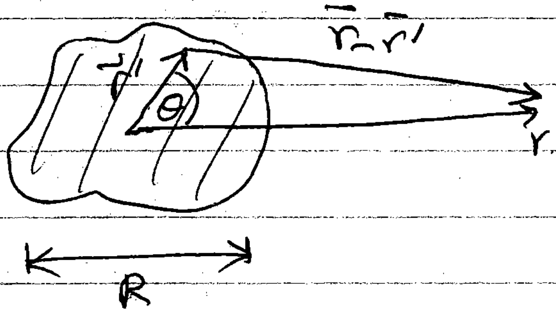
Multipole Expansion

region with $\rho \neq 0$

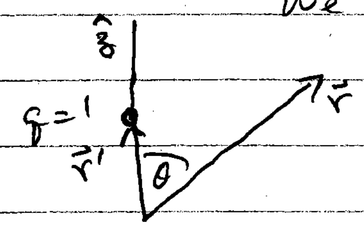


We want to find the potential ϕ for an arbitrary localized distribution of charge ρ, at distances far away $r >> R$.

$$\phi(\vec{r}) = \int d^3r' \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}$$ General Coulomb formula

We want an expansion of $\frac{1}{|\vec{r}-\vec{r}'|}$ in powers of $\left(\frac{r'}{r}\right)$ for $r >> r'$

$\frac{1}{|\vec{r}-\vec{r}'|}$ view this as the potential at $\vec{r}$ due to a unit point charge located at position $\vec{r}'$. We take $\vec{r}'$ on the $\hat{z}$ axis.



The problem has azimuthal symmetry $\Rightarrow \phi$ depends only on r and θ, so we can express it as an expansion in Legendre polynomials.

For $r > r'$,

$$\phi(r,\theta) = \sum_{\ell=0}^{\infty} \frac{B_\ell}{r^{\ell+1}} P_\ell(\cos\theta)$$

all $A_\ell = 0$ as need $\phi \to 0$ as $r \to \infty$

$$= \frac{1}{r} \sum_{\ell=0}^{\infty} \frac{B_\ell}{r^\ell} P_\ell(\cos\theta)$$

We know $\phi(r, \theta=0) = \dfrac{1}{r-r'}$ (for $r > r'$)

$\leftarrow$ scalars here since when $\theta = 0$, $\vec{r}$ and $\vec{r}'$ are both on $\hat{z}$ axis

$$\Rightarrow \phi(r, 0) = \frac{1}{r} \sum_{\ell} \frac{B_\ell}{r^\ell} P_\ell(1)$$

$$= \frac{1}{r} \sum_{\ell=0}^{\infty} \frac{B_\ell}{r^\ell} \quad \text{as } P_\ell(1) = 1$$

$$= \frac{1}{r} \frac{1}{(1 - r'/r)} \leftarrow \text{exact result from Coulomb}$$

Now Taylor expansion $\dfrac{1}{1-\epsilon} = 1 + \epsilon + \epsilon^2 + \epsilon^3 + \epsilon^4 + \cdots$

$$\Rightarrow \frac{1}{r} \sum_{\ell=0}^{\infty} \frac{B_\ell}{r^\ell} = \frac{1}{r}\left(1 + \frac{r'}{r} + \left(\frac{r'}{r}\right)^2 + \left(\frac{r'}{r}\right)^3 + \cdots\right)$$

$\Rightarrow$ $B_\ell = (r')^\ell$ is solution

So for $r > r'$

$$\boxed{\frac{1}{|\vec{r} - \vec{r}'|} = \frac{1}{r} \sum_{\ell=0}^{\infty} \left(\frac{r'}{r}\right)^\ell P_\ell(\cos\theta)}$$

So for the charge distribution ρ,

$$\phi(\vec{r}) = \int d^3r' \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} = \int d^3r' \frac{\rho(\vec{r}')}{r} \sum_{\ell=0}^{\infty} \left(\frac{r'}{r}\right)^\ell P_\ell(\cos\theta)$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{r^{\ell+1}} \int d^3r' \rho(\vec{r}') (r')^\ell P_\ell(\cos\theta)$$

where θ is the angle between the fixed observation point $\vec{r}$ and the integration variable $\vec{r}'$.

This is the multipole expansion, which expresses the potential far from a localized source as a power series in (r'/r). It is exact provided one adds all the infinite l terms. In practice, one generally approximates by summing only up to some finite l.

Note: in doing the integrals

$$\int d^3r' \, \rho(\vec{r}\,')(r')^l \, P_l(\cos\theta)$$

θ is defined as the angle of $\vec{r}\,'$ with respect to observation point $\vec{r}$. We therefore in principle have to repeat this integration every time we change $\vec{r}$.

We will find a way around this by

(i) first looking explicitly at the few lowest order terms

(ii) a general method involving spherical harmonics $Y_{lm}(\theta,\varphi)$

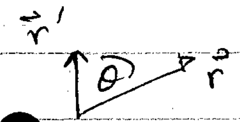
<u>monopole</u>: $l=0$ term

$$\phi^{(0)}(\vec{r}) = \frac{1}{r}\int d^3r'\,\rho(r') \qquad P_0(\cos\theta) = 1$$

$$= \frac{q}{r} \quad \text{where } q \equiv \int d^3r'\,\rho(r') \text{ is } \underline{\text{total}} \text{ charge}$$

<u>dipole</u>: $l=1$ term

$$\phi^{(1)}(\vec{r}) = \frac{1}{r^2}\int d^3r'\,\rho(\vec{r}\,')\,r'\,P_1(\cos\theta)$$



$$= \frac{1}{r^2}\int d^3r'\,\rho(\vec{r}\,')\,r'\cos\theta$$

Now $\vec{r}\cdot\vec{r}\,' = rr'\cos\theta \Rightarrow \hat{r}\cdot\vec{r}\,' = r'\cos\theta$

$$\phi^{(1)}(\vec{r}) = \frac{1}{r^2}\,\hat{r}\cdot\int d^3r'\,\rho(\vec{r}\,')\,\vec{r}\,'$$

$$= \frac{\vec{p}\cdot\hat{r}}{r^2} \quad \text{where } \vec{p} \equiv \int d^3r'\,\rho(\vec{r}\,')\,\vec{r}\,'$$

is the <u>dipole moment</u>

For a set of point charges q_i at $\vec{r}_i$,

$$\vec{p} = \sum_i q_i \vec{r}_i$$

<u>quadrapole</u>: $\ell = 2$ term

$$\phi^{(2)}(\vec{r}) = \frac{1}{r^3} \int d^3r' \, \rho(\vec{r}') \, r'^2 \, P_2(\cos\theta)$$

$$= \frac{1}{r^3} \int d^3r' \, \rho(\vec{r}') \, r'^2 \, \tfrac{1}{2}(3\cos^2\theta - 1)$$

use $\cos\theta = \hat{r}' \cdot \hat{r}$

$$\phi^{(2)}(\vec{r}) = \frac{1}{r^3} \int d^3r' \, \rho(\vec{r}') \, \tfrac{1}{2}\left(3(\vec{r}' \cdot \hat{r})^2 - (r')^2\right)$$

$$= \frac{1}{r^3} \, \hat{r} \cdot \left[\int d^3r' \, \rho(\vec{r}') \, \tfrac{1}{2}\left(3\vec{r}'\vec{r}' - (r')^2 \overleftrightarrow{I}\right) \right] \cdot \hat{r}$$

where $\overleftrightarrow{I}$ is the identity <u>tensor</u> such that for any two vectors $\vec{v}$ and $\vec{u}$, $\vec{u} \cdot \overleftrightarrow{I} \cdot \vec{v} = \vec{u} \cdot \vec{v}$

and $\vec{r}'\vec{r}'$ is the <u>tensor</u> such that for any two vectors $\vec{v}$ and $\vec{u}$, $\vec{u} \cdot [\vec{r}'\vec{r}'] \cdot \vec{v} = (\vec{u} \cdot \vec{r}')(\vec{r}' \cdot \vec{v})$

Define quadrapole tensor $\overleftrightarrow{Q} \equiv \int d^3r' \, \rho(\vec{r}') \, \left(3\vec{r}'\vec{r}' - (r')^2 \overleftrightarrow{I}\right)$

$$\phi^{(2)}(\vec{r}) = \frac{1}{r^3} \, \frac{1}{2} \, \hat{r} \cdot \overleftrightarrow{Q} \cdot \hat{r}$$

So to lowest three terms

$$\phi(\vec{r}) = \frac{q}{r} + \frac{\vec{p} \cdot \hat{r}}{r^2} + \frac{\hat{r} \cdot \overleftrightarrow{Q} \cdot \hat{r}}{2r^3} + \cdots$$

defined in terms of the <u>moments</u> q, $\vec{p}$, $\overleftrightarrow{Q}$ of the charge distribution.

Note, the moments q, $\vec{p}$, $\overleftrightarrow{Q}$ do not depend on the observation point $\vec{r}$ — we can calculate them once and then use them to get $\phi(\vec{r})$ at all $\vec{r}$.

monopole: $q = \int d^3r \, \rho(\vec{r})$ scalar integral

dipole $\vec{p} = \int d^3r \, \rho(\vec{r}) \, \vec{r}$ vector integral

$\hat{e}_1 \equiv \hat{x}$, $\hat{e}_2 \equiv \hat{y}$, $\hat{e}_3 \equiv \hat{z}$

if we pick a coordinate system, we have to do $\underline{\underline{3}}$ integrations to get the three component of $\vec{p}$

$\hat{e}_i \cdot \vec{p} = p_i = \int d^3r \, \rho(\vec{r}) \, r_i$

quadrapole $\overleftrightarrow{Q} = \int d^3r \, \rho(\vec{r}) \left(3\vec{r}\,\vec{r} - (r)^2 \overleftrightarrow{I} \right)$ tensor integral

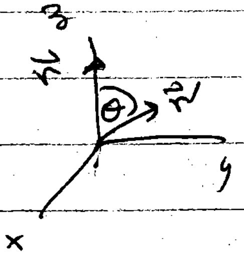
if we pick a coord system $x\,y\,z$ then $\overleftrightarrow{Q}$ is a matrix with components $\hat{e}_1 \equiv \hat{x}$, $\hat{e}_2 \equiv \hat{y}$, $\hat{e}_3 \equiv \hat{z}$

$\hat{e}_i \cdot \overleftrightarrow{Q} \cdot \hat{e}_j = Q_{ij} = \int d^3r \, \rho(\vec{r}) \left[3 r_i r_j - r^2 \delta_{ij} \right]$

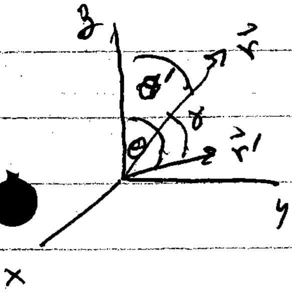
There are 9 elements of the 3×3 matrix Q_{ij}, but $Q_{ij} = Q_{ji}$ is symmetric so there are only 6 independent elements to compute.

General method

$$\phi(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{1}{r^{\ell+1}} \int d^3r' \, \rho(\vec{r}')(r')^\ell P_\ell(\cos\theta)$$



in above, θ is angle between $\vec{r}$ and $\vec{r}'$
if we think of this θ as the spherical coord θ, then in effect, above is choosing $\vec{r}$ to be on $\hat{z}$ axis. We would like a representation in which $\vec{r}$ is positioned arbitrarily with respect to the axes used in describing ρ



Use the addition theorem for spherical harmonics - see Jackson 3.6 for discussion & proof

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta',\phi') \, Y_{\ell m}(\theta,\phi)$$

where (θ,ϕ) are the angles of $\hat{r}$, (θ',ϕ') are the angles of $\hat{r}'$, and γ is the angle between $\hat{r}$ and $\hat{r}'$, ie $\cos\gamma = \hat{r}\cdot\hat{r}'$

$\cos\theta = \hat{z}\cdot\hat{r}$

$\cos\theta' = \hat{z}\cdot\hat{r}'$

$\Rightarrow$

$$\phi(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{1}{r^{\ell+1}} \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} \int d^3r' \, \rho(\vec{r}')(r')^\ell \, Y^*_{\ell m}(\theta',\phi') \, Y_{\ell m}(\theta,$$

Define the moment

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

independent of observation point

Then

$$\phi(\vec{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{q_{lm} Y_{lm}(\theta,\phi)}{(2l+1)\, r^{l+1}}$$

see Jackson equ (4.4), (4-5), (4-6) to relate q_{lm} to q, $\vec{p}$, $\overleftrightarrow{Q}$.

$$\phi(\vec{r}) = \frac{q}{r} + \frac{\vec{p}\cdot\hat{r}}{r^2} + \frac{\hat{r}\cdot\overleftrightarrow{Q}\cdot\hat{r}}{2r^3} \quad \ldots$$

electric field $\vec{E} = -\vec{\nabla}\phi = -\frac{\partial\phi}{\partial r}\hat{r} - \frac{1}{r}\frac{\partial\phi}{\partial\theta}\hat{\theta} - \frac{1}{r\sin\theta}\frac{\partial\phi}{\partial\varphi}\hat{\varphi}$

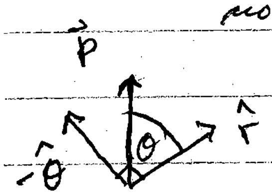
For the monopole term $\vec{E} = \frac{q}{r^2}\hat{r}$

For the dipole term, choose $\vec{p}$ along $\hat{z}$ axis so

$$\phi(\vec{r}) = \frac{p\cos\theta}{r^2}$$

$$\vec{E} = \frac{2p\cos\theta}{r^3}\hat{r} + \frac{p\sin\theta}{r^3}\hat{\theta}$$

$$\vec{E} = \frac{p}{r^3}\left(2\cos\theta\,\hat{r} + \sin\theta\,\hat{\theta}\right)$$



note $p\cos\theta\,\hat{r} = (\vec{p}\cdot\hat{r})\hat{r}$

$p\sin\theta\,\hat{\theta} = -(\vec{p}\cdot\hat{\theta})\hat{\theta}$

Now $\vec{p} = (\vec{p}\cdot\hat{r})\hat{r} + (\vec{p}\cdot\hat{\theta})\hat{\theta}$

$\Rightarrow \quad -(\vec{p}\cdot\hat{\theta})\hat{\theta} = (\vec{p}\cdot\hat{r})\hat{r} - \vec{p}$

So

$$\vec{E} = \frac{1}{r^3}\left[2(\vec{p}\cdot\hat{r})\hat{r} + (\vec{p}\cdot\hat{r})\hat{r} - \vec{p}\right]$$

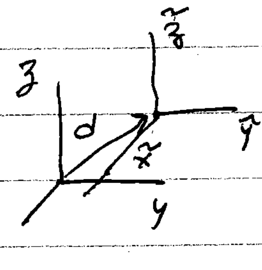
$$= \frac{1}{r^3}\left[3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}\right]$$

expresses $\vec{E}$ in coord free form

$$\vec{E} = \frac{1}{r^3}\left[\,3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}\,\right]$$ expresses $\vec{E}$ of dipole in coord free form

<u>Origin of coordinates</u>

The definition of the multipole moments <u>depends</u> on the choice of origin of the coordinates.



Suppose transform to $\vec{\tilde{r}} = \vec{r} - \vec{d}$

In the $\vec{\tilde{r}}$ cood system

$$\tilde{q} = \int d^3\tilde{r}\,\rho(\tilde{r}) = \int d^3r\,\rho(r) = q$$

monopole <u>does not</u> depend on choice of origin.

$$\vec{\tilde{p}} = \int d^3\tilde{r}\,\rho(\tilde{r})\,\vec{\tilde{r}} = \int d^3r\,\rho\,(\vec{r}-\vec{d})$$

$$= \int d^3r\,\rho\,\vec{r} - \vec{d}\int d^3r\,\rho$$

$$\vec{\tilde{p}} = \vec{p} - \vec{d}q \qquad \vec{\tilde{p}} = \vec{p} \text{ only if } q = 0\,!$$

if $q \neq 0$, then $\vec{\tilde{p}} \neq \vec{p}$

$\Rightarrow$ ~~One cood~~ If $q \neq 0$, one could always choose an origin of coords for which $\vec{p} = 0$!

~~For HW you will show that~~ $\cancel{\tilde{\overleftrightarrow{Q}} = \overleftrightarrow{Q}}$ ~~only if both~~ $\cancel{q = 0}$ ~~and~~ $\cancel{\vec{p} = 0}$.

Quadrupole moment in new coordinates

$$\overleftrightarrow{\tilde{Q}} = \int d^3\tilde{r}\, \rho \left[3\vec{\tilde{r}}\,\vec{\tilde{r}} - (\vec{\tilde{r}})^2 \overleftrightarrow{I} \right]$$

where $\vec{\tilde{r}} = \vec{r} - \vec{d}$

substitute in above

$$\overleftrightarrow{\tilde{Q}} = \int d^3r\, \rho \left[3(\vec{r}-\vec{d})(\vec{r}-\vec{d}) - (\vec{r}-\vec{d})^2 \overleftrightarrow{I} \right]$$

$$= \int d^3r\, \rho \left[3\vec{r}\,\vec{r} - 3\vec{r}\,\vec{d} - 3\vec{d}\,\vec{r} + 3\vec{d}\,\vec{d} - (r^2 + d^2 - 2\vec{r}\cdot\vec{d})\overleftrightarrow{I} \right]$$

$$= \int d^3r\, \rho \left[3\vec{r}\,\vec{r} - r^2 \overleftrightarrow{I} \right] - 3\left[\int d^3r\, \rho\, \vec{r}\right]\vec{d} - 3\vec{d}\left[\int d^3r\, \rho\, \vec{r}\right]$$

$$+ 3\vec{d}\,\vec{d}\left[\int d^3r\, \rho\right] - d^2 \overleftrightarrow{I}\left[\int d^3r\, \rho\right]$$

$$+ 2\left[\int d^3r\, \rho\, \vec{r}\right]\cdot\vec{d}\, \overleftrightarrow{I}$$

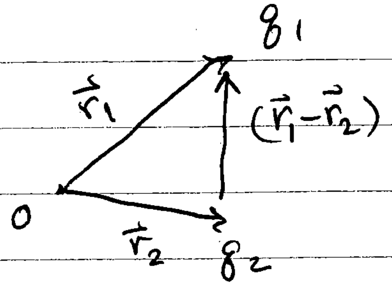
$$\overleftrightarrow{\tilde{Q}} = \overleftrightarrow{Q} - 3\vec{p}\,\vec{d} - 3\vec{d}\,\vec{p} + 3\vec{d}\,\vec{d}\, q - \left(d^2 q - 2\vec{p}\cdot\vec{d} \right)\overleftrightarrow{I}$$

we see that $\overleftrightarrow{Q}$ is independent of choice of origin only when both q and $\vec{p}$ vanish. When this happens the quadrupole term is the <u>leading</u> term in the multipole expansion.

In general, the leading term in multipole expansion will be indep of origin of coordinates.

Example two charges q_1 at $\vec{r}_1$ and q_2 at $\vec{r}_2$

$$q_1 + q_2 = q \neq 0$$



monopole $q_1 + q_2 = q$

dipole $\vec{p} = q_1 \vec{r}_1 + q_2 \vec{r}_2$

quadrupole $\overleftrightarrow{Q} = (3\vec{r}_1\vec{r}_1 - r_1^2 \overleftrightarrow{I}) q_1 + (3\vec{r}_2\vec{r}_2 - r_2^2 \overleftrightarrow{I}) q_2$

We can make the dipole moment vanish by shifting to a new coord system $\vec{r}\,' = \vec{r} - \vec{d}$ where $\vec{d} = \dfrac{\vec{p}}{q}$

$$\vec{r}\,' = \vec{r} - \frac{q_1 \vec{r}_1 + q_2 \vec{r}_2}{q_1 + q_2} = \frac{q_1(\vec{r} - \vec{r}_1) + q_2(\vec{r} - \vec{r}_2)}{q_1 + q_2}$$

positions of q_1, q_2 in new coords are

$$\vec{r}_1\,' = \frac{q_2}{q_1 + q_2}(\vec{r}_1 - \vec{r}_2)$$

$$\vec{r}_2\,' = \frac{-q_1}{q_1 + q_2}(\vec{r}_1 - \vec{r}_2)$$

Origin of new coord system is at

lies along vector from $\vec{r}_2$ to $\vec{r}_1$

$$\vec{r}\,' = 0 \Rightarrow \vec{r} = \frac{q_1 \vec{r}_1 + q_2 \vec{r}_2}{q_1 + q_2}$$ "center of charge"

for many charges q_i at positions $\vec{r}_i$, the origin that makes dipole moment vanish is at

$$\vec{r} = \frac{\sum_i q_i \vec{r}_i}{\sum q_i}$$

In this coord system

$$\vec{p}' = q_1 \vec{r}_1' + q_2 \vec{r}_2' = \frac{q_1 q_2}{q_1+q_2}(\vec{r}_1 - \vec{r}_2) - \frac{q_2 q_1}{q_1+q_2}(\vec{r}_1 - \vec{r}_2)$$

$= 0$ as it must be!

<u>Quadrupole moment</u> in the coord system in which $\vec{p}' = 0$ the quadrupole tensor is

$$\overleftrightarrow{Q}' = \left[3\vec{r}_1'\vec{r}_1' - (r_1')^2 \overleftrightarrow{I}\right] q_1 + \left[3\vec{r}_2'\vec{r}_2' - (r_2')^2 \overleftrightarrow{I}\right] q_2$$

let us choose ~~coord~~ spherical coordinates with origin at O' and $\hat{z}$ axis aligned along $\vec{r}_1 - \vec{r}_2$, so that

$\vec{r}_1 - \vec{r}_2 = s\,\hat{z}$ where $s = |\vec{r}_1 - \vec{r}_2|$ is separation between the charges

then
$$\vec{r}_1' = \frac{q_2}{q_1+q_2} s\,\hat{z}$$
$$\vec{r}_2' = \frac{-q_1}{q_1+q_2} s\,\hat{z}$$

$$\overleftrightarrow{Q}' = \left(\frac{q_2}{q_1+q_2}\right)^2 q_1 \left[3 s^2 \hat{z}\hat{z} - s^2 \overleftrightarrow{I}\right] + \left(\frac{-q_1}{q_1+q_2}\right)^2 q_2 \left[3 s^2 \hat{z}\hat{z} - s^2 \overleftrightarrow{I}\right]$$

$$\overleftrightarrow{Q}' = \frac{q_2^2 q_1 + q_1^2 q_2}{(q_1+q_2)^2} s^2 \left[3\hat{z}\hat{z} - \overleftrightarrow{I} \right]$$

$$= \frac{q_1 q_2}{q_1+q_2} s^2 \left[3\hat{z}\hat{z} - \overleftrightarrow{I} \right]$$

$$Q'_{ij} = \frac{q_1 q_2}{q_1+q_2} s^2 \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$ in xyz coord system

as $\hat{z}\hat{z} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$\overleftrightarrow{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

the contribution of quadrupole to the potential is

$$\Phi_{quad} = \frac{1}{2} \frac{\hat{r} \cdot \overleftrightarrow{Q} \cdot \hat{r}}{r^3}$$ $\hat{r} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$ in xyz coords

with origin at O' this becomes

$$\phi_{quad} = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1+q_2} (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$$

do matrix multiplications

$$\phi_{quad} = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1+q_2} (2\cos^2\theta - \sin^2\theta)$$

independent of φ as it must be due to azimuthal symmetry

Example

sample charge config's

q $\Rightarrow$ monopole is leading term

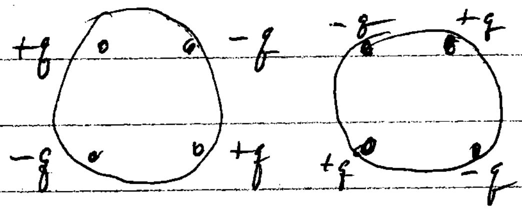
$+q$ $-q$ $\Rightarrow$ monopole $=0$ $\Rightarrow$ dipole is leading term

$\vec{p}$ is indep of origin

$+q$ $-q$ $\Rightarrow$ monopole $=0$ $\Rightarrow$ total dipole is

$-q$ $+q$ sum of dipoles of individual neutral pairs

$\sum = 0$ leading term is quadrapole



when monopole $=0$ and dipole $=0$, quadrapole is indep of origin.
$\rightarrow$ total quadrapole is sum of quadrapoles of individual clusters with $q=0$ and $\vec{p}=0$

$Q = Q_1 + Q_2$

with $Q_2 = -Q_1$

$\Rightarrow$ $Q = 0$ leading term is octopole