26 October 95

We would like to relate a macroscopic quantity $\chi_e$, the electric susceptibility, to a microscopic quantity that is a property of the individual molecules.

We have the relation: $\vec{P} = \chi_e \vec{E}_{macro}$ among macroscopic observables. We seek a microscopic analog.

First notice that the electric field near one molecule is <u>NOT</u> $\vec{E}_{macro}$. To find an expression for the local electric field, we surround the molecule by a sphere which is macroscopically small (because we want the polarization $\vec{P}$ to be approximately constant within), but microscopically large (so it contains very many molecules). We subtract the "smeared out" field due to the Polarization in the continuum approximation, and then add back in the dipole field contribution due to all the molecules in our sphere.

$$\vec{E}_{local}(\vec{r}) = \vec{E}_{macro}(\vec{r}) \underbrace{- \vec{E}_{\substack{\text{AVERAGE}\\ \text{Polarization}}}(\vec{r}) + \vec{E}_{\substack{\text{sum over}\\ \text{molecules}}}(\vec{r})}_{\vec{E}_{internal}(\vec{r})}$$

$$\vec{E}_{local}(\vec{r}) = \vec{E}_{macro}(\vec{r}) + \vec{\nabla}\int_{sphere} dV' \, \frac{\vec{P}\cdot(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3} - \overbrace{\cancel{\vec{\nabla}\sum_{\alpha} \vec{\mu}\cdot\frac{(\vec{r}-\vec{r}_\alpha)}{|\vec{r}-\vec{r}_\alpha|^3}}}^{\text{small}}$$

For a cubic lattice, or for a random (amorphous) arangement of molecules, the sum over $\alpha$ vanishes. For other crystal systems besides cubic, the contribution is small.

In the second term, the polorization $\vec{P}$ is approximately <u>constant</u> over the whole sphere.

$$\vec{\nabla}\int_{sphere} dV' \, \frac{\vec{P}\cdot(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3} = \vec{\nabla}\int_{sphere} dV' \, \vec{P}\cdot\vec{\nabla}_{r'}\frac{1}{|\vec{r}-\vec{r}\,'|}$$

Use the divergence theorem

$$= \vec{\nabla}\oint_{sphere} ds' \, \frac{\vec{P}\cdot\hat{n}'}{|\vec{r}-\vec{r}\,'|} = \oint_{sphere} ds' \, \frac{1}{|\vec{r}-\vec{r}\,'|^2}\,\hat{n}'(\vec{P}\cdot\hat{n}')$$

$$= \int d^2\Omega' \, \hat{n}'(\vec{P}\cdot\hat{n}')$$

choose the polar axis ($+z$-axis) along $\vec{P}$

$$= P\int d^2\Omega' \left[\hat{x}\,\sin\theta'\cancelto{0}{\cos\varphi'} + \hat{y}\,\sin\theta'\cancelto{0}{\sin\varphi'} + \hat{z}\cos\theta'\right]\cos\theta'$$

$$= P\hat{z}\int d^2\Omega' \cos^2\theta' = \vec{P}\,2\pi\left(\tfrac{2}{3}\right) = \frac{4\pi}{3}\vec{P}$$

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$$\vec{E}_{local}(\vec{r}) = \vec{E}_{macro}(\vec{r}) + \frac{4\pi}{3}\vec{P}(\vec{r})$$

The induced dipole moment of the molecules depends on the local electric field; the constant of proportionality is $\gamma$, the molecular polarizability

$$\vec{\mu} = \gamma \vec{E}_{local} .$$

Let $N$ be the number density of molecules in the sample, then

$$\vec{P} = \vec{\mu} N,$$

since $\vec{P}$ the polarization is the dipole moment density.

$$\vec{P} = N \gamma \vec{E}_{local} = N\gamma\left(\vec{E}_{macro} + \frac{4\pi}{3}\vec{P}\right)$$

solve for $\vec{P}$

$$\vec{P} = \frac{N\gamma}{1-\frac{4\pi}{3}N\gamma}\vec{E}_{macro} \qquad \text{but} \qquad \vec{P} = \chi_e \vec{E}_{macro}$$

So the relation we sought between the macroscopic $\chi_e$ and the microscopic $\gamma$ is

$$\chi_e = \frac{N\gamma}{1-\frac{4\pi}{3}N\gamma}$$

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Continuing, the (macroscopic) dielectric constant is:

$$\epsilon = 1 + 4\pi\chi_e = \frac{3+8\pi N\gamma}{3-4\pi N\gamma}$$

or

$$\gamma = \frac{1}{4\pi N}\,\frac{\epsilon-1}{\epsilon+2}$$

this is the Clausius-Mossotti relation.

To good approximation:

$\frac{\epsilon-1}{\epsilon+2}$ for any substance is proportional to its number density.

In fact,

$\frac{\epsilon-1}{\epsilon+2} = 4\pi\gamma N$ is just the first term in a density power series:

$$\frac{\epsilon-1}{\epsilon+2} = \sum_{n=1}^{\infty} C_n(T)\, N^n$$

where $T$ is the absolute temperature.

The first coefficient $C_1(T) = 4\pi\gamma$ just happens to be independent of $T$.

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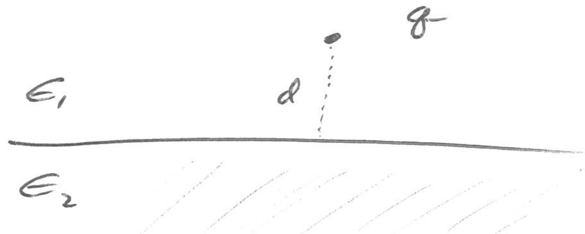
## Boundary-value problems in Dielectric Media

① Consider a point charge $q$ a distance $d$ above the plane interface of two dielectrics




Choose the origin on the interface, directly below $q$ and choose the $+z$-axis to pass through $q$.

If all space were filled with one type of dielectric $\epsilon_1 = \epsilon_2 \equiv \epsilon$, then we could obtain the potential by using Gauss' law.

Since the point charge $\underline{q}$ is the only $\underline{\text{true}}$ charge in the problem and we know one Maxwell equation in matter: $\vec{\nabla} \cdot \vec{D} = 4\pi \rho_{true}$

We know that the displacement field is radial (by symmetry) and

$$|\vec{D}| = \frac{q}{\rho^2 + (z-d)^2} \quad \text{in cylindrical coordinates}$$

$$= \frac{q}{x^2+y^2+(z-d)^2} \quad \text{in Cartesian.}$$

Define

$$r_- \equiv \sqrt{\rho^2 + (z-d)^2}$$

$$r_+ \equiv \sqrt{\rho^2 + (z+d)^2}$$

$$= \frac{q}{r_-^2}$$

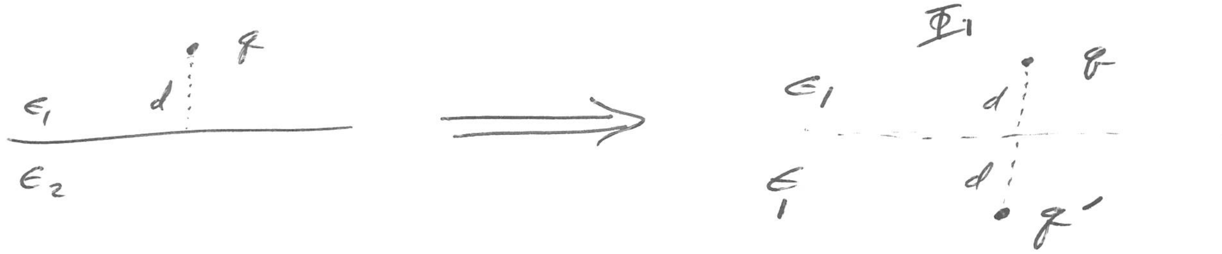
Then since $\vec{D} = \epsilon \vec{E}$ we know

$|\vec{E}| = \dfrac{q}{\epsilon r_-^2}$ and the potential can be obtained by integrating from infinity to position $\vec{r}$.

$$\underline{\Phi} = \frac{q}{\epsilon r_-}$$

But for $\epsilon_1 \neq \epsilon_2$, the situation is more complicated.

We will use image methods. To find the potential in region 1, we imagine altering the original problem in this way: Remove the dielectric constant $\epsilon_2$ and replace it by $\epsilon_1$, so $\epsilon_1$ now fills all space. Put image charges in region 2 since the physical region is region 1.




We will try one image charge of magnitude $q'$ located a distance $d$ below the interface. If this is insufficient, we can change the image distance later. The equal spacing is motivated by the fact that the boundary conditions at $z=0$ must hold for all $\rho$ values.

$$\Phi_1(\vec{r}) = \frac{q}{\epsilon_1 r_-} + \frac{q'}{\epsilon_1 r_+}$$

remember $r_\pm = \sqrt{\rho^2 + (z \pm d)^2}$

same dielectric constant!

To find the potential in region 2, we replace the original problem by one in which $\epsilon_2$ fills all space and the image charge $q''$ is located in region 1, at height $\underline{d}$.


$$\Phi_2(\vec{r}) = \frac{q''}{\epsilon_2 r_-}$$

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Now we apply the two boundary conditions that the fields must satisfy at a dielectric interface. These two equations should enable us to solve for the two unknowns $q'$ and $q''$, the image charges.

i) Continuity of the tangential component of $\vec{E}$ across the dielectric interface in the absence of a <u>true</u> dipole layer.

The two tangential directions are $\hat{\rho}$ and $\hat{\theta}$.

$$\left(E_{1\theta} - E_{2\theta}\right)\Big|_{z=0} = 0 \quad \Rightarrow \quad -\frac{\partial \Phi_1}{\partial \theta}\Big|_{z=0} = -\frac{\partial \Phi_2}{\partial \theta}\Big|_{z=0}$$

Unfortunately, since the potential does not depend on $\theta$ this is the identity $0 = 0$; not helpful!

The other tangential component gives

$$\left(E_{1\rho} - E_{2\rho}\right)\Big|_{z=0} = 0 \quad \Rightarrow \quad -\frac{\partial \Phi_1}{\partial \rho}\Big|_{z=0} = -\frac{\partial \Phi_2}{\partial \rho}\Big|_{z=0}$$

$$\frac{q\rho + q'\rho}{\epsilon_1 (\rho^2+d^2)^{3/2}} = \frac{q''\rho}{\epsilon_2(\rho^2+d^2)^{3/2}}$$

$$\Rightarrow \boxed{\frac{1}{\epsilon_1}(q+q') = \frac{1}{\epsilon_2} q''}$$

Notice that this condition can also be found from the continuity of the potential across the interface without having to take a derivative.

$$\Phi_1\Big|_{z=0} = \Phi_2\Big|_{z=0} \quad \Rightarrow \quad \frac{1}{\epsilon_1}(q+q') = \frac{1}{\epsilon_2} q''$$

since at $z=0$, $r_- = r_+$

ii) Continuity of the normal component of $\vec{D}$ across the interface in the absense of <u>true</u> surface charge.

$$\vec{D} = \epsilon \vec{E} = -\epsilon \vec{\nabla} \Phi$$

$$\left(D_{1z} - D_{2z}\right)\Big|_{z=0} = 0 \implies -\epsilon_1 \frac{\partial \Phi_1}{\partial z}\Big|_{z=0} = -\epsilon_2 \frac{\partial \Phi_2}{\partial z}\Big|_{z=0}$$

$$\frac{-qd + q'd}{(\rho^2 + d^2)^{3/2}} = \frac{-q''d}{(\rho^2+d^2)^{3/2}} \implies \boxed{q = q' + q''}$$

Combining the two boxed relations, we get

$$q' = -\frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + \epsilon_1} q \qquad \underline{\text{and}} \qquad q'' = \frac{2\epsilon_2}{\epsilon_2 + \epsilon_1} q$$

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$$\Phi_1(\vec{r}) = q\left[\frac{1}{\epsilon_1 \sqrt{\rho^2 + (z-d)^2}} + \left(\frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2}\right)\frac{1}{\epsilon_1 \sqrt{\rho^2 + (z+d)^2}}\right]$$

$$\Phi_2(\vec{r}) = \frac{2q}{\epsilon_1 + \epsilon_2} \frac{1}{\sqrt{\rho^2 + (z-d)^2}}$$

Check two limiting cases: $\epsilon_1 = \epsilon_2$ and $\epsilon_2 \to \infty$ (this means that the second medium is a conductor).

(2) A uniform uncharged dielectric sphere of radius $\underline{a}$ embedded in an external field which becomes $\vec{E}_0$ far from the sphere.

Choose the $+z$-axis to be along $\vec{E}_0$ and choose the origin at the center of the sphere.

The boundary condition is:

$$\Phi(|\vec{r}| \to \infty) = -z E_0 = -r \cos\theta \, E_0$$

so $\vec{E} = -\vec{\nabla}\Phi = E_0 \hat{z} = \vec{E}_0$

Some (external) charges at infinity create this field.

In the region $\underline{\text{outside}}$ the sphere, there is no true charge (we neglect the charge at infinity), so $\vec{\nabla} \cdot \vec{D}_{out} = 0$ and since $\vec{E}_{out} = \vec{D}_{out}$ outside the dielectric we have $\vec{\nabla} \cdot \vec{E}_{out} = 0$ so the potential outside satisfies Laplace's equation

$$\nabla^2 \Phi_{out}(\vec{r}) = 0 \Rightarrow \Phi_{out}(\vec{r}) = \frac{1}{r} \sum_{l=0}^{\infty} B_l \left(\frac{a}{r}\right)^l P_l(\cos\theta) - E_0 r \cos\theta$$

For $r < a$, again there are no true charges, so

$$\vec{\nabla} \cdot \vec{D}_{in} = 0 \Rightarrow \vec{\nabla} \cdot \vec{E}_{in} = 0 \Rightarrow \nabla^2 \Phi_{in} = 0$$

$$\Phi_{in}(\vec{r}) = \frac{1}{a}\sum_{l=0}^{\infty} A_l \left(\frac{r}{a}\right)^l P_l(\cos\theta)$$

There is actually no need to keep all those terms. The boundary condition at infinity involves $\cos\theta = P_1(\cos\theta)$ so the solution to Laplace's equation (by the uniqueness theorem) involves only $l=1$. You can also derive this result the hard way by using orthogonality relations on the boundaries $r=a$ and $r=\infty$.

$$\Phi_{in}(\vec{r}) = A_1 \frac{r}{a^2}\cos\theta$$

$$\Phi_{out}(\vec{r}) = B_1 \frac{a}{r^2}\cos\theta - E_0 r\cos\theta$$

The conditions at the dielectric interface $r=a$ are:

i) $\Phi_{in}(a,\theta) = \Phi_{out}(a,\theta)$

$$\Rightarrow A_1 \frac{1}{a}\cos\theta = B_1\frac{1}{a}\cos\theta - E_0 a\cos\theta$$

or $\boxed{B_1 - A_1 = E_0 a^2}$

ii) $D_{in\,r}\Big|_{r=a} = D_{out\,r}\Big|_{r=a} \Rightarrow -\epsilon\frac{\partial}{\partial r}\Phi_{in}\Big|_{r=a} = -\frac{\partial}{\partial r}\Phi_{out}\Big|_{r=a}$

$$\Rightarrow \epsilon A_1 \frac{1}{a^2}\cos\theta = -2B_1\frac{1}{a^2}\cos\theta - E_0\cos\theta$$

or $\boxed{2B_1 + \epsilon A_1 = -E_0 a^2}$

Solving the boxes equations simultaneously gives:

$$A_1 = -\frac{3}{\epsilon+2} E_0 a^2 \qquad\qquad B_1 = \frac{\epsilon-1}{\epsilon+2} E_0 a^2$$

The potential is then:

$$\Phi_{in}(\vec{r}) = \frac{-3E_0}{\epsilon+2} r\cos\theta = -\frac{3E_0}{\epsilon+2} z$$

$$\Phi_{out}(\vec{r}) = \underbrace{\frac{\epsilon-1}{\epsilon+2} E_0 a^3 \frac{1}{r^2}\cos\theta}_{\text{dipole potential}} - E_0 r\cos\theta$$

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The electric field inside the sphere is rather surprizing:

$$\vec{E}_{in} = -\vec{\nabla}\Phi_{in} = \frac{3}{\epsilon+2}\vec{E}_0$$

It is <u>uniform</u>! In general, $\epsilon \geq 1$, so the field inside the dielectric is diminished.

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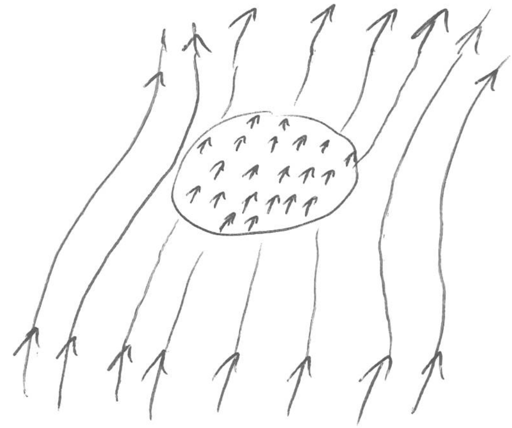
Outside, the electric field is the constant $\vec{E}_0$ plus the field due to a <u>point dipole</u> at the origin of dipole moment:

$$\vec{\mu} = \frac{\epsilon-1}{\epsilon+2}\vec{E}_0 a^3$$



As we said earlier, there is no true charge in the problem. There is, however, polarization charge on the dielectric interface. Since this charge is <u>bound</u>, we can move it slightly and create an excess in one area at the expense of creating a deficit in another area. The <u>net</u> polarization charge over the surface of the sphere should be zero.

$$Q_{pol} = \oint_S ds\, \sigma_{pol} = \oint ds\, \hat{n}\cdot\vec{P} = \int_V dV\, \vec{\nabla}\cdot\vec{P}$$

Since there are no true charges <u>inside</u> the body of the sphere, $V$, we have $\vec{\nabla}\cdot\vec{D} = 0$

but then $\vec{D} = \epsilon\vec{E}$ gives

$$0 = \vec{\nabla}\cdot\vec{D} = \epsilon\,\vec{\nabla}\cdot\vec{E} + \vec{E}\cdot\vec{\nabla}\epsilon$$

If the medium is homogenous, $\vec{\nabla}\epsilon = 0$

and we have $\vec{\nabla}\cdot\vec{E} = 0$

but now $\vec{P} = \chi_e\vec{E}$ and if $\chi_e$ is homogenous also, we see that $\vec{\nabla}\cdot\vec{P} = 0$

so $Q_{pol} = 0$.

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