Chp-10 Electric fields in Matter

- Dielectrics
- Matter comes in many forms
- These respond differently to an applied $\mathbf{E}$-field
- Conductors & Insulators or Dielectrics
- We already considered conductors
- Conductors have charges that can freely move

In metals it is typically one or two electrons per atom. That are not associated with a specific nucleus.

Electron density in a metal.
Chp-10 Electric fields in Matter

- **Insulators or Dielectrics**
- All charges are attached to a specific atom or molecule
- They are not free to roam
- The can move small distances within the confines of an atom or molecule
- Yet the small displacements of charge in an E-field account for the properties of dielectrics
- Two types of displacements are possible...stretching and rotating
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Induced Dipoles

What happens when a neutral atom is placed in an $E$-field?

- Positively charged Nucleus
- Negatively charged Electron cloud

Nucleus is pushed in the direction of the field

Electron cloud is attracted toward the field

If the $E$-field is strong enough it will ionize the atom (hence forming ions and it becomes a conductor)
In the Limit of low magnitude $\mathbf{E}$-field

Equilibrium is reached between the displacement induced by the $\mathbf{E}$-field and Coulombic attraction of nucleus and electrons.

The atom is polarized in the $\mathbf{E}$-field.

Get an induced dipole moment $\mathbf{p}$ points in the same direction as the applied $\mathbf{E}$-field.
In the Limit of low magnitude $\mathbf{E}$-field

\[ \mathbf{p} = \alpha \mathbf{E} \]

$\alpha = \text{atomic polarizability}$

<table>
<thead>
<tr>
<th></th>
<th>H</th>
<th>He</th>
<th>Li</th>
<th>Be</th>
<th>C</th>
<th>Ne</th>
<th>Na</th>
<th>Ar</th>
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<td>0.205</td>
<td>24.3</td>
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<td>24.1</td>
<td>1.64</td>
<td>43.4</td>
<td>59.4</td>
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Atomic Polarizabilities $\alpha/4\pi\varepsilon_0$ in units of $10^{-30}$ m$^3$

Handbook of Chemistry & Physics 91$^{\text{st}}$ Edition CRC Press
Assuming that the electron cloud retains its spherical symmetry under small displacement in an E-field, calculate the atomic polarizability for the atom.

No E-field

Applied E-field

\[ E = E_e \]

Internal field due to e⁻ pulling nucleus left Is balanced by the external E-field pushing right

What is the field a distance d from the center of a uniformly charged Sphere?
The charge from outside shell does not contribute

\[ V_{\text{sphere}} = \frac{4\pi d^3}{3} \]

\[ \rho = ch \arg e \text{ density} \]

so \( q' = \frac{4\pi d^3}{3} \rho \)

\[ E = \frac{q}{4\pi \varepsilon_0 r^2} \text{ so} \]

\[ E' = \frac{q'}{4\pi \varepsilon_0 d^2} = \frac{4\pi d^3 \rho}{4\pi \varepsilon_0 d^2} = \frac{\rho d}{3 \varepsilon_0} \]

\[ E' = \frac{4\pi d^3 \left( \frac{3q}{4\pi r^3} \right)}{4\pi \varepsilon_0 d^2} = \frac{qd}{4\pi \varepsilon_0 r^3} \]

What is the field a distance \( d \) from the center of a uniformly charged Sphere?
Electric fields in Matter

Very crude atomic model but accurate within a factor of ~4

\[ E' = E_e = \frac{q d}{4 \pi \varepsilon_0 r^3} \]

but \( p = q d \)

\[ p = (4 \pi \varepsilon_0 r^3)E' \]

but \( p = \alpha E \)

\[ \alpha = 4 \pi \varepsilon_0 r^3 = 3 \varepsilon_0 V_{\text{atom}} \]

Estimate the atomic polarizability of an H atom

\[ \alpha = 4 \pi \varepsilon_0 r^3 = 4 \pi (8.85 \times 10^{-12} \text{ F/m})(52.9 \times 10^{-12} \text{ m})^3 \]

\[ \alpha = 1.64 \times 10^{-41} \text{ Fm}^2 \]

\[ \frac{\alpha}{4 \pi \varepsilon_0} = 1.48 \times 10^{-31} \text{ m}^3 \]

\[ \frac{\alpha}{4 \pi \varepsilon_0} = 0.667 \times 10^{-30} \text{ m}^3 \]
What about molecules? They are not isotropic in their polarizability.

\[
\begin{align*}
\text{CO}_2 & \quad \alpha_\perp = 2 \times 10^{-40} \text{ C}^2\text{m/N} \\
& \quad \alpha_\parallel = 4.5 \times 10^{-40} \text{ C}^2\text{m/N}
\end{align*}
\]

Applied \( \mathbf{E} \)-field perpendicular or parallel to molecular axis.

If applied field is at an angle then resolve into components:

\[
\mathbf{p} = \alpha_\perp \mathbf{E}_\perp + \alpha_\parallel \mathbf{E}_\parallel
\]

However, the induced dipole moment may not be pointing in the same direction as the \( \mathbf{E} \)-field.

For an asymmetrical molecule the most general linear relationship between \( \mathbf{E} \) and \( \mathbf{p} \) is via a tensor.
Tensor: magnitude and multiple directions

Polarizability tensor (tensor of rank 2 so for 3D space $3^2=9$ elements)

\[ p_x = \alpha_{xx} E_x + \alpha_{xy} E_y + \alpha_{xz} E_z \]
\[ p_y = \alpha_{yx} E_x + \alpha_{yy} E_y + \alpha_{yz} E_z \]
\[ p_z = \alpha_{zx} E_x + \alpha_{zy} E_y + \alpha_{zz} E_z \]

Matrix of $\alpha_{ij}$ elements = Polarizability Tensor

The values of $\alpha_{ij}$ depend on orientation of the axes you use

Orient so you have the “principal” axes so that all off-diagonal elements are zero leaving: $\alpha_{xx} \quad \alpha_{yy} \quad \alpha_{zz}$

Characterize an asymmetric molecule with 3 polarizabilities
Griffiths Prob. 4.1

A H atom (with Bohr radius of 0.5 angstrom) is situated between two metal plates 1 mm apart, which are connected to opposite terminals of a 500 V battery. What fraction of the atomic radius does the separation distance \( d \) amount to, roughly? Estimate the voltage you would need with this apparatus to ionize the atom [Use the value of \( \alpha \) in Table 4.1]

Expectation…The displacements due to polarization will be quite small
Griffiths Prob. 4.1

\[ E = \frac{V}{x} = \frac{500 \text{V}}{10^{-3} \text{m}} = 5 \times 10^5 \text{ V/m} \]

\[ \frac{\alpha}{4\pi\varepsilon_0} = 0.667 \times 10^{-30} \text{ m}^3 \]

\[ \alpha = 4\pi\varepsilon_0 r^3 = 4\pi (8.85 \times 10^{-12} \text{ F/m})(0.667 \times 10^{-30} \text{ m}^3) = 7.42 \times 10^{-41} \text{ F/m}^2 \]

\[ p = \alpha E = ed \quad \text{so} \quad d = \frac{\alpha E}{e} = \frac{(7.42 \times 10^{-41} \text{ F/m}^2)(5 \times 10^{-5} \text{ V/m})}{1.602 \times 10^{-19} \text{ C}} = 2.32 \times 10^{-16} \text{ m} \]

\[ \text{Ratio} \quad \frac{d}{r} = \frac{2.32 \times 10^{-16} \text{ m}}{52.9 \times 10^{-12} \text{ m}} = 4.39 \times 10^{-6} \]

Or \( 4.39 \times 10^{-4}\% \)
Griffiths Prob. 4.1…To ionize let $d=$radius of atom

\[ r = \frac{\alpha E}{e} = \frac{\alpha V}{E_{\text{ex}}} \]

\[
so \quad V = \frac{r_{\text{ex}}}{\alpha} = \frac{(52.9 \times 10^{-12} \text{ m})(1.602 \times 10^{-19} \text{ C})(1 \times 10^{-3} \text{ m})}{7.42 \times 10^{-41} \text{ F/m}^2} = 1.14 \times 10^8 \text{ V}
\]
Griffiths 4.1.3 Alignment of Polar Molecules

What about molecules with a permanent dipole moment?

E.g. Water has a large electronegativity difference between hydrogen and oxygen & OH bonds are 105° apart.

Electrons are more tightly pulled toward oxygen (although it is still a covalent compound)

\[ p = 6.1 \times 10^{-30} \text{ Cm} \]

What happens when an E-field is applied?

Large dipole moment so water is a good polar solvent.
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- Place water molecule in a uniform E-field
- The force on the positive end will be exactly balance the force on the negative end but there will be a torque

\[ F_+ = qE \quad \text{and} \quad F_- = -qE \]

**torque**

\[ N = (r_+ \times F_+) + (r_- \times F_-) \]

\[ N = \left[ \left( \frac{d}{2} \right) \times (qE) \right] + \left[ \left( -\frac{d}{2} \right) \times (-qE) \right] = qd \times E \]
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The dipole moment in a uniform \(\mathbf{E}\)-field experiences a torque:
\[
\mathbf{p} = q\mathbf{d}
\]
\[
\mathbf{N} = \mathbf{p} \times \mathbf{E}
\]

Note \(\mathbf{N}\) is in a direction to line up \(\mathbf{p}\) parallel to \(\mathbf{E}\).

A polar molecule that is rotationally free will rotate in an applied \(\mathbf{E}\)-field.

A non uniform \(\mathbf{E}\)-field will mean a net force in addition to \(\mathbf{N}\).

Over the molecular dimensions:
Variation in \(\mathbf{E}\) is usually small.
A non uniform $\mathbf{E}$-field will mean a net force in addition to $\mathbf{N}$.

There will be a difference in $\mathbf{E}$-field from + to - end

$$\mathbf{F} = \mathbf{F}_+ + \mathbf{F}_- = q(\mathbf{E}_+ - \mathbf{E}_-) = q(\Delta \mathbf{E})$$

Recall that

$$dT = \left(\frac{\partial T}{\partial x}\right)dx + \left(\frac{\partial T}{\partial y}\right)dy + \left(\frac{\partial T}{\partial z}\right)dz$$

$$dT = \left(\left(\frac{\partial T}{\partial x}\right)\hat{x} + \left(\frac{\partial T}{\partial y}\right)\hat{y} + \left(\frac{\partial T}{\partial z}\right)\hat{z}\right) \bullet (dx\hat{x} + dy\hat{y} + dz\hat{z})$$

$$dT = (\nabla T) \bullet (d\mathbf{I})$$

So if the dipole is very short

And for $x$ & $y$

$$\Delta \mathbf{E}_x = (\nabla \mathbf{E}_x) \bullet \mathbf{d}$$

$$\Delta \mathbf{E} = (\mathbf{d} \bullet \nabla)\mathbf{E}$$

And since $\mathbf{p} = q\mathbf{d}$

$$\mathbf{F} = (\mathbf{p} \bullet \nabla)\mathbf{E}$$
Polarization*

What happens when we put a slab of a dielectric material in an electric field (E-field)?

If the dielectric is made of neutral atoms or nonpolar molecules, the electric field will induce a tiny dipole moment pointing in the field direction. In asymmetric molecules, the induced dipole will not be parallel to the field, but if they are randomly oriented, the components perpendicular to the field will cancel. If it is a crystalline solid, the cancellation does not occur.

If the dielectric is made of polar molecules, each molecular dipole will experience a torque and rotate if free. Note that temperature-dependent random thermal motions will always compete with the alignment in the applied field.

* Note that this is NOT the same polarization as in light polarization…which refers to the time-dependent orientation of the E-field vector during propagation of an EM wave.
Dielectric material becomes *polarized* in the \( \mathbf{E} \)-field.

We measure this effect as the polarization \( \mathbf{P} \)

\[ \mathbf{P} \text{ Dipole moment per unit volume} \]

The polarized material will produce its own field…what will this do?
Induced fields in nanoparticles

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Induced fields in nanoparticles

We now have two $E$-fields

1. External applied $E$-field

Induce many dipole moments (each atom or molecule)

2. ``Internal field`` due to the induced Polarization

These fields will combine by superposition
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- The field of a Polarized object
- Concept of bound charges
- What is the field produced by the induced dipoles?
- Strategy…We know the field/potential (far field limit) for a single dipole

Field Lines & Potential surfaces for a single dipole

Subdivide the dielectric into infinitesimal dipoles & integrate

It is easier to work with the potential
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Notational Warning to Physics 242 & 340 students

\[ \phi(r) \] Purcell’s Notation for the potential (Phys 242)

\[ V(r) \] Griffiths Notation for the potential (Phys 340)

Generalized Multipole Expansion

Expansion for the potential for any Localized charge distribution (previously we considered one isolated dipole)
**Chp-10 Electric fields in Matter**

**Generalized Multipole Expansion**

\[ \phi(r) = \frac{1}{4\pi\epsilon_o} \int \frac{\rho(r') dv'}{R} \]

**Law of cosines**

\[ R^2 = r^2 + r'^2 - 2rr'\cos\alpha = r^2 \left[ 1 + \left( \frac{r'}{r} \right)^2 - 2\left( \frac{r'}{r} \right)\cos\alpha \right] \]

\[ R = r\sqrt{1 + \epsilon} \quad \epsilon = \left( \frac{r'}{r} \right)\left( \frac{r'}{r} - 2\cos\alpha \right) \]

\( \epsilon << 1 \) for large \( r \)

i.e. for point P far from charge distribution

Suggests a binomial expansion for \( 1/R \) (see integral above)

\[ (1+x)^n = \left[ 1 + nx + \frac{n(n-1)}{2!}x^2 + ... \right] \]
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Generalized Multipole Expansion

\[
\frac{1}{R} = \frac{1}{r} (1 + \varepsilon)^{-\frac{1}{2}} = \frac{1}{r} \left( 1 - \frac{1}{2} \varepsilon + \frac{3}{8} \varepsilon^2 - \frac{5}{16} \varepsilon^3 + \ldots \right)
\]

Substitute back in for \( \varepsilon \)

\[
\varepsilon = \left( \frac{r'}{r} \right) \left( \frac{r'}{r} - 2\cos \alpha \right)
\]

\[
\frac{1}{R} = \frac{1}{r} \left( 1 - \frac{1}{2} \left( \frac{r'}{r} \right) \left( \frac{r'}{r} - 2\cos \alpha \right) + \frac{3}{8} \left( \frac{r'}{r} \right)^2 \left( \frac{r'}{r} - 2\cos \alpha \right)^2 - \frac{5}{16} \left( \frac{r'}{r} \right)^3 \left( \frac{r'}{r} - 2\cos \alpha \right)^3 + \ldots \right)
\]

Collect terms in powers of \( (r'/r) \)

\[
\frac{1}{R} = \frac{1}{r} \left( 1 + \left( \frac{r'}{r} \right) \cos \alpha + \left( \frac{r'}{r} \right)^2 \left( \frac{3\cos^2 \alpha - 1}{2} \right) + \left( \frac{r'}{r} \right)^3 \left( \frac{5\cos^3 \alpha - 3\cos \alpha}{2} \right) + \ldots \right)
\]

\[
P_n \text{ are the Legendre polynomials... It is a generating function for multipole expansions}
\]

Now substitute back into the integral
**Chp-10 Electric fields in Matter**

**Generalized Multipole Expansion**

The potential \( \phi(\mathbf{r}) \) at a point \( \mathbf{r} \) due to a distribution of charge densities \( \rho(\mathbf{r}') \) over a region defined by \( \mathbf{r}' \) can be expressed as a series expansion known as the Generalized Multipole Expansion (GME).

\[
\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}')}{\mathbf{R}} \, d\mathbf{v}'
\]

Where

\[
\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \sum_{n=0}^{\infty} \frac{1}{r^{(n+1)}} \int (r')^n P_n(\cos \alpha) \rho(\mathbf{r}') \, d\mathbf{v}'
\]

The potential can be written as:

\[
\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \left[ \frac{1}{r} \int \rho(\mathbf{r}') \, d\mathbf{v}' + \frac{1}{r^2} \int r' \cos \alpha \, \rho(\mathbf{r}') \, d\mathbf{v}' + \frac{1}{r^3} \int (r')^2 \left( \frac{3}{2} \cos^2 \alpha - \frac{1}{2} \right) \rho(\mathbf{r}') \, d\mathbf{v}' \right] + ...
\]

**Monopole**

**Dipole**

**Quadrupole**

**Multipole Expansion for the potential in terms of 1/r**

(Exact expression if all terms included)

Integral depends on the angle \( \alpha \) between \( \mathbf{r} \) & \( \mathbf{r}' \)

If you orient so \( \mathbf{r} \) is on \( z' \) axis (i.e. \( P \) on \( z' \) axis)

\( \alpha \) becomes the polar angle \( \theta' \)
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Multipole Expansion as an approximation to the potential

\[ \phi_{\text{monopole}}(r) = \frac{1}{4\pi\varepsilon_0} \frac{Q}{r} \quad \text{where} \quad Q = \int \rho dv \]

Monopole term dominates at large \( r \)

**Dipole term**

\[ \phi_{\text{dipole}}(r) = \frac{1}{4\pi\varepsilon_0} \frac{1}{r^2} \int r' \cos \alpha \rho(r')dv' \]

\[ \cos \alpha = \frac{r \cdot r'}{r r'} \quad \text{so} \quad r' \cos \alpha = \hat{r} \cdot r' \]

\[ \phi_{\text{dipole}}(r) = \frac{1}{4\pi\varepsilon_0} \frac{1}{r^2} \hat{r} \cdot \int r' \rho(r')dv' \]

\[ p = \int r' \rho(r')dv' \quad p = \text{dipole moment of the charge distribution} \]

\[ \phi_{\text{dipole}}(r) = \frac{1}{4\pi\varepsilon_0} \frac{p \cdot \hat{r}}{r^2} \quad \text{For a single dipole} \]
Where were we? Bound charges

Subdivide the dielectric into infinitesimal dipoles & integrate

\[
\phi_{\text{dipole}}(\mathbf{r}) = \frac{1}{4\pi \varepsilon_0} \frac{p \cdot \hat{\mathbf{r}}}{r^2}
\]

\[ \mathbf{P} \] Dipole moment per unit volume

\[ p = \mathbf{P} \, dv' \]

\[
\phi(\mathbf{r}) = \frac{1}{4\pi \varepsilon_0} \int_{\text{volume}} \frac{\mathbf{P}(\mathbf{r}')}{r'^2} \, dv'
\]

But note…

\[
\nabla' \left( \frac{1}{r} \right) = \hat{\mathbf{r}} \frac{1}{r^2}
\]

‘ notation indicates differentiation wrt the source coordinates (r’).
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Where were we? Bound charges

Subdivide the dielectric into infinitesimal dipoles & integrate

\[ \phi(r) = \frac{1}{4\pi\varepsilon_o} \int_{\text{volume}} P \cdot \nabla' \left( \frac{1}{r} \right) \, dv' \]

Integrate by parts using the product rule \( \nabla \cdot (fA) = f(\nabla \cdot A) + A \cdot (\nabla f) \)

\[ \phi(r) = \frac{1}{4\pi\varepsilon_o} \left[ \int_{\text{volume}} \nabla' \cdot \left( \frac{P}{r} \right) \, dv' - \int_{\text{volume}} \frac{1}{r} (\nabla' \cdot P) \, dv' \right] \]

\[ \phi(r) = \frac{1}{4\pi\varepsilon_o} \int_{\text{Surface}} \frac{1}{r} P \cdot \hat{n} \, da' - \frac{1}{4\pi\varepsilon_o} \int_{\text{volume}} \frac{1}{r} (\nabla' \cdot P) \, dv' \]
Resembles potentials of surface & volume charges

\[ \phi(r) = \frac{1}{4\pi\varepsilon_o} \int \frac{1}{r} \mathbf{P} \cdot \hat{n} \, d\mathbf{a}' - \frac{1}{4\pi\varepsilon_o} \int \frac{1}{r} (\nabla' \cdot \mathbf{P}) \, d\mathbf{v}' \]

\[ \sigma_b = \mathbf{P} \cdot \hat{n} \]
\[ \rho_b = -\nabla \cdot \mathbf{P} \]

The potential of a polarized dielectric material is the same as is produced by:

1. Surface charge density \( \sigma_b = \mathbf{P} \cdot \hat{n} \)

2. Volume charge density \( \rho_b = -\nabla \cdot \mathbf{P} \)

This is true for the \( \mathbf{E} \)-field too since the gradient is a linear operator

\[ \mathbf{E} = -\nabla \phi \]
Net result we can avoid integrating all the dipoles

We find the **bound charges** then calculate their fields

E.g. we could apply Gauss’s Law as we have seen

\[
\phi(r) = \frac{1}{4\pi \varepsilon_0} \int_{\text{Surface}} \frac{\sigma_b}{r} d\mathbf{a}' + \frac{1}{4\pi \varepsilon_0} \int_{\text{Volume}} \frac{\rho_b}{r} d\mathbf{v}'
\]

\[
\sigma_b = \mathbf{P} \cdot \mathbf{\hat{n}} \\
\rho_b = -\nabla \cdot \mathbf{P}
\]
Find the electric field produced by a uniformly polarized sphere, radius $R$

Set $z$ axis in the direction of polarization

Then determine bound charge densities

$$\sigma_b = \mathbf{P} \cdot \mathbf{n}$$
$$\rho_b = -\nabla \cdot \mathbf{P}$$

$$\rho_b = -\nabla \cdot \mathbf{P} = 0 \quad \text{Vol. bound charge density zero (since Polarization is uniform)}$$

$$\sigma_b = \mathbf{P} \cdot \mathbf{n} = P \cos \theta \quad \text{Surface bound charge density integrated over a sphere}$$

Solved in Ex 3.9 in Griffiths

$$\phi(r, \theta) = \frac{P}{3\varepsilon_o} \frac{r \cos \theta}{r^2} \quad \text{for } r < R \quad \text{Inside}$$

$$z = r \cos \theta$$

$$\phi(r, \theta) = \frac{P}{3\varepsilon_o} \frac{R^3}{r^2} \cos \theta \quad \text{for } r \geq R \quad \text{Outside}$$
Find the electric field produced by a uniformly polarized sphere, radius $R$.

\[
\phi(r, \theta) = \frac{P}{3\varepsilon_0} r \cos \theta \quad \text{for} \quad r < R
\]

Inside

\[
\phi(r, \theta) = \frac{P}{3\varepsilon_0} z
\]

Potential varies linearly in $z$ inside the sphere.

\[
E = -\nabla \phi = -\nabla \left[ \frac{P}{3\varepsilon_0} z \right] = -\frac{P}{3\varepsilon_0} \hat{z} = -\frac{1}{3\varepsilon_0} P \quad \text{for} \quad r < R
\]

Potential

http://homepage.ntu.edu.tw/~chernrl/
Find the electric field produced by a uniformly polarized sphere, radius $R$.

Inside

$$\phi(r, \theta) = \frac{P}{3\varepsilon_0} r \cos \theta \quad \text{for } r < R$$

Outside

$$\phi(r, \theta) = \frac{P}{3\varepsilon_0} \frac{R^3}{r^2} \cos \theta \quad \text{for } r \geq R$$

Potential outside the sphere is identical to perfect dipole at the origin!

$$\phi(r, \theta) = \frac{1}{4\pi\varepsilon_0} \frac{p \cdot \hat{r}}{r^2} \quad \text{for } r \geq r$$

$$p = \frac{4\pi}{3} R^3 P$$

http://homepage.ntu.edu.tw/~chernrl/
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- Physical Interpretation of bound charges
- E-field of a polarized dielectric is produced by the combined distribution of bound volume and surface charges

$$\rho_b = -\nabla \cdot \mathbf{P} \quad \sigma_b = \mathbf{P} \cdot \hat{n}$$

- Was this just abstract mathematical wizardry/bookkeeping?
  No the bound charges represent physical accumulations of charge!

- How do we understand this? Consider a line of dipoles in a polarized material…We get effective cancelation except at the end points
  Looks like a large charge displacement but really many small displacements

We call the net charge at the ends a bound charge

It is still attached (bound) to a specific atom or molecule

But it is still a charge!

How do we calculate the amount of bound charge?

Consider a cylinder of dielectric parallel to \( \mathbf{P} \)

Bound charge accumulated on right face

\[
p = P(A d) = qd
\]

\[
q = PA
\]
How do we calculate the amount of bound charge?

Consider a cylinder

Of dielectric parallel to $\mathbf{P}$

$p = P(Ad) = qd$

$q = PA$ ↔ Bound charge accumulated on right face

If the slab is cut perpendicular to the cylinder

$\sigma_b = \frac{q}{A} = P$

If the slab is cut at angle to the cylinder, charge is the same

$\sigma_b = \frac{q}{A_{\text{end}}} = P \cos \theta = \mathbf{P} \cdot \mathbf{\hat{n}}$

Physically, Polarization “paints” bound charge over the surface
If the polarization is nonuniform bound charge will also accumulate inside the dielectric as well as at the surface.

Without polarization Charges cancel (neutral)

With polarization Charges separate into Caps (surface bound charge)

The Integrated bound volume charge will be equal and opposite to the charge pushed out to the surface:

\[
\int_{Vol} \rho_b \, dv' = - \int_{Surface} \mathbf{P} \cdot \hat{n} \, da = - \int_{Vol} \nabla \cdot \mathbf{P} \, dv'
\]

Conclude

\[\rho_b = -\nabla \cdot \mathbf{P}\]
The field inside a dielectric

We started the derivation with formula for the potential for an ideal or perfect dipole

Atoms or molecules are real or physical dipoles (but tiny!)

Also the Polarization $\mathbf{P}$ is a continuous vector function

Does this raise flags of concern?

Outside the dielectric we are in the far field ($R \gg d$) so the dipole term dominates the expansion and we do not notice the discrete graininess of the real dipole
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What about inside the dielectric?

At the microscopic level of atoms/subatomic particles it would be impossible to integrate

Electric field would vary wildly in space and time at the microscopic level

But we are interested in the macroscopic field

i.e. the average over regions containing thousands of atoms

But not too large!

So we average (integrate) over regions smaller than object itself

\[ \int_{Vol} \rho_b \, dv' \]

Physicists and Mathematicians will Diverge here!
Assume we want to measure the macroscopic field near a point \( r \).

Integrate over a sphere of radius \( R \)

Macroscopic Field at \( r \) will be the sum of \( E \)-fields due to charges Inside & Outside the sphere

\[
E_r = E_{\text{out}} + E_{\text{in}}
\]

\[ R = 1000 \cdot 2a_o \]

\( a_o = \text{atomic radius} \)
Macroscopic Field at $\mathbf{r}$ will be the sum of $\mathbf{E}$-fields due to charges Inside & Outside the sphere

$\mathbf{E}_r = \mathbf{E}_{\text{out}} + \mathbf{E}_{\text{in}}$

The average $\mathbf{E}$-field over a sphere produced by charges outside, is equal to the field they produce at the center

$\mathbf{E}_{\text{out}}$ is the field at $\mathbf{r}$ due to dipoles outside the sphere

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int_{\text{outside}} \frac{\mathbf{P}(\mathbf{r}') \cdot \hat{\mathbf{r}}}{r^2} \, dV'$$
Chp-10 Electric fields in Matter

Macroscopic Field at \( r \) will be the sum of \( \mathbf{E} \)-fields due to charges Inside & Outside the sphere

\[
\mathbf{E}_r = \mathbf{E}_{\text{out}} + \mathbf{E}_{\text{in}}
\]

\( \mathbf{E}_{\text{in}} \) dipoles are too close...we can’t integrate safely!

But wait...we just need the average field

The average field within a sphere of radius \( R \) due to all the charge contained in the volume is

\[
\mathbf{E}_{\text{Ave}} = -\frac{1}{4\pi\varepsilon_0} \frac{\mathbf{p}}{R^3}
\]

(This is Eqn 3.105 in Griffiths)

(\( \mathbf{p} \) is the total dipole moment)
Chp-10 Electric fields in Matter

Macroscopic Field at \( \mathbf{r} \) will be the sum of \( \mathbf{E} \)-fields due to charges Inside & Outside the sphere

\[
\mathbf{E}_r = \mathbf{E}_{\text{out}} + \mathbf{E}_{\text{in}}
\]

Inside the sphere

\[
\mathbf{E}_{\text{in}} = -\frac{1}{3\varepsilon_o} \mathbf{P}
\]

Regardless of the charge distribution

Outside the sphere

\[
\mathbf{E}_{\text{in}} = -\frac{1}{4\pi\varepsilon_o} \frac{\mathbf{P}}{R^3}
\]

where \( \mathbf{p} = \frac{4}{3}\pi R^3 \mathbf{P} \)

We implicitly assumed our sphere is small enough that \( \mathbf{P} \) does not vary much over its volume… Wait what was the field of a uniformly polarized sphere?

\[
\mathbf{E} = -\nabla \phi = -\frac{1}{3\varepsilon_o} \mathbf{P}
\]

The term omitted for the outside integration gets put back in by \( \mathbf{E}_{\text{in}} \)!

See last lecture
Thus the macroscopic $E$-field can be obtained from the potential which is obtained by integrating over the entire dielectric!

$$
\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int_{\text{Volume}} \frac{\mathbf{P}(\mathbf{r}') \cdot \hat{\mathbf{r}}}{r^2} dV'
$$

We were properly calculating the average macroscopic field for inside the dielectric. All due to the fact that...

The average field over any sphere due to the charge inside is the same as the field at the center of a uniformly polarized sphere with the same total dipole moment.

*It would hold for other averaging geometries…but harder to prove*
**Chp-10 Electric fields in Matter**

- The Electric Displacement
- Gauss’s Law in the Presence of Dielectrics
- \( \mathbf{E} \)-field due to Polarization is the field due to bound charges

Bound Surface Charge
\[
\sigma_b = \mathbf{P} \cdot \hat{n}
\]

Bound Volume Charge
\[
\rho_b = -\nabla \cdot \mathbf{P}
\]

Let’s put it all together!

The \( \mathbf{E} \)-field due to all other charges (e.g. electrons in a conductor, ions in the material, etc.) is called the *free charge*

Any charge that is not due to Polarization of the dielectric material
In the Dielectric total charge density

\[ \rho = \rho_b + \rho_f \]  
Total Charge Density

Gauss’s law for a dielectric material is

\[ \varepsilon_o \nabla \cdot \mathbf{E} = \rho = \rho_b + \rho_f = -\nabla \cdot \mathbf{P} + \rho_f \]

\( \mathbf{E} \) is the total field not just that due to Polarization \( \mathbf{P} \)

Combine the two divergence terms and re-write defining the Electric Displacement \( \mathbf{D} \)

\[ \nabla \cdot (\varepsilon_o \mathbf{E} + \mathbf{P}) = \rho_f \]

define \( \mathbf{D} = \varepsilon_o \mathbf{E} + \mathbf{P} \)  
\( \mathbf{D} \) is the Electric Displacement

\[ \nabla \cdot \mathbf{D} = \rho_f \]  
Gauss’s Law for Dielectrics in Differential Form
Gauss’s Law in terms of the electric displacement

\[ \nabla \cdot \mathbf{D} = \rho_f \]

**Differential Form**

Griffith’s Eqn 4.22

\[ \int \mathbf{D} \cdot \hat{n} \, da = Q_{f \text{ enclosed}} \]

**Integral Form**

Griffith’s Eqn 4.23

Note this only refers to the free charge

But we can only control the free charge

Bond charge “comes along for the ride” once we put the free charge in place (creating an E-field…which induces the Polorization \( \mathbf{P} \))

Initially we start with knowing the free charge
But we do not initially know the bound charge

Given the correct symmetry, we can use Eqn 4.23 to calculate \( \mathbf{D} \) using the usual Gauss’s Law methods
Ex. 4.4 A long straight wire of charge line density \( \lambda \) is surrounded by rubber insulation out to radius \( a \). Find \( \mathbf{D} \)

\[
\lambda \quad a \\
\hspace{2cm} \hat{n} \quad \mathbf{D} \quad \mathbf{L}
\]

Gaussian surface

Flux through the cylinder ends
Will be zero by symmetry

Apply Integral form of Gauss’s Law (Eqn 4.23)

\[
\int \mathbf{D} \cdot \hat{n} \, da = \mathbf{D} \quad \int da = Q_{\text{f \, enclosed}} \\
\text{Surface} \quad \text{Surface}
\]

\[
A = 2\pi \, s L
\]

\[
2\pi \, s L \mathbf{D}_s = \lambda L \quad \text{so} \quad \mathbf{D} = \frac{\lambda}{2\pi \, s} \hat{s}
\]

This equation holds both inside & outside
The insulator…Outside \( \mathbf{P} = 0 \)

\[
\mathbf{D} = \varepsilon_o \mathbf{E} + \mathbf{P} \quad \text{so} \quad \mathbf{E} = \frac{\mathbf{D}}{\varepsilon_o} = \frac{\lambda}{2\pi \varepsilon_o s} \hat{s} \quad \text{for} \ s > a \\
\text{Outside}
\]

(we would need to know \( \mathbf{P} \) to calculate \( \mathbf{E} \) inside)
Gauss’s Law in terms of the electric displacement

\[ \nabla \cdot \mathbf{D} = \rho_f \]
Differential Form
Griffith’s Eqn 4.22

\[ \int_{\text{Surface}} \mathbf{D} \cdot \mathbf{n} \, da = Q_{\text{f enclosed}} \]
Integral Form
Griffith’s Eqn 4.23

Wait a minute…what about the surface bound charge \( \sigma_b \)?

We cannot apply the *differential* form of Gauss’s law precisely at the surface of a dielectric surface as \( \rho_b \) blows up along with the \( \text{Div} \mathbf{E} \)

The *integral* form of Gauss’s law is free of this issue

We can also treat the edge as having a finite thickness so the Polarization decays to zero…in which case there is no \( \sigma_b \)

* The polarization drops precipitously to zero outside the dielectric material…so its derivative is a delta function…The surface bound charge is this term (see Griffith’s Prob. 1.46)
A Deception Parallel…beware!

Griffith’s Eqn 4.22
\[ \nabla \cdot \mathbf{D} = \rho_f \]
Differential Form

Griffith’s Eqn 4.23
\[ \int \mathbf{D} \cdot \hat{n} \, da = Q_{\text{enclosed}} \]
Integral Form

Eq. 4.22 Looks exactly like Gauss’s law except with the free charge density and \( \mathbf{D} \)

Can we treat \( \mathbf{D} \) and \( \mathbf{E} \) the same way? No!

There is no Coulomb’s law for \( \mathbf{D} \)

\[ \mathbf{D}(\mathbf{r}) \neq \frac{1}{4\pi} \int \frac{\hat{\mathbf{r}}' \rho_f(\mathbf{r}') \, dv'}{r'^2} \]

Moreover the curl of \( \mathbf{D} \) is not always zero

\[ \nabla \times \mathbf{D} = \varepsilon_0 (\nabla \times \mathbf{E}) + (\nabla \times \mathbf{P}) = \nabla \times \mathbf{P} \]
Research Aside Linear & Nonlinear Optics

Introduction

Second Harmonic Generation (SHG) Microscopy

Collagen Imaging

Third Harmonic Generation (THG) Microscopy

Sensitive Imaging of Malaria Infection

Nonlinear Optical Effects

Tightly Focused Femtosecond Laser

Specific Material Properties
Nonlinear Harmonic Microscopy

SHG Changes With Membrane Potential
Nuriya et al. PNAS 103, 786 (2006)
Sacconi et al. PNAS 103, 3124 (2006)
Time Dependent Polarization

Linear optics
\[ P(t) = \chi^{(1)} E(t) \]

Nonlinear optics
if E field is very large
\[ P(t) = \chi^{(1)} E(t) + \chi^{(2)} E^2(t) + \chi^{(3)} E^3(t) + \ldots \]

SHG
THG

The nonlinear polarization produces an electric field
\[ \nabla^2 E - \frac{n^2}{c^2} \frac{\partial^2 E}{\partial t^2} = \frac{4\pi}{c^2} \frac{\partial^2 P^{NL}}{\partial t^2} \]
Consider the following electric field

\[ E(t) = E e^{-i\omega t} + E^* e^{i\omega t} \]

The second order nonlinear polarization will give

\[ P^{(2)}(t) = 2\chi^{(2)} E E^* + \chi^{(2)} \left( E^2 e^{-2i\omega t} + (E^*)^2 e^{2i\omega t} \right) \]

Virtual State

No generation of light

2 photons laser fundamental frequency

Jablonski energy diagram for SHG

Medium Must be Non centro-symmetric
Consider the same electric field

\[ E(t) = E e^{-i\omega t} + E^* e^{i\omega t} \]

The third order nonlinear polarization will give

\[ P^{(3)}(t) = 3\chi^{(3)}(E^2 E^* e^{-i\omega t} + E (E^*)^2 e^{i\omega t}) + \chi^{(3)}(E^3 e^{-3i\omega t} + (E^*)^3 e^{3i\omega t}) \]

Virtual State

Jablonski energy diagram for THG

- Changes refractive index of material
- 3 photons laser fundamental frequency
- Non resonant No energy deposition
- Sensitive to gradients in n or \( \chi^{(3)} \)

THG
SHG Imaging of Healthy Pericardium

Optical Sections from a z-stack from Human Heart Pericardium (fibrous layer)

SHG (green)
Collagen

2PAF (red)
elastin
SHG Imaging of Healthy Pericardium

Optical z-stack (64 µm) from Healthy Human Heart Pericardium

SHG (green) Collagen
Pericarditis is an Inflammation of the pericardium.
SHG Imaging of Human Pericarditis

Optical z-stack (64 μm) from Human Heart Pericarditis Case

SHG (green)
Collagen