Phi_{lm}}{\partial \phi} = -\frac{4\pi}{2l+1} q_{lm} \frac{im}{r^{l+2}\sin\theta} Y_{l,m}(\theta,\phi). \end{aligned} \tag{160}$$

The leading moments are

$$q_{00} = \int d^3x\, \rho(\mathbf{x}) \frac{1}{\sqrt{4\pi}} = \frac{q}{\sqrt{4\pi}} \tag{161}$$

where q is precisely the total charge of the system. This term is the *monopole moment* of the charge distribution; it is fundamentally just the total charge. Similarly,

$$q_{10} = \sqrt{\frac{3}{4\pi}} \int d^3x\, \rho(\mathbf{x}) r \cos\theta = \sqrt{\frac{3}{4\pi}} \int d^3x\, \rho(\mathbf{x}) z \tag{162}$$

and

$$q_{11} = -q^*_{1,-1} = -\sqrt{\frac{3}{8\pi}} \int d^3x\, \rho(\mathbf{x}) r \sin\theta e^{-i\phi} = -\sqrt{\frac{3}{8\pi}} \int d^3x\, \rho(\mathbf{x})(x - iy). \tag{163}$$

From these equations we can see that the information contained in the coefficients q_{1m} is the same as what is contained in the components of the electric dipole moment $\mathbf{p}$ of the charge distribution,

$$\mathbf{p} \equiv \int d^3x\, \rho(\mathbf{x}) \mathbf{x}. \tag{164}$$

The explicit connection is

$$\mathbf{p} = \left\{ \frac{1}{2}\sqrt{\frac{8\pi}{3}}(q_{11} - q_{1,-1})\hat{\mathbf{x}} - \frac{1}{2}\sqrt{\frac{8\pi}{3}}i(q_{11} + q_{1,-1})\hat{\mathbf{y}} + \sqrt{\frac{4\pi}{3}}q_{10}\hat{\mathbf{z}} \right\} \quad (165)$$

The $l = 2$ moments, called *electric quadrupole moments*, are easily shown to be

$$\begin{aligned} q_{22} &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\int d^3x\,\rho(\mathbf{x}')(x - iy)^2 \\ q_{21} &= -\sqrt{\frac{15}{8\pi}}\int d^3x\,\rho(\mathbf{x})(x - iy)z \\ q_{20} &= \frac{1}{2}\sqrt{\frac{5}{4\pi}}\int d^3x\,\rho(\mathbf{x})(3z^2 - r^2). \end{aligned} \quad (166)$$

These multipole moments are traditionally written in terms of the components of the *traceless quadrupole moment tensor*, defined by

$$Q_{ij} \equiv \int d^3x\,\rho(\mathbf{x})(3x_ix_j - r^2\delta_{ij}); \quad (167)$$

the subscripts i and j stand for Cartesian components x, y, and z, or 1,2,3. With a little algebra, one can show that

$$\begin{aligned} q_{22} &= \frac{1}{12}\sqrt{\frac{15}{2\pi}}(Q_{11} - 2iQ_{12} - Q_{22}) \\ q_{21} &= -\frac{1}{3}\sqrt{\frac{15}{8\pi}}(Q_{13} - iQ_{23}) \\ q_{20} &= \frac{1}{2}\sqrt{\frac{5}{4\pi}}Q_{33} \end{aligned} \quad (168)$$

It seems a little strange to be replacing at most five independent numbers (contained in the moments q_{2m}) by nine numbers Q_{ij}; however, the quadrupole moment tensor is symmetric, $Q_{ij} = Q_{ji}$, reducing the number of possible independent components to six, and it also has, as its name suggests and as may be shown easily from the definition, zero trace so that $Q_{33} = -Q_{11} - Q_{22}$ and only two of the diagonal components are independent. Thus the tensor can have at most five independent components also.