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Physics 15b (Hoffman)
Lecture #19
Thurs, Nov 29, 2007

Title: "Electric Dipoles"

Recap:

Electric fields:
- how to calculate them from charge distribution
- how they act on single charges

Magnetic fields:
- how to calculate them from current distribution
- how they act on moving charges

Maxwell's eqns:

$$\vec{\nabla}\cdot\vec{E} = 4\pi\rho \qquad \vec{\nabla}\cdot\vec{B} = 0$$

$$\vec{\nabla}\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \qquad \vec{\nabla}\times\vec{B} = \frac{4\pi}{c}\vec{J} + \frac{1}{c}\frac{\partial\vec{E}}{\partial t}$$

EM waves:

$$\left.\begin{array}{l}\vec{E} = \vec{E}_0\sin(\vec{k}\cdot\vec{r} - \omega t)\\ \vec{B} = \vec{B}_0\sin(\vec{k}\cdot\vec{r} - \omega t)\end{array}\right\} \text{ where: }$$

$\omega = kc = 2\pi f \leftarrow$ frequency

$|\vec{E}_0| = |\vec{B}_0|$

$\hat{k} = \hat{E}\times\hat{B}$ = propagation direction

$k = \frac{2\pi}{\lambda} \swarrow$ wavelength

energy flow:

Poynting vector: $\vec{S} = \frac{c}{4\pi}\vec{E}\times\vec{B} = \frac{\text{energy}}{\text{time}\cdot\text{area}}$

radiation pressure (momentum flow): $\frac{\vec{S}}{c} = \frac{1}{4\pi}\vec{E}\times\vec{B}$

ALL of this takes place in vacuum!

But most of the world around us is not vacuum!
How to proceed & make everything we've learned apply to the real world?

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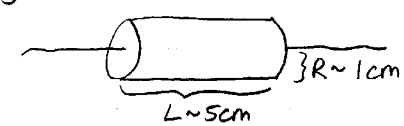
EM fields in <u>matter</u>: We will spend the remainder of the course (only 6 lectures!) on this.

Today:
- example to show that EM in matter can be quite different (our vacuum theories don't cut it)
- start at the bottom (most microscopic level)
- what is the E-field from a single molecule?
  - → develop some mathematical framework to simplify the expression for the "far field" of a molecule (we usually don't care about the $\vec{E}$-field produced Ångstroms away from a single molecule = the "near field"; rather we care about the average field from a number of molecules at some distance = the "far field")
- multipole expansion
  - → often dominated by "dipoles"
  - torque on dipole
  - force on dipole
- atomic polarizability
- polarizability of molecules

Next week:
- put together the tools we'll develop today for understanding single molecules
- → understand macroscopic materials

Motivating example: 1 Farad capacitor



Assume this must be a parallel plate capacitor all rolled up (or some form of concentric parallel plates)

$$C = \frac{A}{4\pi d} \text{ (cgs)} \qquad C = \frac{\varepsilon_0 A}{d} \text{ (SI)}$$

→ need to estimate A and d

Suppose the plates are only as far apart as a piece of paper is thick (after all, we do need <u>something</u> between the plates to keep them apart, or they will just snap together b/c they're oppositely charged).

How thick is a piece of paper?
ream of 500 sheets ~ 5 cm thick
$\rightarrow$ 1 sheet ~ 0.01 cm $= 10^{-4}$ m

Ok, so $d \sim 10^{-4}$ m, what about A?

Let's assume we stuff the capacitor into that cylinder as efficiently as possible, so $A \sim V/d$

$$A \sim \frac{\pi (1\,cm)^2 (5\,cm)}{0.01\,cm} \approx \frac{15\ cm^3}{0.01\ cm} = 0.15\ m^2$$

$$\Rightarrow C = \frac{\varepsilon_0 A}{d} \approx \frac{\varepsilon_0 V}{d^2} \quad \frac{\left(8.85\times10^{-12}\frac{C^2}{N\cdot m^2}\right)(15\times10^{-6}\,m^3)}{(10^{-4}\,m)^2} \approx 10^{-8}\,\underbrace{\frac{C^2}{N\cdot m}}$$

$$\frac{C^2}{J} = \frac{C}{(J/C)} = \frac{\text{Coulomb}}{\text{Volt}} = \text{Farad}$$

Oops! Our calculated <u>capacitance</u> is off by <u>8 orders of magnitude</u>!

Even if we make d thinner, we can't fix this problem. (We'd have to make d 4 orders of magnitude thinner $= 10^{-8}$ m $\rightarrow$ approaching the size of a single atom!)

$\Rightarrow$ Something has gone horribly wrong w/ our estimate, and that something is that we neglected the effect of whatever material it is that's holding the plates a distance d apart.

So we really <u>do</u> need to investigate fields in matter.

Let's start w/ the field from a single molecule, and build up from there.

Multipole expansion: the "far field" of a small charge distribution

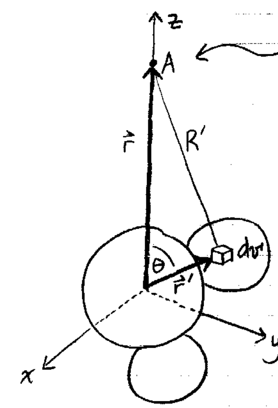
Start by looking at an arbitrary small charge distribution.

What is the $\vec{E}$-field at an arbitrary point A, far away?

(far away means $r \gg$ the size of the charge distribution)

We need to pick a coordinate system to get started (we'll try to get a coordinate-independent formula later).

Arbitrarily pick an origin somewhere within the charge distribution. Then for ease of calculation, let's orient our coordinates so the z-axis lies along the line from our chosen origin to point A.



the electric potential here is:

$$\varphi_A = \int \frac{\rho(x', y', z')\, dv'}{R'}$$

Note: Purcell doesn't put a prime on R. I prefer to put a prime on R, to emphasize that R' changes as we integrate over our volume, because R' is the distance from A to the particular volume element dv'.

The only distance which doesn't change as we integrate over our charge distribution is $\vec{r}$. The vector $\vec{r}$ depends only on our choice of origin and on A, so our goal is going to be to pull all $\vec{r}$-dependence out of the integral.

$$\varphi_A = \int \frac{\rho(x', y', z')\,dv'}{R'}$$

Law of cosines: $R' = (r^2 + r'^2 - 2rr'\cos\theta)^{1/2}$

(this is just geometry, not physics; don't stress if you don't remember this formula)

$$\varphi_A = \int \rho\,dv'\,(r^2 + r'^2 - 2rr'\cos\theta)^{-1/2}$$

Remember we're looking for the "far field" so $r \gg r'$.

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

$$= \frac{1}{r}\Big[1 + \underbrace{\left(\frac{r'}{r}\right)^2 - 2\frac{r'}{r}\cos\theta}_{\text{this should be small!}}\Big]^{-1/2}$$

Use the Taylor expansion: $(1+\delta)^{-1/2} = 1 - \frac{1}{2}\delta + \frac{3}{8}\delta^2 + \ldots$

$$= \frac{1}{r}\left\{1 - \frac{1}{2}\left[\left(\frac{r'}{r}\right)^2 - 2\frac{r'}{r}\cos\theta\right] + \frac{3}{8}\left[\left(\frac{r'}{r}\right)^2 - 2\frac{r'}{r}\cos\theta\right]^2 + \ldots\right\}$$

The $\frac{r'}{r}$ terms will be $\ll 1$, and the $\left(\frac{r'}{r}\right)^2$ terms will be $\ll$ the $\frac{r'}{r}$ terms, and so on.

Let's keep up to the $\left(\frac{r'}{r}\right)^2$ terms, although in principle we could continue this expansion to $\left(\frac{r'}{r}\right)^3$, etc.

Grouping terms, we're left with:

$$(r^2 + r'^2 - 2rr'\cos\theta)^{-1/2} = \frac{1}{r}\left[1 + \frac{r'}{r}\cos\theta + \left(\frac{r'}{r}\right)^2 \frac{(3\cos^2\theta - 1)}{2} + \text{higher order terms}\right]$$

Ah-hah! Now we can take r out of the integration.

$$\varphi_A = \int \frac{\rho\,dv'}{R'} = \frac{1}{r}\underbrace{\int \rho\,dv'}_{K_0} + \frac{1}{r^2}\underbrace{\int r'\cos\theta\,\rho\,dv'}_{K_1} + \frac{1}{r^3}\underbrace{\int r'^2\,\frac{(3\cos\theta - 1)}{2}\,\rho\,dv'}_{K_2} + \ldots$$

Each of the K integrals now depend only on the structure of the charge distribution, not on the choice of point A. We've pulled the A-dependence out of the integrals, so now we have a prescription for finding φ at any point, based on a few integrals that we only have to compute once for a given charge distribution.

$$\varphi(\vec{r}) = \frac{1}{r}K_0 + \frac{1}{r^2}K_1 + \frac{1}{r^3}K_2 + \ldots$$

these terms are getting rapidly smaller

For the "far field", $\varphi(\vec{r})$ is dominated by the first non-vanishing term, given by the first non-vanishing K-integral.

$K_0 = \int \rho\,dv'$ = total charge in the distribution

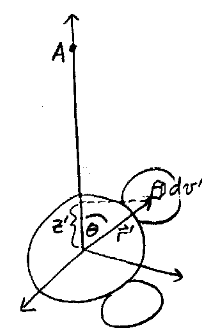
→ vanishes for a neutral molecule

(called the "monopole moment" of the charge distribution)

$$K_1 = \int \underbrace{r'\cos\theta}_{\text{this is just } z'}\,\rho\,dv'$$

⇒ K_1 measures the relative displacement, in the direction towards A, of the positive & negative charge

Clearly, K_1 doesn't depend on our choice of origin in the x-y direction, but what about z?



Does K_1 depend on our choice of origin in the z-direction?

Let's replace z' by $z'+z_0'$, in effect shifting the origin:

$$K_1 = \int r'\cos\theta\,\rho\,d\tau' = \int z'\rho\,d\tau' \rightarrow K_1^{shift} = \int (z'+z_0')\,\rho\,d\tau'$$

$$K_1^{shift} = \underbrace{\int z'\rho\,d\tau'}_{K_1} + \int z_0'\rho\,d\tau'$$

this z_0' is our constant origin shift, so it comes out of the integral

$$K_1^{shift} = K_1 + z_0'\int \rho\,d\tau' = K_1 + z_0' K_0$$

K_0 ← 0, for no net charge

⇒ for a neutral molecule, K_1 doesn't depend on our choice of origin

⇒ K_1 is a coordinate-independent property of a neutral molecule, called the "dipole moment"

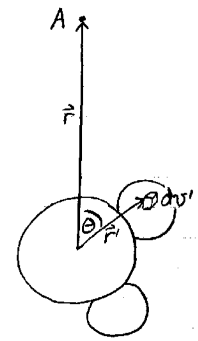
Summary: if $K_0 \neq 0$ then potential behaves like $1/r$ at large distances ("monopole")

if $K_0 = 0$ but $K_1 \neq 0$, then potential behaves like $1/r^2$ at large distances "dipole moment"

if $K_0 = K_1 = 0$ but $K_2 \neq 0$, then potential behaves like $1/r^3$ at large distances "quadrupole moment" is only important if dipole moment vanishes, which is a rather uncommon physical situation, so we'll just focus on the dipole moment for now

Remember: this description (decomposition into "moments" or powers of $1/r^n$) is only useful in the "far field" for large r.

Potential & E-field <u>produced</u> by a dipole:



the dipole contribution to the potential at A is

$$\frac{1}{r^2}\int \underbrace{r'\cos\theta}\,\rho\,d\tau'$$

this is just the projection of $\vec{r}'$ onto $\hat{r}$

$= \vec{r}' \cdot \hat{r}$

depends only on charge distribution ($\vec{r}'$)

depends only on direction and distance of A ($\hat{r}$) → we can pull this out of integral

$$\varphi_A = \frac{\hat{r}}{r^2}\cdot \underbrace{\int \vec{r}'\rho\,d\tau'}$$

this is a vector quantity ≡ dipole moment ≡ $\vec{p}$

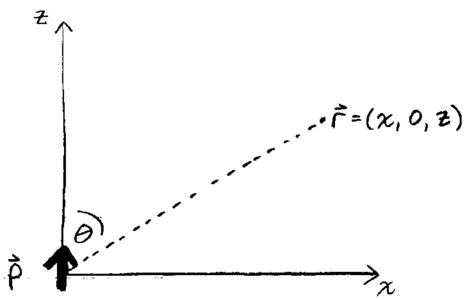
Now, finally, we can write $\varphi(\vec{r})$ in a coordinate-independent way:

$$\varphi(\vec{r}) = \frac{\hat{r}\cdot\vec{p}}{r^2} \quad \text{where } \vec{p} = \int \vec{r}'\rho\,d\tau'$$

this is the dominate "far-field" potential for a neutral molecule.

$\vec{E} = -\vec{\nabla}\varphi$, so can you derive the $\vec{E}$-field of a dipole (the "far field" of a neutral molecule)?

Hint: to get $\vec{E}$, it's easiest to go back into a coordinate system, e.g. choose the origin at the center of the dipole $\vec{p}$, and choose the z-axis to lie along the direction of $\vec{p}$.



What are the components of $\vec E$ at point $\vec r$?

$$\varphi(\vec r) = \frac{\hat r \cdot \vec p}{r^2} = \frac{p\cos\theta}{r^2} = \frac{p\,\frac{z}{(x^2+z^2)^{1/2}}}{x^2+z^2} = \frac{pz}{(x^2+z^2)^{3/2}}$$

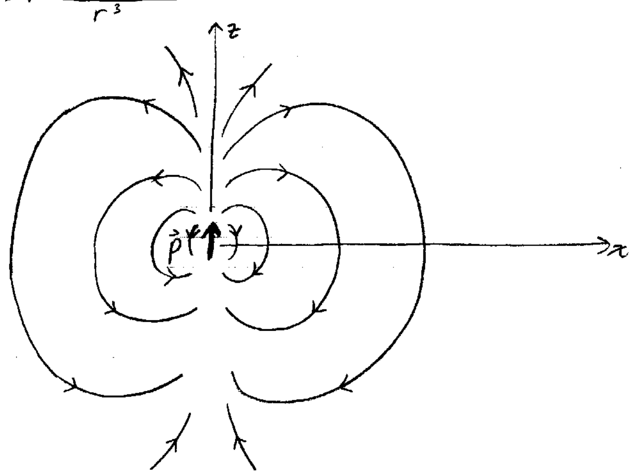
The components of the $\vec E$-field follow from $\vec E = -\vec\nabla\varphi$

$$E_x = -\frac{\partial\varphi}{\partial x} = \frac{-\left(-\frac{3}{2}\cdot 2x\right)pz}{(x^2+z^2)^{5/2}} = \frac{3pxz}{(x^2+z^2)^{5/2}}$$

$$= \frac{3p}{(x^2+z^2)^{3/2}}\cdot\frac{x}{(x^2+z^2)^{1/2}}\cdot\frac{z}{(x^2+z^2)^{1/2}} = \frac{3p\cos\theta\sin\theta}{r^3}$$

$$E_z = -\frac{\partial\varphi}{\partial z} = \frac{-p}{(x^2+z^2)^{3/2}} - \frac{\left(-\frac{3}{2}\cdot 2z\right)pz}{(x^2+z^2)^{5/2}} = \frac{p}{(x^2+z^2)^{3/2}}\left[\frac{3z^2}{x^2+z^2} - 1\right]$$

$$= p\frac{(3\cos^2\theta - 1)}{r^3}$$

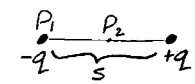


How does a dipole <u>respond</u> to an external $\vec E$-field?

Let's start with the simplest example of a dipole:

2 charges, $\pm q$, stuck together at a fixed distance by an insulating rod of length s

What is $\vec p$? try 2 different origins:



P_1) $\vec p = -q(0) + q(\vec s) = qs\hat x$

P_2) $\vec p = -q\left(-\frac{\vec s}{2}\right) + q\left(\frac{\vec s}{2}\right) = qs\hat x$

What is the net force on the dipole in a uniform applied field $\vec E = E\hat x$?

$$\vec F_{tot} = \vec F_1 + \vec F_2 = -qE\hat x + qE\hat x = 0$$

What about a uniform applied field $\vec E = E\hat z$?

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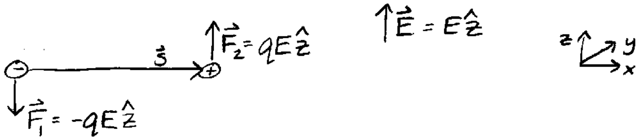
Torque on a dipole in a uniform field:



① pick the origin at the negative charge

$\vec{F}_1$ does not contribute to torque

$$\vec{N} = \vec{s} \times \vec{F}_2 = q\vec{s} \times \vec{E} = \vec{p} \times \vec{E}$$

② or pick origin at midpoint between charges

$$\vec{N} = \frac{\vec{s}}{2} \times \vec{F}_2 - \frac{\vec{s}}{2} \times \vec{F}_1$$
$$= \tfrac{1}{2} q\vec{s} \times \vec{E} - \tfrac{1}{2}(-q)\vec{s} \times \vec{E}$$
$$= q\vec{s} \times \vec{E} = \vec{p} \times \vec{E}$$

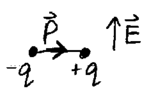
(Torque is independent of origin choice.)

⇒ Dipole "wants" to rotate to align with the applied E-field, to minimize its energy.

How much energy does it gain from rotating?

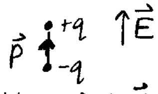
Hint: increment of work is $N\,d\theta$

position 1



θ btwn $\vec{p}$ & $\vec{E} = \frac{\pi}{2}$

position 2



θ btwn $\vec{p}$ & $\vec{E} = 0$

$$W_{tot} = \int_{\pi/2}^{0} N\,d\theta = \int_{\pi/2}^{0} pE\sin\theta\,d\theta = pE(-\cos\theta)\Big|_{\pi/2}^{0} = -pE$$

We gain energy pE by allowing dipole to rotate parallel to E field

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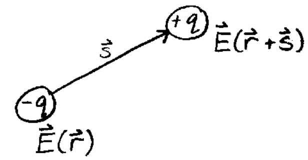
What about the force on a dipole in a non-uniform E-field?



$\vec{E}(\vec{r})$ acts on the charge $-q$
$\vec{E}(\vec{r}+\vec{s})$ acts on the charge $+q$

We assume that the dipole is small compared to the length scale over which $\vec{E}$ changes significantly, so we expand $\vec{E}(\vec{r}+\vec{s})$ for small $\vec{s}$:

$$\vec{F}_{tot} = -q\vec{E}(\vec{r}) + \underbrace{q\vec{E}(\vec{r}+\vec{s})}_{q\left[\vec{E}(\vec{r}) + s_x \frac{\partial \vec{E}}{\partial x} + s_y \frac{\partial \vec{E}}{\partial y} + s_z \frac{\partial \vec{E}}{\partial z}\right]}$$

$$= q\vec{E}(\vec{r}) + (q\vec{s}\cdot\vec{\nabla})\vec{E}$$

$$\vec{F}_{tot} = -q\vec{E}(\vec{r}) + q\vec{E}(\vec{r}) + (\vec{p}\cdot\vec{\nabla})\vec{E}$$

$$\vec{F}_{tot} = (\vec{p}\cdot\vec{\nabla})\vec{E}$$

<u>Example</u> what is the force on a dipole $\vec{p}$ from a point charge Q, if $\vec{p}$ is oriented radially?

$$\vec{F}_{tot} = \left[p\hat{r}\cdot\left(\frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\hat{\phi}\right)\right]\vec{E} = p\frac{\partial}{\partial r}\vec{E}$$

$$= p\frac{\partial}{\partial r}\left(\frac{Q}{r^2}\hat{r}\right) = -\frac{2pQ}{r^3}\hat{r}$$

Force points radially inward b/c the negative part of the dipole feels the larger force, b/c it is closer.