Last time | <u>Multipole Expansion</u> (cont'd)

$\rho(\vec{x})$

$$\boxed{\Phi(\vec{x}) = \frac{1}{\varepsilon_0} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{1}{2\ell+1} \frac{q_{\ell m}}{r^{\ell+1}} Y_{\ell m}(\theta, \varphi)}$$

where the <u>multipole moments</u> are

$$\boxed{q_{\ell m} \equiv \int d^3x' \, \rho(\vec{x}') \, (r')^{\ell} \, Y^*_{\ell m}(\theta', \varphi')}$$

We worked out the 1st few moments:

$$q_{00} = \frac{q}{\sqrt{4\pi}}, \qquad q_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \, (p_x \mp i p_y)$$

$$q_{1,0} = \sqrt{\frac{3}{4\pi}} \, p_z$$

where $\boxed{\vec{p} = \int d^3x \, \rho(\vec{x}) \, \vec{x}'}$ electric dipole moment (EDM).

q_{2m}'s are <u>expressed in terms of</u>

$$\boxed{Q_{ij} = \int d^3x \, \rho(\vec{x}) \left[3 x_i x_j - r^2 \delta_{ij} \right].}$$

quadrupole moments

$$\boxed{\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0} \left[\frac{q}{r} + \frac{\vec{p} \cdot \vec{r}}{r^3} + \frac{1}{2} \sum_{i,j} Q_{ij} \frac{r_i r_j}{r^5} + \ldots \right]}$$

$$= \frac{1}{12}\sqrt{\frac{15}{2\pi}}\left(Q_{11} - 2i\,Q_{12} - Q_{22}\right)$$

where we've defined (traceless) <u>quadrupole moment tensor</u>

$$\boxed{Q_{ij} = \int d^3x'\,\rho(\vec{x}')\left[3x_i'x_j' - r'^2\delta_{ij}\right]}$$

By analogy, $Y_{21} = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\varphi} =$

$$= -\sqrt{\frac{15}{8\pi}}\,\frac{z}{r^2}(x+iy) \Rightarrow q_{21} = -\sqrt{\frac{15}{8\pi}}\int d^3x'\rho(\vec{x}')\cdot$$

$$\cdot z'(x'-iy') = -\frac{1}{3}\sqrt{\frac{15}{8\pi}}\left(Q_{13} - i\,Q_{23}\right)$$

One can also show that $q_{20} = \frac{1}{2}\sqrt{\frac{5}{4\pi}}\,Q_{33}$.

As $Y_{l,-m}(\theta,\varphi) = (-1)^m\, Y^*_{lm}(\theta,\varphi) \Rightarrow \boxed{q_{l,-m} = (-1)^m\, q^*_{lm}}$.

can use to obtain other $q_{l,-m}$'s.

Using the found multipole moments we get

$$\Phi(\vec{x}) = \frac{1}{\varepsilon_0}\,\frac{q_{00}}{r}\,Y_{00} + \frac{1}{3\varepsilon_0}\,\frac{1}{r^2}\left(q_{11}Y_{11} + q_{10}Y_{10} + q_{1,-1}Y_{1,-1}\right)\cdot$$

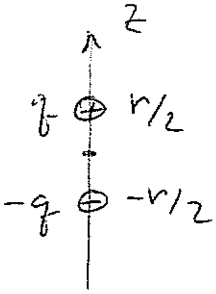
$$+ \ldots = \frac{1}{4\pi\varepsilon_0}\,\frac{q}{r} + \frac{1}{\cancel{3}\varepsilon_0}\,\frac{\cancel{3}}{8\pi}\,\frac{1}{r^2}\Big(+(p_x - ip_y)\cdot\frac{x+iy}{r} +$$

$$+ (p_x + ip_y)\,\frac{x-iy}{r} + 2p_z\,\frac{z}{r}\Big) + \ldots \Rightarrow$$

$$\boxed{\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0}\left[\frac{q}{r} + \frac{\vec{p}\cdot\vec{x}}{r^3} + \frac{1}{2}\sum_{i,j} Q_{ij}\,\frac{x_i x_j}{r^5} + \dots\right]}$$

can also be derived.

Examples:



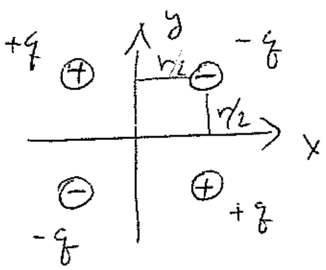
dipole: $q=0$.

$$\vec{p} = q\,\frac{\vec{r}}{2} - (-q)\left(-\frac{\vec{r}}{2}\right) = q\vec{r} \quad \checkmark \text{ok.}$$

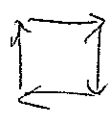
$$Q_{zz} = 3\left(\frac{r}{2}\right)^2 q - 3\left(\frac{r}{2}\right)^2 q - \left(\frac{r}{2}\right)^2 q + \left(\frac{r}{2}\right)^2 q = 0$$

all $Q_{ij} = 0$, ...

quadrupole:



$=$



$q = 0$

$\Rightarrow \vec{p} = 0$

$$Q_{xx} = -q\cdot\left(3\left(\frac{r}{2}\right)^2 - \frac{r^2}{2}\right)2 + 2q\left(+3\left(\frac{r}{2}\right)^2 - \frac{r^2}{2}\right) = 0$$

$$Q_{xy} = -q\cdot 3\left(\frac{r}{2}\right)^2\cdot 2 + q\cdot 3\left(\frac{r}{2}\right)\left(-\frac{r}{2}\right)\cdot 2 = -3qr^2 \neq 0.$$

$Q_{yy} = 0$. $\quad Q_{zz} = 0, \dots$

non-zero quadrupole moment.

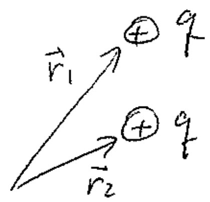
If we know Φ, we know $\vec{E} = -\vec{\nabla}\Phi \Rightarrow$

$$\Rightarrow \boxed{\vec{E} = \frac{1}{4\pi\varepsilon_0}\left[\frac{q}{r^3}\vec{r} + \underbrace{\frac{3\hat{n}(\vec{p}\cdot\hat{n}) - \vec{p}}{r^3}}_{\text{dipole's electric field}} + \dots\right]}$$

$\hat{n} = \dfrac{\vec{r}}{r}.$

All, but the <u>lowest non-vanishing</u> multipole moments depend on the choice of origin!

e.g.



$$q_{00} = \frac{2q}{\sqrt{4\pi}} \neq 0$$

$$q_{1m} \rightarrow \vec p = q\vec r_1 + q\vec r_2$$ ↖ depends on origin

⋮

etc.

However, we've been a bit sloppy: for a dipole

$$\Phi(\vec r) = \frac{1}{4\pi\varepsilon_0}\frac{\vec p\cdot\vec r}{r^3} = \frac{-1}{4\pi\varepsilon_0}\vec p\cdot\vec\nabla\frac{1}{r} = -\frac{1}{4\pi\varepsilon_0}\sum_j p_j\frac{\partial}{\partial x_j}\frac{1}{r}$$

Start by regulating $\quad \frac{1}{r} = \lim_{\varepsilon\to 0}\frac{1}{\sqrt{x^2+y^2+z^2+\varepsilon^2}}$

$$E_i \overset{= -\frac{\partial}{\partial x_i}\Phi}{=} +\frac{1}{4\pi\varepsilon_0}p_j\frac{\partial^2}{\partial x_i\partial x_j}\frac{1}{\sqrt{x^2+y^2+z^2+\varepsilon^2}} = \frac{1}{4\pi\varepsilon_0}p_j\cdot$$

$$\cdot\left[\frac{3x_i x_j}{(r^2+\varepsilon^2)^{5/2}} - \frac{\delta_{ij}}{(r^2+\varepsilon^2)^{3/2}}\right] = \frac{1}{4\pi\varepsilon_0}p_j\cdot\frac{3x_ix_j - \delta_{ij}(r^2+\varepsilon^2)}{(r^2+\varepsilon^2)^{5/2}}$$

$$= \frac{1}{4\pi\varepsilon_0}\frac{3x_i\,\vec p\cdot\vec r - p_i r^2}{r^5} - \frac{1}{4\pi\varepsilon_0}p_i\underbrace{\frac{\varepsilon^2}{(r^2+\varepsilon^2)^{5/2}}}_{\delta_\varepsilon(r)}$$

(i) $r\neq 0,\ \varepsilon\to 0 \Rightarrow \delta_\varepsilon \to 0$

$r = 0,\ \varepsilon\to 0 \Rightarrow \delta_\varepsilon(0) = \infty$

(ii) $\displaystyle\int d^3r\,\frac{\varepsilon^2}{(r^2+\varepsilon^2)^{5/2}} = 4\pi\int_0^\infty dr\cdot r^2\,\frac{\varepsilon^2}{(r^2+\varepsilon^2)^{5/2}} = \Big|\ \tilde r = \frac{r}{\varepsilon}$

$$= 4\pi \int_0^{\infty} d\tilde{r}\, \frac{\tilde{r}^2}{(1+\tilde{r}^2)^{5/2}} = \frac{4\pi}{3} \Rightarrow \delta_\varepsilon(r) \xrightarrow[\varepsilon \to 0]{} \frac{4\pi}{3}\delta^3(\vec{r})$$

$\Rightarrow$ field of a dipole is, in fact:

$$\vec{E} = \frac{1}{4\pi\varepsilon_0}\left[\underbrace{\frac{3\vec{r}\,(\vec{p}\cdot\vec{r}) - \vec{p}\,r^2}{r^5}}_{\text{part known from undergraduate E\&M}} - \underbrace{\frac{4\pi}{3}\vec{p}\,\delta^3(\vec{r})}_{\text{new piece. makes } \int d^3x\, \vec{E} \text{ finite.}} \right]$$

Electrostatic energy & multipole expansion

put our system of charges in external field $\Phi(\vec{x})$: potential energy will be

$$W = \int d^3x\, \rho(\vec{x})\, \Phi(\vec{x})$$

Suppose $\Phi(\vec{x})$ is slowly varying $\Rightarrow$ expand

$$\Phi(\vec{x}) \simeq \Phi(0) + \vec{x}\cdot\vec{\nabla}\Phi(0) + \frac{1}{2}\sum_{i,j} x_i x_j \frac{\partial^2 \Phi}{\partial x_i \partial x_j}(0) + \dots$$

$\Rightarrow$ as $\vec{E} = -\vec{\nabla}\Phi$ and as $\vec{\nabla}\cdot\vec{E} = -\nabla^2\Phi = \frac{1}{\varepsilon_0}\rho_{ext} = 0$ in absense of external charges $\Rightarrow$

$$\Phi(\vec{x}) \simeq \Phi(0) - \vec{x}\cdot\vec{E} - \frac{1}{6}\sum_{i,j}\Big(3x_i x_j \underbrace{- r^2\delta_{ij}}_{\text{added a zero since } \vec{\nabla}\cdot\vec{E} = 0}\Big)\frac{\partial E_j}{\partial x_i}(0) + \dots$$

Therefore,

$$W = q\,\Phi(0) - \vec{p}\cdot\vec{E} - \frac{1}{6}\sum_{i,j} Q_{ij}\,\frac{\partial E_j}{\partial x_i}(0) + \ldots$$

Dielectrics.

Suppose we have two types of charges:

"free charges" and "bound charges".

The potential is then the sum of potentials of free and bound charges: $\Phi = \Phi_{free} + \Phi_{bound}$

$$\Phi_{free}(\vec{x}) = \frac{1}{4\pi\varepsilon_0}\int d^3x'\,\frac{\rho_f(\vec{x}')}{|\vec{x}-\vec{x}'|}$$

Bound charges give charge-neutral media (e^- & p in the atoms & molecules). The dominant multipole is dipole. (It's easy to polarize a molecule.) Potential of a point dipole $\vec{p}$ (at $\vec{x}'$) is

$$\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0}\,\frac{\vec{p}\cdot(\vec{x}-\vec{x}')}{|\vec{x}-\vec{x}'|^3}$$

Def. Defining polarization $\vec{P}(\vec{x})$ as dipole moment per unit volume, we write

$$\Phi_{bound}(\vec{x}) = \frac{1}{4\pi\varepsilon_0} \int_V d^3x' \, \frac{\vec{P}(\vec{x}') \cdot (\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^3}$$

where V is the region containing polarization $\vec{P}$.

As $\dfrac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} = \vec{\nabla}' \dfrac{1}{|\vec{x} - \vec{x}'|} \Rightarrow$

$$\Phi_{bound}(\vec{x}) = \frac{1}{4\pi\varepsilon_0} \int d^3x' \, \vec{P}(\vec{x}') \cdot \vec{\nabla}' \frac{1}{|\vec{x} - \vec{x}'|} = (\text{parts})$$

$$= -\frac{1}{4\pi\varepsilon_0} \int d^3x' \, \frac{1}{|\vec{x} - \vec{x}'|} \cdot \vec{\nabla}' \cdot \vec{P}(\vec{x}')$$

Finally, $\Phi(\vec{x}) = \Phi_{free}(\vec{x}) + \Phi_{bound}(\vec{x}) =$

$$= \boxed{\frac{1}{4\pi\varepsilon_0} \int d^3x' \, \frac{1}{|\vec{x} - \vec{x}'|} \left[\rho_f(\vec{x}') - \vec{\nabla}' \cdot \vec{P}(\vec{x}') \right] = \Phi(\vec{x})}$$

given ρ_f & $\vec{P}(\vec{x}) \Rightarrow$ get Φ.

$\Rightarrow$ There seems to be two components to <u>total</u> charge density: $\rho_{tot} = \rho_f - \vec{\nabla} \cdot \vec{P}$

Now, $\vec{E} = -\vec{\nabla}\Phi \Rightarrow \boxed{\vec{\nabla} \times \vec{E} = 0}$ true in dielectrics

$$\vec{\nabla} \cdot \vec{E} = -\nabla^2 \Phi = \frac{1}{\varepsilon_0} \left[\rho_f(\vec{x}) - \vec{\nabla} \cdot \vec{P}(\vec{x}) \right]$$

as $\nabla^2 \dfrac{1}{|\vec{x} - \vec{x}'|} = -4\pi \, \delta^3(\vec{x} - \vec{x}')$