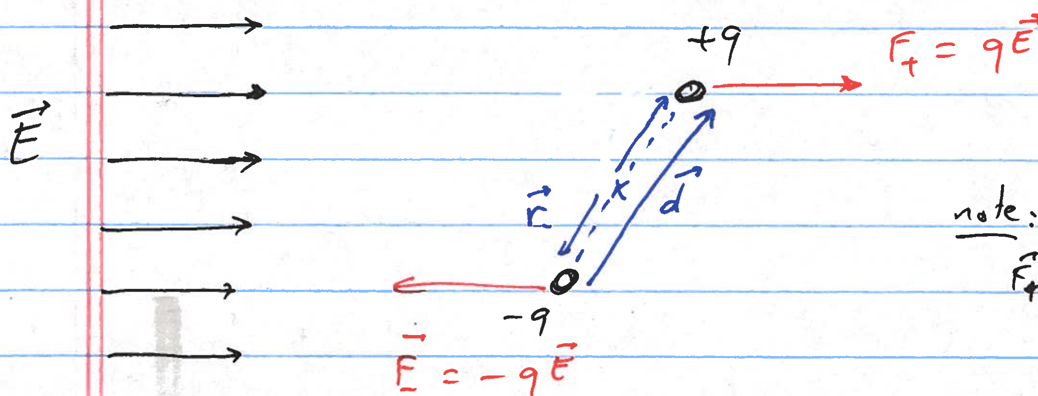
Wednesday, March 29, 2023

Dipole Forces [chpt 4.1.3]

A) Torque on a dipole in a uniform E-field



note: net force
$\vec{F}_{total} = \vec{F}_+ + \vec{F}_-$
$= 0$

Torque: $\vec{\tau} = \vec{r}_+ \times \vec{F}_+ + \vec{r}_- \times \vec{F}_-$

$\vdots$ some algebra (short)

$= \underbrace{q\vec{d}}_{\vec{p}} \times \vec{E}$

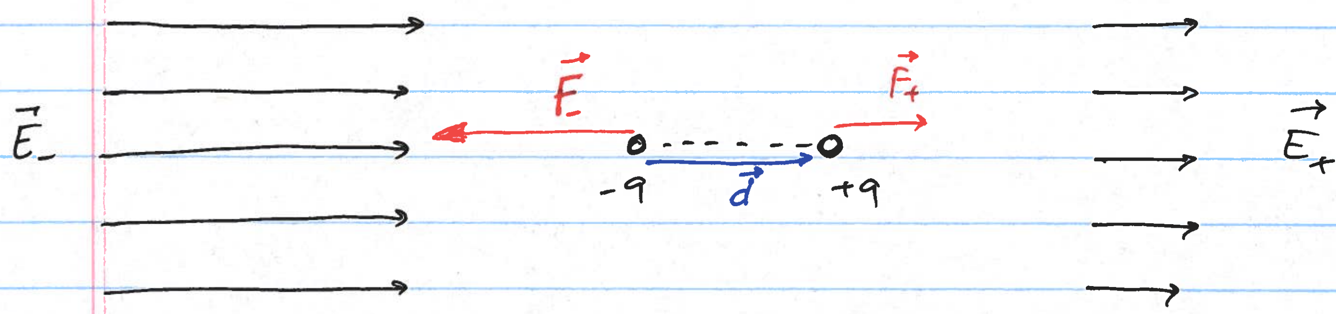
$\Rightarrow$ $\boxed{\vec{\tau} = \vec{p} \times \vec{E}}$ = torque on a dipole

note: Torque is zero when $\vec{p} \parallel \vec{E}$ ($\underbrace{\text{parallel}}_{\text{stable}}$ or $\underbrace{\text{anti-parallel}}_{\text{unstable}}$)

↳ a molecule with a $\underbrace{\text{permanent dipole moment}}$ will align with the electric field.

→ i.e. a polar molecule
↳ e.g. water

B) Force on a dipole in a non-uniform E-field



$$\vec{F}_{total} = \vec{F}_+ + \vec{F}_- = q\underbrace{(\vec{E}_+ - \vec{E}_-)}_{\Delta\vec{E} \,=\, \ldots\ldots \,=\, (\vec{d}\cdot\vec{\nabla})\vec{E}}$$

some algebra

note: $(\vec{d}\cdot\vec{\nabla})\vec{E} = \left(d_x \frac{\partial}{\partial x} + d_y \frac{\partial}{\partial y} + d_z \frac{\partial}{\partial z}\right)\vec{E}$

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

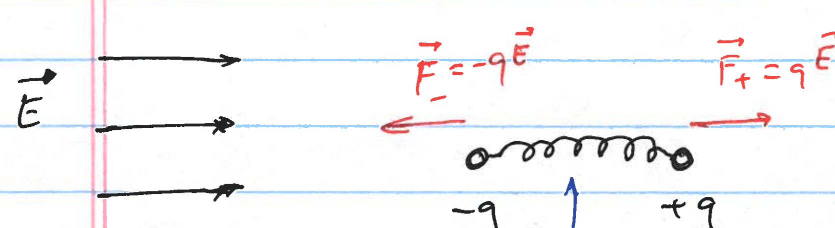
$\Rightarrow$ $\boxed{\vec{F} = (\vec{p}\cdot\vec{\nabla})\vec{E}}$ = force on a dipole in a non-uniform E-field.

note: if $\vec{p} = cst$ (i.e. does not change orientation or magnitude)
then $\vec{F} = \vec{\nabla}(\vec{p}\cdot\vec{E})$

↳ The potential energy U of the dipole is then obtained from
$\vec{F}_{dipole} = -\vec{\nabla} U_{dipole} \Rightarrow \boxed{U_{dipole} = -\vec{p}\cdot\vec{E}}$

C) Internal force on a dipole, atom, molecule: Induced dipole moment

[chpt. 4.1.2]



$\Rightarrow \Delta\vec{F} = 2q\vec{E}$

"spring" = force that binds the $+q$ & $-q$ charges (generally, an internal Coulomb force)

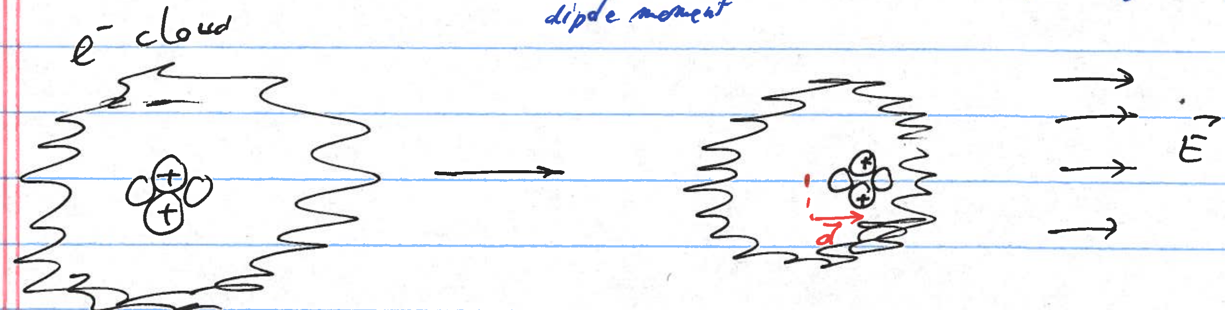
(uniform E-field)

Internal "spring" displacement: $\vec{F} = -k \underbrace{\Delta \vec{x}}_{\text{"}\vec{d}\text{"}}$

gives rise to a dipole moment $q \Delta \vec{x} = q\vec{d}$

Typically, for atoms & molecules, $\boxed{\vec{p} = \alpha \vec{E}}$

induced dipole moment ($\vec{p}$); atomic polarizability (α); applied E-field ($\vec{E}$)



α = DC polarizability > 0 [see Stark effect in QM]

Back to dipole force: $\vec{F} = (\vec{p} \cdot \vec{\nabla})\vec{E} = (\alpha \vec{E} \cdot \vec{\nabla})\vec{E} = \vec{\nabla}\left(\frac{1}{2}\alpha \vec{E}^2\right)$

$\Rightarrow$ potential energy: $\boxed{U_{atom} = -\frac{1}{2}\alpha \vec{E}^2}$

Energy of atom becomes more negative as the E-field increases.

$\Rightarrow$ atoms are attracted to regions of high E-field (and molecules)

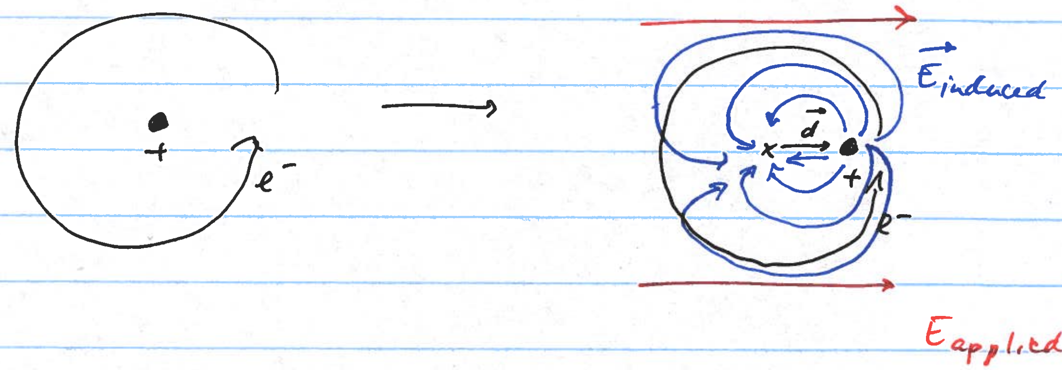
$\Rightarrow$ $\boxed{\text{atoms \& molecules are high-field seekers}}$ (E-field)

Example: For an IR laser, far from any atomic resonances, the laser is quasistatic to an atom (e^- dynamics/response is much faster than f_{laser} = laser frequency)

$\hookrightarrow$ atoms are attracted to the laser focus (where E_{laser} is highest) (high intensity)

Electrostatics in Matter

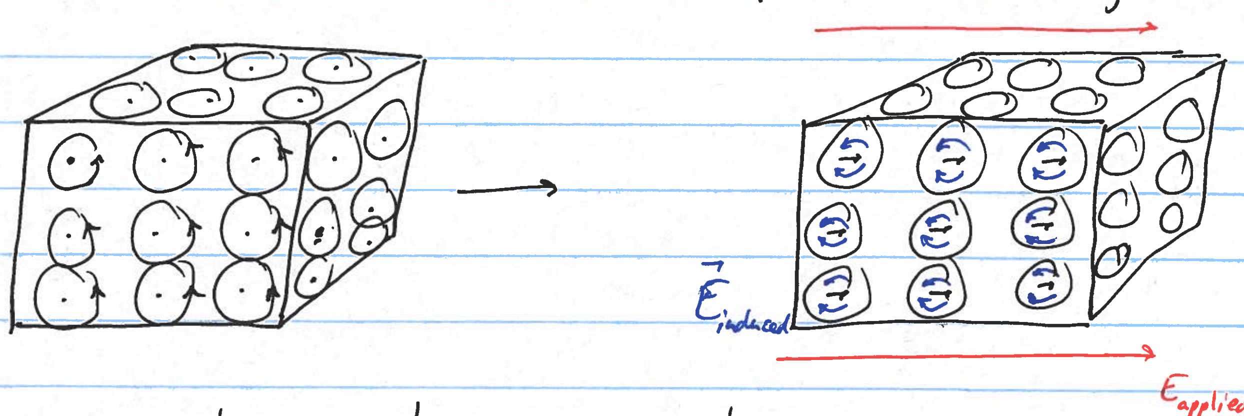
1) Consider a classical atom in an E-field:



$$\vec{P}_{induced} = \alpha \vec{E}$$

$\Rightarrow$ The induced dipole $\vec{P}_{induced}$ produces its own E-field, $\vec{E}_{induced}$, which partially counteracts the applied E-field, $\vec{E}_{applied}$.

2) Consider a block of matter made up of similar-behaving atoms:



$\Rightarrow$ you expect to polarize the material and so there should be an associated $\vec{E}_{induced}$

$\hookrightarrow$ dipole moment per unit volume: $\underbrace{\vec{P} \overset{?}{=} \alpha \vec{E}}_{\text{we'll come back to this later}}$

Thus $\vec{E}_{total}$ is given by $\vec{E}_{total} = \vec{E}_{applied} + \underbrace{\vec{E}_{induced}}_{\vec{E}_{self} \text{ or } \vec{E}_{internal}}$

→ you expect the charges in the material to not exactly cancel (i.e. you get local dipoles)

↳ $\begin{cases} \text{Volume bound charge } \rho_b \\ \text{Surface bound charge } \sigma_b \end{cases}$

↳ total charge density: $\rho_{total}(\vec{r}) = \rho_{applied}(\vec{r}) + \rho_b(\vec{r}) + \sigma_b(\vec{r})$

ρ_{free} = free charge
= charge put there by the experimentalist

We also require $\displaystyle\int_{V \text{ of material}} \rho_b(\vec{r})\, d^3r + \int_{S \text{ of material}} \sigma_b(\vec{r})\, ds = 0 =$ total bound charge

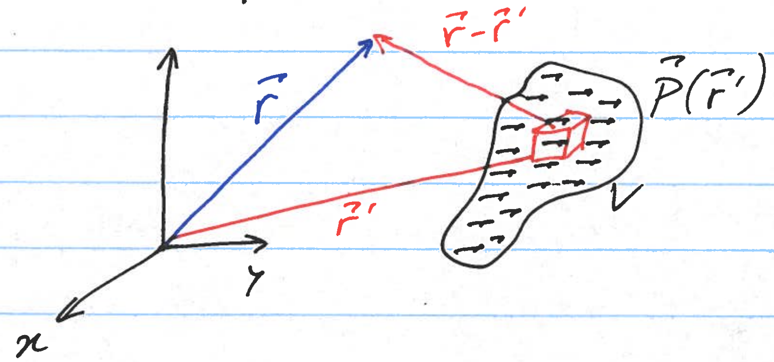
<u>definition</u>: $\vec{P} \equiv$ dipole moment per unit volume

↳ we will model polarized matter as a collection of dipoles (no quadrupoles)

<u>Q</u>: What is the relationship between $\vec{P}$, ρ_b, and σ_b?

<u>A</u>: Let's derive it!

Consider the potential $V(\vec{r})$ produced by a polarized material:



For a single dipole $\vec{p}$: $V(\vec{r}) = \dfrac{1}{4\pi\varepsilon_0}\dfrac{\vec{p}\cdot\hat{r}}{r^2}$

For a continuous distribution of $\vec{p}$'s: $V(\vec{r}) = \dfrac{1}{4\pi\varepsilon_0}\displaystyle\int_V \dfrac{\vec{P}(\vec{r}\,')\cdot\widehat{(\vec{r}-\vec{r}\,')}}{|\vec{r}-\vec{r}\,'|^2}\,d^3r'$

stopped here (i.e. our material)

However, we note that $\vec{\nabla}_{r'}\left(\dfrac{1}{|\vec{r}-\vec{r}\,'|}\right) = \dfrac{\widehat{(\vec{r}-\vec{r}\,')}}{|\vec{r}-\vec{r}\,'|^2}$

a few lines of algebra

Thus $V(\vec{r}) = \dfrac{1}{4\pi\varepsilon_0}\displaystyle\int_V \underbrace{\vec{P}(\vec{r}\,')\cdot\vec{\nabla}_{r'}\left(\dfrac{1}{|\vec{r}-\vec{r}\,'|}\right)}_{\vec{\nabla}\cdot\left(\vec{P}\frac{1}{|\vec{r}-\vec{r}\,'|}\right) - \frac{1}{|\vec{r}-\vec{r}\,'|}\vec{\nabla}\cdot\vec{P}}\,d^3r'$

$$= \frac{1}{4\pi\varepsilon}\left\{\underbrace{\int_V \vec{\nabla}\cdot\left(\frac{\vec{P}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\right)d^3r'}_{\text{divergence theorem}} + \int_V \frac{(-\vec{\nabla}\cdot\vec{P})\,d^3r'}{|\vec{r}-\vec{r}\,'|}\right\}$$

surface charge distribution

volume charge distribution

$$\Rightarrow\quad V(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_S \frac{\vec{P}(\vec{r}\,')\cdot\hat{n}'\,ds'}{|\vec{r}-\vec{r}\,'|} + \frac{1}{4\pi\varepsilon}\int_V \frac{\left(-\vec{\nabla}_{r'}\cdot\vec{P}(\vec{r}\,')\right)d^3r'}{|\vec{r}-\vec{r}\,'|}$$

Thus we infer (or define):

volume bound charge: $\boxed{\rho_b(\vec{r}) \equiv -\vec{\nabla}\cdot\vec{P}(\vec{r})}$

~~surface~~

surface bound charge: $\boxed{\sigma_b(\vec{r}) \equiv \vec{P}(\vec{r})\cdot\hat{n}}$ where $\hat{n}$ = normal vector pointing out of surface