Dielectric & Polarization

by Tony Shing

Overview:

- Model of electric dipole

- How to describe dipole arrangement: Polarization field $\vec{\boldsymbol{P}}$, bound charges ρ_b, σ_b

- Material under external $\vec{\boldsymbol{E}}$ field:

    - A special case of material model: <u>Linear dielectric</u>
    - Describe external field: Free charges ρ_f, σ_f, electric displacement field $\vec{\boldsymbol{D}}$

    (If linear dielectric is all you need, feel free to skip all vector calculus)

1　Electric Dipole

1.1　Insulators as Mixture of Dipoles

From chemistry, atoms in non-metalic substance join together by sharing electrons. The difference in atoms' electronegativity (i.e. strength of attracting outer shell electrons) causes uneven charge distribution around the atoms. For example,

- <u>Ionic bond</u> - One atom completely takes an electron from another, forming a pair of positive and negative ions.

    (add figure here: ionic bond)

- <u>Covalent bond</u> - Bonding electrons are shared by two atoms, but the atom with higher electronegativity pulls the electrons closer to itself, forming a polar covalent bond.

    (add figure here: covalent bond)

In the classical model, we can view a non-metal object (i.e. insulator, also called **dielectric**) as a structure of charges, but using **electric dipoles** as the basic unit.

(add figure here: stacking dipoles in ionic bond/ covalent bond)

Since electric dipoles emit E-field, theoretically all materials are sources of E-field. However the dipoles in real life are at atomic scale ($\sim 10^{-10}$ m) and are usually packed in random orientations, the net field can be treated as zero if we view the dipoles from a very large distance.

(add figure here: view at short distance vs long distance)

So electric properties of materials are normally unobservable, unless we apply an external E-field to align the dipoles in some direction, i.e. we **polarize** the material.

(add figure here: many dipole from random direction flip to the same direction)

1.2   Fields of Electric Dipole

Since electric dipole is the basic unit of dielectric, we can first analyze the field emitted by a single dipole, then sum the contributions from all dipoles according to the material structure. Rhe classical model of electric dipole is as follows:

(add figure here: electric dipole model)

- Both ends of the dipole have equal but opposite *point* charge $+q$ and $-q$.

- Separation between the charges is labelled by a vector $\vec{d}$, which points from the negative charge to the positive charge.

- We are only interested in the potential/field far away from the dipole, i.e. $|\vec{r}| \gg |\vec{d}|$. The position vector $\vec{r}$ is referenced from the center of the dipole.

1.2.1   Potential by Electric Dipole

Deriving electric potential from a dipole is straightforward by Coulomb's law, while applying Taylor approximation in the middle step.

1. The total potential contributions from the two charges towards position $\vec{r}$ is

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0} \left(\frac{q}{|\vec{r}_+|} + \frac{-q}{|\vec{r}_-|} \right)$$

$$= \frac{q}{4\pi\epsilon_0} \left(\underbrace{\frac{1}{\sqrt{|\vec{r}|^2 + \left|\frac{\vec{d}}{2}\right|^2 - 2|\vec{r}|\left|\frac{\vec{d}}{2}\right|\cos\theta}}}_{} - \underbrace{\frac{1}{\sqrt{|\vec{r}|^2 + \left|\frac{\vec{d}}{2}\right|^2 + 2|\vec{r}|\left|\frac{\vec{d}}{2}\right|\cos\theta}}}_{} \right)$$

<div align="center">↑————— These are just cosine law —————↑</div>

$$= \frac{q}{4\pi\epsilon_0|\vec{r}|} \left(\frac{1}{\sqrt{1 + \frac{1}{4}\frac{|\vec{d}|^2}{|\vec{r}|^2} - \frac{|\vec{d}|}{|\vec{r}|}\cos\theta}} - \frac{1}{\sqrt{1 + \frac{1}{4}\frac{|\vec{d}|^2}{|\vec{r}|^2} + \frac{|\vec{d}|}{|\vec{r}|}\cos\theta}} \right)$$

2. Taylor expansion "$(1+x)^n \approx 1 + nx$ for $x \ll 1$" is always applied at this step. Because we are only interested in the potential far from the dipole, $\frac{|\vec{d}|}{|\vec{r}|} \ll 1$,

- $\frac{1}{4}\frac{|\vec{d}|^2}{|\vec{r}|^2} \approx 0$

- $\frac{1}{\sqrt{1 - \frac{|\vec{d}|}{|\vec{r}|}\cos\theta}} = \left(1 - \frac{|\vec{d}|}{|\vec{r}|}\cos\theta\right)^{-\frac{1}{2}} \approx 1 + \frac{1}{2}\cdot\frac{|\vec{d}|}{|\vec{r}|}\cos\theta$

So the potential becomes

$$V(\vec{r}) = \frac{q}{4\pi\epsilon_0|\vec{r}|} \left[\left(1 + \frac{1}{2}\frac{|\vec{d}|}{|\vec{r}|}\cos\theta\right) - \left(1 - \frac{1}{2}\frac{|\vec{d}|}{|\vec{r}|}\cos\theta\right) \right]$$

$$= \frac{q}{4\pi\epsilon_0|\vec{r}|}\frac{|\vec{d}|}{|\vec{r}|}\cos\theta$$

3. From geometry, θ is the angle between $\vec{d}$ and $\vec{r}$. We can replace $\cos\theta$ by $\cos\theta = \frac{\vec{d}\cdot\vec{r}}{|\vec{d}||\vec{r}|}$

$$V(\vec{r}) = \frac{q}{4\pi\epsilon_0}\frac{|\vec{d}|}{|\vec{r}|^2}\frac{\vec{d}\cdot\vec{r}}{|\vec{d}||\vec{r}|}$$

$$= \frac{1}{4\pi\epsilon_0}\frac{q\vec{d}}{|\vec{r}|^2}\underbrace{\left(\frac{\vec{r}}{|\vec{r}|}\right)}_{\text{Unit vector of }\vec{r}}$$

4. To emphasize that we now treat an electric dipoles as "one unit of source", We define the **electric dipole moment $\vec{p}$**,

$$\boxed{\vec{p} \overset{\text{def}}{=} q\vec{d}}$$

Finally we reach the standard formula of electric potential from an electric dipole:

$$\boxed{V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{\vec{p}\cdot\hat{r}}{|\vec{r}|^2}}$$

As a comparison with Columb's law formula from point charge

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{q}{|\vec{r}|}$$

(add figure here: V from point charge source)

- Charge is just a number, not directional.
- Dependance on distance is $\frac{1}{r}$.

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{\vec{p}\cdot\hat{r}}{|\vec{r}|^2}$$

(add figure here: V from dipole source)

- Dipole is directional. Magnitude of potential depends on the charges' magnitude AND the angle (dot product) between $\vec{p}$ and $\hat{r}$.
- Dependance on distance is $\frac{1}{r^2}$.

1.2.2   E-field by Electric Dipole

The standard derivation of E-field from dipole is through the relation $\vec{\boldsymbol{E}} = -\vec{\boldsymbol{\nabla}}V$. It is nothing more than some boring calculus. Here I quote the final result:

$$\vec{\boldsymbol{E}}(\vec{\boldsymbol{r}}) = \frac{1}{4\pi\epsilon_0}\frac{3(\vec{\boldsymbol{p}}\cdot\hat{\boldsymbol{r}})\hat{\boldsymbol{r}} - \vec{\boldsymbol{p}}}{|\vec{\boldsymbol{r}}|^3}$$

And this formula is rarely used because vector calculation is annoying.

The boring derivation:

1. Derivation is possible with high school calculus if we turn all vectors into x-y-z form: $\vec{r} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}}$, $|\vec{r}| = \sqrt{x^2 + y^2 + z^2}$ and $\vec{\boldsymbol{p}} = p_x\hat{\boldsymbol{x}} + p_y\hat{\boldsymbol{y}} + p_z\hat{\boldsymbol{z}}$:

$$\frac{\vec{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}}}{|\vec{r}|^2} = \frac{\vec{\boldsymbol{p}}}{|\vec{r}|^2} \cdot \frac{\vec{r}}{|\vec{r}|} = \frac{1}{|\vec{r}|^3}(\vec{\boldsymbol{p}} \cdot \vec{r}) = \frac{1}{(x^2 + y^2 + z^2)^{\frac{3}{2}}}(p_x x + p_y y + p_z z)$$

2. First the x term in gradient, $\hat{\boldsymbol{x}}\dfrac{\partial}{\partial x}(\cdots)$, can be calculated by:

$$\hat{\boldsymbol{x}}\frac{\partial}{\partial x}\left[\frac{1}{(x^2+y^2+z^2)^{\frac{3}{2}}}(p_x x + p_y y + p_z z)\right] \quad \textcolor{blue}{\text{This is just quotient rule}}$$

$$= \frac{\hat{\boldsymbol{x}}}{(x^2+y^2+z^2)^3}\left[p_x(x^2+y^2+z^2)^{\frac{3}{2}} - (p_x x + p_y y + p_z z) \cdot 3x(x^2+y^2+z^2)^{\frac{1}{2}}\right]$$

$$= \frac{1}{(x^2+y^2+z^2)^{\frac{5}{2}}}\left[p_x\hat{\boldsymbol{x}}\underline{(x^2+y^2+z^2)} - \underline{(p_x x + p_y y + p_z z)} \cdot 3x\hat{\boldsymbol{x}}\right]$$

$$= \frac{1}{|\vec{r}|^5}\left[p_x\hat{\boldsymbol{x}}\underline{|\vec{r}|^2} - 3\underline{(\vec{\boldsymbol{p}} \cdot \vec{r})}x\hat{\boldsymbol{x}}\right]$$

3. Similar for y and z terms:

$$\hat{\boldsymbol{y}}\frac{\partial}{\partial y}(\cdots) = \frac{1}{|\vec{r}|^5}\left[p_y\hat{\boldsymbol{y}}|\vec{r}|^2 - 3(\vec{\boldsymbol{p}} \cdot \vec{r})y\hat{\boldsymbol{y}}\right]$$

$$\hat{\boldsymbol{z}}\frac{\partial}{\partial z}(\cdots) = \frac{1}{|\vec{r}|^5}\left[p_z\hat{\boldsymbol{z}}|\vec{r}|^2 - 3(\vec{\boldsymbol{p}} \cdot \vec{r})z\hat{\boldsymbol{z}}\right]$$

4. Summing all 3 components gives:

$$-\vec{\boldsymbol{\nabla}}V(\vec{r}) = -\left(\hat{\boldsymbol{x}}\frac{\partial V}{\partial x} + \hat{\boldsymbol{y}}\frac{\partial V}{\partial y} + \hat{\boldsymbol{z}}\frac{\partial V}{\partial z}\right)$$

$$= -\frac{1}{4\pi\epsilon_0}\frac{1}{|\vec{r}|^5}\left[\underline{(p_x\hat{\boldsymbol{x}} + p_y\hat{\boldsymbol{y}} + p_z\hat{\boldsymbol{z}})}|\vec{r}|^2 - 3(\vec{\boldsymbol{p}} \cdot \vec{r})\underline{(x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}})}\right]$$

$$= \frac{1}{4\pi\epsilon_0}\frac{1}{|\vec{r}|^5}\left[3(\vec{\boldsymbol{p}} \cdot \vec{r})\underline{\vec{r}} - \underline{\vec{\boldsymbol{p}}}|\vec{r}|^2\right]$$

$$\textcolor{red}{\text{Take out magnitude to become unit vector}}$$

$$= \frac{1}{4\pi\epsilon_0}\frac{1}{|\vec{r}|^5}\left[3(\vec{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}})\hat{\boldsymbol{r}}\,|\vec{r}|^2 - \vec{\boldsymbol{p}}|\vec{r}|^2\right]$$

$$\boxed{\vec{\boldsymbol{E}}(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{3(\vec{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}})\hat{\boldsymbol{r}} - \vec{\boldsymbol{p}}}{|\vec{r}|^3}}$$

2 Describing Dipole Arrangement

In general, all dielectric materials are made of many tiny electric dipoles. To analyze the material's electric properties, we can begin with the property of a single dipole, then sum the contributions of all dipoles according to the dipole arrangement in the material.

(add figure here: NaCl, H2O by dipole arrangement)

For example, the electric potential created by the material can be treated as a sum of potentials from all dipoles.

$$\underbrace{V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{\vec{p}}{|\vec{r}|^2}\cdot\left(\frac{\vec{r}}{|\vec{r}|}\right)}_{\text{By a single dipole from origin}} \qquad\Rightarrow\qquad \underbrace{V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\sum_{\text{All dipoles } i}\frac{\vec{p}_i}{|\vec{r}-\vec{r}_i|^2}\cdot\left(\frac{\vec{r}-\vec{r}_i}{|\vec{r}-\vec{r}_i|}\right)}_{\text{By many dipoles at different positions } \vec{r}_i}$$

(add figure here: single dipole point to r vs many dipoles at different ri to r)

Here we introduce two quantities that describe electric dipole arrangements in materials.

- **Polarization field** - $\vec{P}(\vec{r})$

- **Bound charge distributions** - $\rho_b(\vec{r})$ and $\sigma_b(\vec{r})$

2.1 Polarization Field

When the dipoles in the material are so dense such that we can treat them as a continuous distribution, we can replace

- Sum of all dipoles $\xRightarrow{\text{become}}$ Volume integral over the whole object.

- Discrete dipoles source $\xRightarrow{\text{become}}$ A vector distribution called **polarization field** $\vec{P}(\vec{r})$.

$$\boxed{V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\iiint\limits_{\substack{\text{Whole}\\\text{material}}}\frac{\vec{P}(\vec{r}')}{|\vec{r}-\vec{r}'|^2}\cdot\left(\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right)\mathrm{d}^3\vec{r}'}$$

(add figure here: dispole arrangement is similar to some vector field in the object)

The polarization field $\vec{P}(\vec{r})$ can also be interpreted as **electric dipole density** because its usage is similar to charge density $\rho(\vec{r})$. Comparing with the Coulomb's law for electric potential:

- When the source is made of charges:

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\iiint\frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}\,\mathrm{d}^3\vec{r}' \quad\sim\quad \frac{1}{4\pi\epsilon_0}\sum\frac{(\text{charge density})}{(\text{distance})}$$

- When the source is made of dipoles:

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\iiint\frac{\vec{P}(\vec{r}')}{|\vec{r}-\vec{r}'|^2}\cdot\left(\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right)\mathrm{d}^3\vec{r}' \quad\sim\quad \frac{1}{4\pi\epsilon_0}\sum\frac{(\text{dipole density})}{(\text{distance})^2}\cdot\left(\substack{\text{unit}\\\text{vector}}\right)$$

(add figure here: charge density vs dipole density in the same material)

2.2 Bound Charge Distribution

Ultimately, electric dipoles are just pairs of charges. If the dipoles are aligned non-uniformly in a material, some regions may appear to have a higher density of positive heads than its surroundings, and so as negative tails.

<p style="color:red; text-align:center">(add figure here: dipole heads and tails non uniform)</p>

These regions with extra dipole heads / tails are described as **bound charges** distribution in the material - they are always "bounded" to regions where there are more dipole heads/tails. So bound charge distribution can be used to describe electric dipole arrangement in the material.

2.2.1 Mathematical Origin

With vector calculus, the potential formula can be rewritten into a "charge densities form".

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0} \iiint_{\substack{\text{Whole} \\ \text{material}}} \frac{\vec{P}(\vec{r}')}{|\vec{r} - \vec{r}'|^2} \cdot \left(\frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|} \right) \mathrm{d}^3\vec{r}'$$

$$= (\cdots \text{ After more boring vector calculus } \cdots)$$

$$= \frac{1}{4\pi\epsilon_0} \iiint_{\substack{\text{Whole} \\ \text{material}}} \frac{-\vec{\nabla} \cdot \vec{P}(\vec{r}')}{|\vec{r} - \vec{r}'|} \mathrm{d}^3\vec{r}' + \frac{1}{4\pi\epsilon_0} \oiint_{\substack{\text{Surface} \\ \text{of material}}} \frac{\vec{P}(\vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \mathrm{d}^2\vec{r}'$$

By comparing with the Coulomb's law for electric potential $V \sim \frac{1}{4\pi\epsilon_0} \sum \frac{(\text{charge density})}{(\text{distance})}$, we identify the 2 source terms as the **bound charge densities**:

– **The 1ˢᵗ term:**

$$\frac{1}{4\pi\epsilon_0} \iiint_{\substack{\text{Whole} \\ \text{material}}} \frac{-\vec{\nabla} \cdot \vec{P}(\vec{r}')}{|\vec{r} - \vec{r}'|} \mathrm{d}^3\vec{r}' \quad \sim \quad \frac{1}{4\pi\epsilon_0} \sum_{\substack{\text{Inside} \\ \text{material}}} \frac{(-\vec{\nabla} \cdot \vec{P})}{(\text{distance})}$$

$-\vec{\nabla} \cdot \vec{P}$ appears as some charge density distributed <u>inside</u> the material. Therefore it is defined as the **volume bound charge density** ρ_b.

$$\boxed{\rho_b(\vec{r}) \overset{\text{def}}{=} -\vec{\nabla} \cdot \vec{P}(\vec{r})}$$

– **The 2ⁿᵈ term:**

$$\frac{1}{4\pi\epsilon_0} \oiint_{\substack{\text{Surface} \\ \text{of material}}} \frac{\vec{P}(\vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \mathrm{d}^2\vec{r}' \quad \sim \quad \frac{1}{4\pi\epsilon_0} \sum_{\substack{\text{On material} \\ \text{surface}}} \frac{(\text{Flux of } \vec{P})}{(\text{distance})}$$

Flux of $\vec{P}$ on the material surface appears as some charge density distributed <u>on the surface</u> of the material. Therefore it is defined as the **surface bound charge density** σ_b.

$$\boxed{\sigma_b(\vec{r}) \overset{\text{def}}{=} \vec{P}(\vec{r}) \cdot \hat{n}}$$

where $\hat{n}$ is the (outward) unit normal vector on the material surface. Dot product with it to represent out-flux.

<p style="text-align:center">P.7</p>

Finally, the expression of the "charge densities form" is nothing more than saying that the electric potential from a material is the result of the two kinds of charges distributions.

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0} \underbrace{\iiint}_{\substack{\text{Whole} \\ \text{material}}} \frac{\rho_b(\vec{r'})}{|\vec{r} - \vec{r'}|} \, \mathrm{d}^3\vec{r'} \;+\; \frac{1}{4\pi\epsilon_0} \underbrace{\oiint}_{\substack{\text{Surface} \\ \text{of material}}} \frac{\sigma_b(\vec{r'})}{|\vec{r} - \vec{r'}|} \, \mathrm{d}^2\vec{r'}$$

$$= \begin{pmatrix} \text{Contribution} \\ \text{by charges inside} \\ \text{the material} \end{pmatrix} \;+\; \begin{pmatrix} \text{Contribution} \\ \text{by charges on} \\ \text{material's surface} \end{pmatrix}$$

The boring derivation:

1. Deriving the "charge densities" form begins with a vector calculus identity:

$$\vec{\boldsymbol{\nabla}}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right) = \left(\hat{\boldsymbol{x}}\frac{\partial}{\partial \underline{x'}} + \hat{\boldsymbol{y}}\frac{\partial}{\partial \underline{y'}} + \hat{\boldsymbol{z}}\frac{\partial}{\partial \underline{z'}}\right)\left(\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\right)$$

Note: Differentiation is w.r.t. x', y', z'

$$= \frac{\hat{\boldsymbol{x}}(x-x')+\hat{\boldsymbol{y}}(y-y')+\hat{\boldsymbol{z}}(z-z')}{[(x-x')^2+(y-y')^2+(z-z')^2]^{\frac{3}{2}}}$$

$$= \frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|^3}$$

This part is just a unit vector

$$= \frac{1}{|\vec{r}-\vec{r}'|^2}\left(\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right)$$

$\left(\text{This is basically } \frac{\mathrm{d}}{\mathrm{d}r'}\left(\frac{1}{r-r'}\right)=\frac{1}{(r-r')^2} \text{ but in vector version}\right)$

2. So the potential formula can be rewritten as:

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\iiint \frac{\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|^2}\cdot\left(\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right)\mathrm{d}^3\vec{r}'$$

$$= \frac{1}{4\pi\epsilon_0}\iiint \underbrace{\vec{\boldsymbol{P}}(\vec{r}')\cdot\vec{\boldsymbol{\nabla}}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)}_{\vec{G}\cdot\vec{\nabla}f}\mathrm{d}^3\vec{r}'$$

$$= \frac{1}{4\pi\epsilon_0}\iiint \underbrace{\vec{\boldsymbol{\nabla}}\cdot\left(\frac{\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|}\right)}_{\vec{\nabla}\cdot(f\vec{G})} - \underbrace{\frac{\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|}}_{-f(\vec{\nabla}\cdot\vec{G})}\mathrm{d}^3\vec{r}'$$

Here used the product rule of divergence $\boxed{\vec{\boldsymbol{\nabla}}\cdot(f\vec{G}) = f(\vec{\boldsymbol{\nabla}}\cdot\vec{G}) + (\vec{\boldsymbol{\nabla}}f)\cdot\vec{G}}$, where f is a scalar function (like $\frac{1}{|\vec{r}-\vec{r}'|}$) and $\vec{G}$ is a vector function (like $\vec{\boldsymbol{P}}$).

3. Finally use divergence theorem to convert the 1$^{\text{st}}$ term's volume integral into a surface integral over the volume's surface:

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\iiint \vec{\boldsymbol{\nabla}}\cdot\left(\frac{\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|}\right)\mathrm{d}^3\vec{r}' \ - \ \frac{1}{4\pi\epsilon_0}\iiint \frac{\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}^3\vec{r}'$$

Divergence theorem

$$= \frac{1}{4\pi\epsilon_0}\oiint \frac{\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|}\cdot\mathrm{d}^2\vec{r}' \ - \ \frac{1}{4\pi\epsilon_0}\iiint \frac{\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{P}}(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}^3\vec{r}'$$

$$= \left(\begin{array}{c}\text{Contribution}\\\text{from material's}\\\text{surface}\end{array}\right) \ + \ \left(\begin{array}{c}\text{Contribution}\\\text{from inside}\\\text{the material}\end{array}\right)$$

Remind that we are integrating regions where dipoles exist. So this volume integral corresponds to the whole material and surface integral corresponds to only the surface of the material.

2.2.2 Visualization

The bound charge densities are related to $\vec{P}$ pretty much like normal charge density are related to $\vec{E}$ in Gauss's law.

– **Volume bound charge**: By circling the regions with more dipole heads and treat the circle like a Gaussian surface, we can see

$$\boxed{\begin{array}{c}\text{More dipole} \\ \text{pointing into the circle}\end{array} \quad \Leftrightarrow \quad \begin{array}{c}\text{More positive charge} \\ \text{contained in the circle}\end{array}}$$

(add figure here: contain region dipole head)

Recall that we can use sign of flux to identify positions with converging/diverging vector field, and divergence operator $\vec{\nabla}\cdot$ is equivalent to finding flux per volume.

$$\begin{pmatrix}\text{Bound charge} \\ \text{volume density}\end{pmatrix} \sim \rho_b = -\vec{\nabla}\cdot\vec{P} \sim \begin{pmatrix}\text{\color{red}In}\text{-flux of dipole} \\ \text{per volume}\end{pmatrix}$$

– **Surface bound charge**: On the material surface, we can see that

$$\boxed{\begin{array}{c}\text{More dipole} \\ \text{pointing outward}\end{array} \quad \Leftrightarrow \quad \begin{array}{c}\text{More positive charge} \\ \text{on the material surface}\end{array}}$$

(add figure here: surface dipole head)

As we have defined the normal vector $\hat{n}$ of the material surface to be pointing outward, the more dipoles in the same direction as $\hat{n}$, the more positive charges on the surface. Therefore the definition of surface bound charge density involve dot product with $\hat{n}$.

$$\begin{pmatrix}\text{Bound charge} \\ \text{surface density}\end{pmatrix} \sim \sigma_b = \vec{P}\cdot\hat{n} \sim \begin{pmatrix}\text{Out-flux of dipole} \\ \text{per surface area}\end{pmatrix}$$

Side note:

Although all dielectric materials are made of dipoles, we almost never observe the $\vec{P}$ field or bound charges on daily-life objects because

– Magnitude of a dipole is too small. Typical atomic separation $d \sim 10^{-10}$ m, and so a dipole moment is of magnitude $\vec{p} = q\vec{d} \sim 1.6 \times 10^{-29}$ C·m.

– The dipoles are usually randomly arranged, or in patterns such that their effects cancel out. Especially when the material is large.

To most material, polarization effect is neligible unless it is placed under an external E-field, which forces its dipoles to align and "stretch" them harder (increase the $\vec{d}$ in dipole moment).

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3 Material under External E-field

If we place a single electric dipole under an external E-field, the dipole will rotate itself until it is in the same direction as the E-field.

(add figure here: single dipole under external E-field, flip)

However in a material structure, bondings/interactions exist between dipoles, which prevent the dipoles from freely rotating. So the final dipole alignment might not always align with the external E-field!

(add figure here: many dipoles under external E-field, not fully align)

In reality, fully model a material's response to E-field can be very complicated. The general theory assumes the polarization field $\vec{P}$ (i.e. new dipole alignment) as some function to the total E-field $\vec{E}_{\text{total}}$:

$$\vec{P} \;=\; f(\vec{E}_{\text{total}}) \;\sim\; \underbrace{\vec{a}_i^{(1)} E_i + \vec{a}_{ij}^{(2)} E_i E_j + \vec{a}_{ijk}^{(3)} E_i E_j E_k + \cdots}_{\text{Like a Taylor expansion}}$$

This f function denotes a theoretical model that we have choosen to investigate the material. And the model parameters $\vec{a}^{(1)}, \vec{a}^{(2)}, \vec{a}^{(3)}...$ shall be determined from experiment.

(add figure here: random spherical dipole + regular external E-field = irregular align ellipse dipole)

3.1 Special Case: Linear Dielectric

Linear dielectric is the simplest model of E-field reponse - where the dipoles are completely free to rotate, such that new dipole alignment is directly proportional to the external E-field's magnitude and direction. This assumption is applicable to most daily life materials.

(add figure here: dipoles uniform under external E-field)

The linear model only has 1 parameter to be determined from experiments - the proportionality constant between $\vec{P}$ and $\vec{E}_{\text{total}}$.

$$\boxed{\vec{P} = \epsilon_0 \chi_e \vec{E}_{\text{total}}}$$

Here the χ_e is called **electric susceptibility**, a pure number (no unit) whose value depends on the type of material. ϵ_0 is multiplied to match the units.

- $\chi_e = 0$ for vacuum (by defintion), because there are no dipoles in a vacuum.

- $\chi_e > 0$ for normal materials, because dipoles normally follow E-field's direction.

3.2 Describing External Field

The total E-field is a result of the external E-field plus the field induced by dipole alignment. After we have chosen the model about dipole alignment, now we look at the external E-field.

3.2.1 Free Charge Distribution

In order to create an external E-field around the material, we need a "setup" to build an external source of charges. For example, apply voltage between two very large parallel plates:

(add figure here: free charge vs bound charge in dielectric setup)

The charges that build up in the setup are given the name **free charges**, to distinguish from the bound charges (dipole alignment) in the material. The are "free" because we can always control them by varying the setup, making them known quantities in calculation.

(add figure here: adjust parallel plate voltage -¿ adjust free charge amount)

$$\frac{\sigma_{\text{free}}}{\epsilon_0} = |\vec{E}| = \frac{V}{d}$$

For calculation, free charge densities are denoted like bound charges:

- **Volume free charge density** $\rho_f(\vec{r})$ - Charge distribution <u>inside</u> the setup.
- **Surface free charge density** $\sigma_f(\vec{r})$ - Charge <u>on any surfaces</u> of the setup.

In real practices, a pair of parallel plates is the most common setup to create external E-field. So surface free charge is mostly all you need. No reason to make things complicated.

3.2.2 Displacement Field $\vec{D}$

Previously, we have relate bound charges to a vector field quantity - the polarization field $\vec{P}$. Similarly, free charges distributions can be related with another vector field. From Gauss's law,

$$
\begin{aligned}
\epsilon_0 \vec{\nabla} \cdot \vec{E}_{\text{total}} = \quad \rho_{\text{total}} &= \left(\begin{matrix} \text{All} \\ \text{charges} \end{matrix} \right) \\
= \rho_f + \rho_b &= \left(\begin{matrix} \text{Free charges} \\ \text{on setup} \end{matrix} \right) + \left(\begin{matrix} \text{Bound charges} \\ \text{on material} \end{matrix} \right) \\
&= \rho_f + (-\vec{\nabla} \cdot \vec{P}) \\
\vec{\nabla} \cdot \left(\epsilon_0 \vec{E}_{\text{total}} + \vec{P} \right) &= \rho_f
\end{aligned}
$$

Here we define the **displacement field $\vec{D}$**:

$$\boxed{\vec{D} \overset{\text{def}}{=} \epsilon_0 \vec{E}_{\text{total}} + \vec{P}} \quad \longleftarrow \quad \text{\color{red}{This relation connects all 3 field quantities}}$$

Such that it is related to the free charge density by:

$$\boxed{\begin{cases} \rho_f(\vec{r}) \overset{\text{def}}{=} \vec{\nabla} \cdot \vec{D}(\vec{r}) \\ \sigma_f(\vec{r}) \overset{\text{def}}{=} \vec{D}(\vec{r}) \cdot \hat{n} \end{cases}}$$

where $\hat{n}$ is the (outward) unit normal vector on the equipment surface. Dot product with it to represent out-flux.

Notice the relations of $\vec{D}$ with free charges are almost identical to $\vec{E}$ with total charges in Gauss's law. In the special case of linear dielectric, we can solve for $\vec{D}$ from the given free charges like the Gauss's law integral form or with Coulomb's law.

$$Q_f = \oiint \vec{D}(\vec{r}) \cdot \mathrm{d}\vec{s}$$

$$= \oiint |\vec{D}||\,\mathrm{d}\vec{s}\,|\cos\theta \quad \longleftarrow \quad \text{Just dot product} \atop \vec{a}\cdot\vec{b} = |\vec{a}||\vec{b}|\cos\theta$$

$$= |\vec{D}|\,\cos\theta \oiint |\,\mathrm{d}\vec{s}\,|$$

Same magnitude everywhere — Can move out of integral   Form same angle everywhere — Can move out of integral

$$= |\vec{D}|\,\cos\theta\,(\text{Total surface area})$$

$$\boxed{|\vec{D}| = \frac{Q_f}{(\text{Total surface area})\cos\theta}}$$

But note that this can be wrong for other models of dielectrics.

Side Note:

Although $\vec{D}$ forms a PDE relationship to free charge just like $\vec{E}_{\text{total}}$ with total charge, we cannot solve for $\vec{D}$ exactly by free charge if we don't know the material's model. This is because:

- $\vec{E}_{\text{total}}$ is guarenteed to be "curl-less" in electrostatics, such that we can define a potential function V and solve for $\vec{E}_{\text{total}}$ uniquely.

- $\vec{P}$ may not be "curl-less" since the dipole arrangement can be arbituary, e.g. if they arrange into some vortex-like pattern. Then by $\vec{D} = \epsilon_0\vec{E}_{\text{total}} + \vec{P}$, there is no guarenteed that $\vec{D}$ is "curl-less" either.

   (add figure here: vortex dipole arrangement -¿ P field not curl 0)

But in the special case of linear dielectric,

$$\boxed{\vec{P} \text{ aligns} \atop \text{with } \vec{E}_{\text{total}}} \quad \Rightarrow \quad \boxed{\vec{P} \text{ is} \atop \text{"curl-less"}} \quad \Rightarrow \quad \boxed{\vec{D} = \epsilon_0\vec{E}_{\text{total}} + \vec{P} \atop \text{is also "curl-less"}}$$

So it is fine to solve for $\vec{D}$ like normal Gauss's law problems for linear dielectric.

3.3   Measurement in Practice

In problems that involve dielectric,

- The material's polarization (dipole alignment) is the cause of all troubles. But usually we are only told which material model we need to apply. *(E.g. Given a linear dielectric ...)*

– Actual calculation requires measurements from equipment setup. In electrostatic experiments, usually the control/measure-able parameters are

  – Applied voltage - Directly connect with a power source. All you need is a voltmeter.
  – Free charge - If the amount of charge is manually placed on the setup.

(add figure here: control set up with voltage or free charge procedure)

Note that

  – Applied voltage can be used to determine to total E-field $\vec{E}_{\text{total}}$

  – Free charge can be used to determine to displacement field $\vec{D}$.

Once we have chosen a model of the material, we can connect the two measurables by:

$$\vec{D} = \epsilon_0 \vec{E}_{\text{total}} + f(\vec{E}_{\text{total}})$$

Then the model parameters in $f(\cdots)$ can be determined by experiments. But in the special case of linear dielectric, since there is only 1 constant parameter χ_e for each material,

$$\vec{D} = \epsilon_0 \vec{E}_{\text{total}} + \epsilon_0 \chi_e \vec{E}_{\text{total}}$$
$$= \epsilon_0 (1 + \chi_e) \vec{E}_{\text{total}}$$
$$= (\text{A constant}) \cdot \vec{E}_{\text{total}}$$

We usually use this new constant to represent the material's response to E-field, by defining

$$\boxed{\epsilon \overset{\text{def}}{=} \epsilon_0 (1 + \chi_e) \overset{\text{def}}{=} \epsilon_0 \epsilon_r} \qquad \text{such that} \qquad \vec{D} = \epsilon \vec{E}_{\text{total}}$$

where

  – ϵ = **Absolute permittivity**, or **dielectric constant**. Has the same unit as ϵ_0.

  – ϵ_r = **Relative permittivity**. A pure number that normally > 1. Material handbooks usually tabulate values of ϵ_r of different materials.

Material scientists prefer using ϵ instead of χ_e is likely for convenience - since $\vec{D}$ and $\vec{E}_{\text{total}}$ are the measureables (through free charge and voltage), the slope in a $|\vec{D}|$ v.s. $|\vec{E}_{\text{total}}|$ graph immediately gives the value of ϵ. *Too lazy to convert it back to χ_e.*

(add figure here: D v.s. E plot -¿ slope = epsilon)

3.4   Calculation Example

Here are some examples of questions you may see in the chapter of linear dielectric. In principle, one of the information about $\vec{D}$ (free charge) or $\vec{E}_{\text{total}}$ (voltage) will be given, then you are asked to find the other, and so as $\vec{P}$ and bound charges.

Example 3.1. Consider two pieces of material, each with relativity permittivity ϵ_1, ϵ_2, being placed between two large parallel plates. The plates are initially charged up to a surface density $\pm \sigma$ before putting in the materials. Assume the plates to be large enough such that the charged density and total E-field are uniform.

1. A good start is to label all the charges locations, and if they are free/bounded.

2. Always remember that $\vec{D}$ is only related to the free charges. In this configuration, $\pm\sigma$ is the exact amount of free charge density on the plates since they are the manually placed in. This $\vec{D}$ is the same everywhere between the plates.

$$|\vec{D}| = \sigma_f = \sigma$$

3. According to the linear dielectric model, E-field is proportional to the $\vec{D}$ by the dielectric constant at that location, i.e. $\vec{D} = \epsilon\vec{E}$. Because we have the same $\vec{D}$ everywhere,

   - In vacuum, $|\vec{E}| = \dfrac{|\vec{D}|}{\epsilon_0} = \dfrac{\sigma}{\epsilon_0}$

   - In material 1, $|\vec{E}| = \dfrac{|\vec{D}|}{\epsilon_1} = \dfrac{\sigma}{\epsilon_1}$

   - In material 2, $|\vec{E}| = \dfrac{|\vec{D}|}{\epsilon_2} = \dfrac{\sigma}{\epsilon_2}$

4. Then we can find $\vec{P}$ by $\vec{P} = \vec{D} - \epsilon_0\vec{E}$:

   - In vacuum, $|\vec{P}| = |\vec{D}| - |\vec{D}| = 0$ (Obviously)

   - In material 1, $|\vec{P}| = |\vec{D}| - \epsilon_0|\vec{E}| = |\vec{D}| - \epsilon_0 \cdot \dfrac{|\vec{D}|}{\epsilon_1} = \left(1 - \dfrac{\epsilon_0}{\epsilon_1}\right)\sigma$

   - In material 2, $|\vec{P}| = |\vec{D}| - \epsilon_0|\vec{E}| = |\vec{D}| - \epsilon_0 \cdot \dfrac{|\vec{D}|}{\epsilon_2} = \left(1 - \dfrac{\epsilon_0}{\epsilon_2}\right)\sigma$

   According to $\vec{P} \cdot \hat{\boldsymbol{n}} = \sigma_b$, the $|\vec{P}|$ on each material are also the amount of surface bound charge densities on each of the materials' surfaces.

Example 3.2. Consider two uniform spherical shells of radius R_1, R_2 connected by a voltage source V. A layer of material with dielectric constant ϵ and thickness w is covering the inner shell.

1. This time we are only given the applied voltage but not the free charge. However we can always tell that there must be some free charges on the shells. Let the total free charges to be $\pm Q_f$.

(add figure here: label free charge on spherical shell)

2. By symmetry, $\vec{D}$ must be uniform and radially outward. We can apply Gauss's law integral form for $\vec{D}$:

$$Q_f = \oiint \vec{D} \cdot \mathrm{d}\vec{s} = |\vec{D}| \cdot 4\pi r^2 \qquad \Rightarrow \qquad |\vec{D}| = \frac{Q_f}{4\pi r^2}$$

This is the $\vec{D}$ everywhere between the shells, which is function to radial distance r.

3. According to the linear dielectric model, E-field is proportional to the $\vec{D}$ by the dielectric constant at that location.

   – In the dielectric layer, $|\vec{E}| = \dfrac{|\vec{D}|}{\epsilon} = \dfrac{Q_f}{4\pi\epsilon r^2}$

   – In the vacuum layer, $|\vec{E}| = \dfrac{|\vec{D}|}{\epsilon_0} = \dfrac{Q_f}{4\pi\epsilon_0 r^2}$

4. Now we can find the free charge by relating the applied voltage V to the E-field by integrating along radial direction:

$$V = \int \vec{E} \cdot \mathrm{d}\vec{r}$$

$$= \int_{R_1}^{R_1+w} \frac{Q_f}{4\pi\epsilon r^2}\,\mathrm{d}r \; + \; \int_{R_1+w}^{R_2} \frac{Q_f}{4\pi\epsilon_0 r^2}\,\mathrm{d}r$$

$$= \frac{Q_f}{4\pi\epsilon}\left(\frac{1}{R_1} - \frac{1}{R_1+w}\right) + \frac{Q_f}{4\pi\epsilon_0}\left(\frac{1}{R_1+w} - \frac{1}{R_2}\right)$$

$$Q_f = \frac{4\pi V}{\frac{1}{\epsilon}\left(\frac{1}{R_1} - \frac{1}{R_1+w}\right) + \frac{1}{\epsilon_0}\left(\frac{1}{R_1+w} - \frac{1}{R_2}\right)}$$

5. Also $\vec{P}$ by $\vec{P} = \vec{D} - \epsilon_0\vec{E}$:

   – In the dielectric layer, $|\vec{P}| = |\vec{D}| - \epsilon_0|\vec{E}| = |\vec{D}| - \epsilon_0 \cdot \dfrac{|\vec{D}|}{\epsilon} = \left(1 - \dfrac{\epsilon_0}{\epsilon}\right)\dfrac{Q_f}{4\pi r^2}$

   – In the vacuum layer, $|\vec{P}| = 0$ (Obviously)

6. This time $\vec{P}$ is a function of r, so the surface bound charge *density* are different on the inner and outer surfaces.

   – On inner surface: $\sigma_b = |\vec{P}|_{(r=R_1)} = \left(1 - \dfrac{\epsilon_0}{\epsilon}\right)\dfrac{Q_f}{4\pi R_1^2}$

   – On outer surface: $\sigma_b = |\vec{P}|_{(r=R_1+w)} = \left(1 - \dfrac{\epsilon_0}{\epsilon}\right)\dfrac{Q_f}{4\pi(R_1+w)^2}$

P.16

But notice that the total bound charge on each surface are the same.

$$Q_b = \sigma_b \cdot (4\pi r^2) = \left(1 - \frac{\epsilon_0}{\epsilon}\right) Q_f$$

(add figure here: different bound charge density on spherical shell)

Also, checking for volume bound charge in the material is more annoying.

$$\rho_b = -\vec{\nabla} \cdot \vec{P}$$

$$= -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 |\vec{P}|\right)$$

$$= -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \left(1 - \frac{\epsilon_0}{\epsilon}\right)\frac{Q_f}{4\pi r^2}\right)$$

$$= 0$$

— The End —