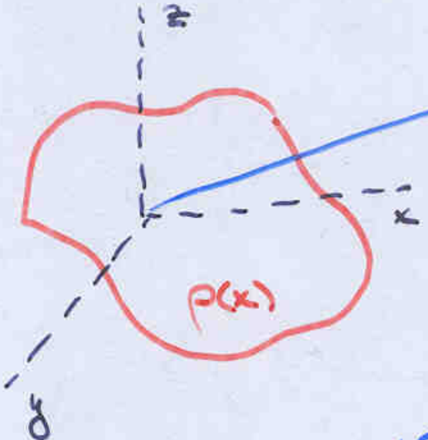
Multipole Expansion



$\varphi(x')$ $\quad$ $x' >$ any x where $\rho(x) \neq 0$

$$\varphi(x') = \int \frac{\rho(x)}{4\pi\varepsilon_0} \frac{1}{|x - x'|} d^3x$$

$$\frac{1}{|x-x'|} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta_{(x;x')})$$

$$= \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} Y_{lm}(\theta', \phi') Y_{lm}^*(\theta, \phi)$$

$r_< = r$

$r_> = r'$

$$\varphi(x') = \int \frac{\rho(x)}{4\pi\varepsilon_0} \sum_{l=0}^{\infty} \frac{r^l}{r'^{l+1}} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} Y_{lm}(\theta', \phi') Y_{lm}^*(\theta\phi) d^3x$$

$$= \frac{1}{\varepsilon_0} \sum_{l=0}^{\infty} \frac{1}{2l+1} \sum_{m=-l}^{l} \left[\int r^l \rho(x) Y_{lm}^*(\theta, \phi) d^3x \right] \frac{Y_{lm}(\theta', \phi')}{r'^{l+1}}$$

$$= \frac{1}{\varepsilon_0} \sum_{l=0}^{\infty} \frac{1}{2l+1} \sum_{m=-l}^{l} \underbrace{q_{lm}}_{\text{multipole moment.}} \frac{Y_{lm}(\theta', \phi')}{r'^{l+1}}$$

Multipole Expansion

$$\phi = \sum_{\ell m} \phi_{\ell m}$$

$$\phi_{\ell m} = \frac{1}{\varepsilon_0} \frac{1}{2\ell+1} q_{\ell m} \frac{Y_{\ell m}(\theta,\phi)}{r^{\ell+1}}$$

$$\vec{E} = \sum_{\ell m} \vec{E}^{\ell m}$$

$$E_r^{\ell m} = \frac{1}{\varepsilon_0} \frac{\ell+1}{2\ell+1} q_{\ell m} \frac{Y_{\ell m}(\theta,\phi)}{r^{\ell+2}}$$

$$E_\theta^{\ell m} = \frac{1}{\varepsilon_0} \frac{1}{2\ell+1} q_{\ell m} \frac{1}{r^{\ell+2}} \frac{\partial}{\partial\theta} Y_{\ell m}(\theta,\phi)$$

$$E_\phi^{\ell m} = \frac{1}{\varepsilon_0} \frac{1}{2\ell+1} q_{\ell m} \frac{1}{r^{\ell+2}} \frac{im}{\sin\theta} Y_{\ell m}(\theta,\phi)$$

Note on $q_{\ell m}$'s

Only lowest moment is independent of position

if $q_{00} \neq 0 \Rightarrow q_{1n}$ is a function of coordinate system

if $q_{00} = 0 \Rightarrow q_1$'s independent of coordinates, but q_2 are not.

if $q_0, q_{1n} = 0 \Rightarrow q_2$'s independent, etc.

Multipole Moments:

$$q_{mn} = \int \rho(x)\, r^m\, Y_{mn}(\theta,\phi)\, d^3x$$

Monopole Moment = charge

$$q_{00} = \int \rho(\vec{x})\, Y_{00}(\vec{x})\, d^3\vec{x} = \frac{1}{\sqrt{4\pi}} \int \rho(\vec{x})\, d^3x = \frac{q}{\sqrt{4\pi}}$$

Just a term $\quad \phi = \frac{1}{4\pi\varepsilon_0}\frac{q}{r} \qquad E_r = \frac{1}{4\pi\varepsilon_0}\frac{q}{r^2}$

Dipole Moment = dipole

$$q_{11} = \int r\rho(x)\, Y_{11}(x)\, d^3x = -\sqrt{\frac{3}{8\pi}} \int r\rho(x)\, e^{i\phi} \sin\theta\, d^3x$$

$$= -\sqrt{\frac{3}{8\pi}} \int \rho(\vec{x})\, (x - iy)\, d^3x$$

If we define the dipole moment as

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

$$\Rightarrow q_{11} = -\sqrt{\frac{3}{8\pi}}\,(p_x - i p_y) \qquad q_{1-1} = q_{11}^* = \sqrt{\frac{3}{8\pi}}\,(p_x + i p_y)$$

Likewise:

$$q_{10} = \sqrt{\frac{3}{4\pi}} \int \rho(\vec{x})\, r\cos\theta\, d^3x = \sqrt{\frac{3}{4\pi}}\, p_z$$

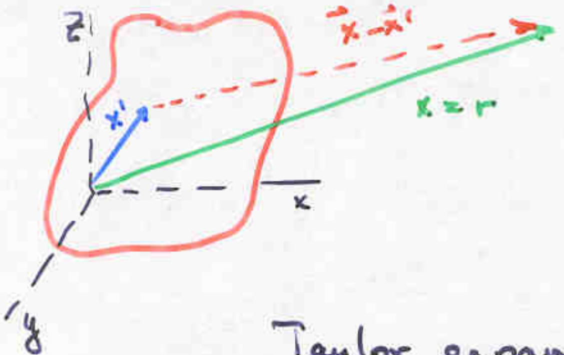
Dipole term

$$\sum_{i=-1}^{1} \phi_{1i} = \frac{1}{3\varepsilon_0}\frac{1}{r^2}\left[-\sqrt{\frac{3}{8\pi}}\,(p_x - i p_y)\, e^{i\phi} \sin\theta \cdot -\sqrt{\frac{3}{8\pi}} + \right.$$

$$\left. \sqrt{\frac{3}{4\pi}}\, p_z \cos\theta + -\sqrt{\frac{3}{8\pi}}\,(p_x + i p_y)\, e^{-i\phi} \sin\theta\, -\sqrt{\frac{3}{8\pi}} \right]$$

$$= \frac{1}{4\pi\varepsilon_0}\frac{\vec{p}\cdot\vec{x}}{r^3}$$

Multipole Expansion:
Alternate Interpretation



Taylor expansion of $\frac{1}{|x-x'|}$

$$\frac{1}{|x-x'|} = \frac{1}{|x|} + \vec{x}' \cdot \left[\nabla' \frac{1}{|x-x'|}\right]_{x'=0} + \sum_{ij} \frac{1}{2} x_i' x_j' \underbrace{\left[\frac{\partial}{\partial x_i'} \frac{\partial}{\partial x_j'} \frac{1}{|x-x'|}\right]_{x'=0}}_{\text{Double Gradient} \Rightarrow \text{matrix}} + \cdots$$

$$= \frac{1}{r} + x' \cdot \frac{\hat{r}}{r^2} + \frac{1}{2} \sum_{ij} \frac{x_i x_j}{r^5} \left(3 x_i' x_j' - r'^2 \delta_{ij}\right) + \cdots$$

$$\Phi(r) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(x')}{|x-x'|} d^3x'$$

$$= \frac{1}{4\pi\varepsilon_0} \left[\frac{q}{r} + \frac{\hat{r}}{r^2} \cdot \int x' \rho(x') d^3x' + \frac{1}{2} \sum_{ij} \frac{x_i x_j}{r^5} \cdot \right.$$

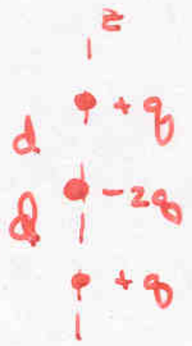
$$\left. \int \rho(x') \left(3x_i' x_j' - r'^2 \delta_{ij}\right) d^3x' + \cdots \right.$$

$$= \frac{q}{4\pi\varepsilon_0 r} + \frac{\vec{r} \cdot \vec{p}}{4\pi\varepsilon_0 r^3} + \frac{1}{8\pi\varepsilon_0} \sum_{ij} \frac{x_i x_j}{r^5} \cdot Q_{ij} + \cdots$$

electric dipole

electric Quadrupole

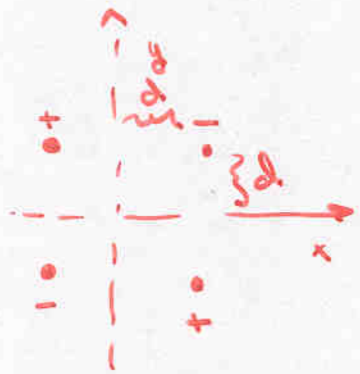
Examples: ELECTRIC QUADRUPOLE



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

$$= \begin{bmatrix} -2qd^2 & 0 & 0 \\ 0 & -2qd^2 & 0 \\ 0 & 0 & 4qd^2 \end{bmatrix}$$

quadrupole matrix the same even if −2q were missing!



$$Q_{ij} = \begin{bmatrix} 0 & -4qd^2 & 0 \\ -4qd^2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Properties of Q_{ij}

(1) Symmetric $\quad Q_{ij} = Q_{ji}$

(2) Traceless $\quad \mathrm{Tr}(Q_{ij}) = 0$

$\Rightarrow$ 5 independent quantities:

Q_{ij} related to $q_{2\ell}$'s

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

$$q_{21} = -\frac{1}{3}\sqrt{\frac{15}{8\pi}}\left(Q_{13} - iQ_{23}\right)$$

$$q_{20} = \frac{1}{2}\sqrt{\frac{5}{4\pi}}\, Q_{33}$$

Energy of Charge Distribution in External field

$$W = \int \rho(x)\, \Phi_{ext}(x)\, d^3x$$

$$\Phi_{ext}(x) = \Phi(0) + \vec{x}\cdot\nabla\Phi\Big|_{x=0} + \frac{1}{2}\sum_{i,j} x_i x_j \frac{\partial^2 \Phi}{\partial x_i \partial x_j}\Big|_{\substack{x_i=0\\ x_j=0}} + \cdots$$

$$= \Phi(0) - \vec{x}\cdot\vec{E}(0) - \frac{1}{2}\sum_{ij} x_i x_j \frac{\partial E_j(0)}{\partial x_i} \cdots$$

$$W = \Phi(0)\int \rho(x)\, d^3x - \vec{E}(0)\cdot\int x\,\rho(x)\, d^3x - \frac{1}{2}\sum_{ij}\frac{\partial E_j(0)}{\partial x_i}\int x_i x_j\, \rho(x)\, d^3x + \cdots$$

since $\sum_i \frac{\partial E_i}{\partial x_i} = 0$ $[\nabla\cdot E = 0]$

last term

$$= \frac{1}{6}\sum_{ij}\frac{\partial E_j(0)}{\partial x_i}\int (3x_i x_j - r^2\delta_{ij})\,\rho(x)\, d^3x$$

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

Dipole – Dipole Interaction Energies.

$$\Phi_{\text{at 2 from 1}} = \frac{1}{4\pi\varepsilon_0}\frac{\vec{p}\cdot\vec{r}}{r^3}$$

$$\vec{E}_2 = -\vec{\nabla}\Phi = \frac{1}{4\pi\varepsilon_0}\frac{3\hat{r}(p_1\cdot\hat{r}) - \vec{p}_1}{r^3}$$

$$W_2 = -p_2\cdot E_2 = -\frac{1}{4\pi\varepsilon_0}\frac{3(p_2\cdot\hat{r})(\hat{p}_1\cdot\hat{r}) - p_1\cdot p_2}{r^3}$$

Quadrupole Interactions

Nucleus: Net charge ⇒ choose axis where $\vec{p} = 0$.

⇒ first interesting term is quadrupole

angular momentum eigen states

⇒ charge distribution invariant around z axis ⇒ $Q_{xy} = Q_{yz} = Q_{xz} = 0$

$$Q_{xx} = Q_{yy} = -\frac{Q_{zz}}{2}$$

axis defined by gradient in electric field:

$$\Rightarrow W = -\frac{1}{6} Q_{zz}\frac{\partial E_z(0)}{\partial z}$$

⇒ lifts degeneracy for various L states