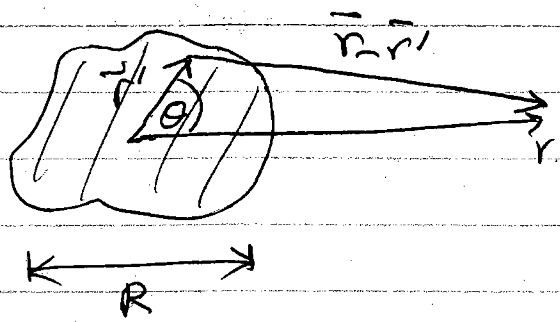
Multipole Expansion

region with $\rho \neq 0$

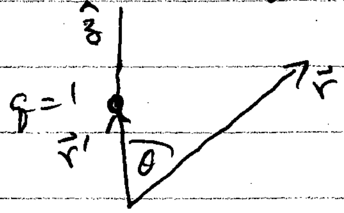


We want to find the potential ϕ for an arbitrary *localized* distribution of charge ρ, at distances far away $r >> R$.

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

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

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

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

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

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

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

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

$\Rightarrow B_\ell = (r')^\ell$ 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 $Y_{lm}(\theta, \varphi)$

monopole: $l=0$ term

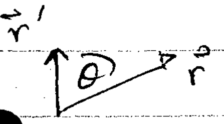
$$\Phi^{(0)}(\vec{r}) = \frac{1}{r}\int d^3r'\,\rho(r') \qquad P_0(\cos\theta) = 1$$

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

total charge

dipole: $l=1$ 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 $\vec{r}\cdot\vec{r}\,' = r r'\cos\theta \Rightarrow \hat{r}\cdot\vec{r}\,' = r'\cos\theta$

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

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

is the dipole moment

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 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

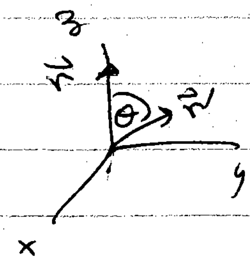
if we pick a coord system $x\, y\, z$ then $\overleftrightarrow{Q}$ is a matrix with components $\hat{e}_1 \equiv \hat{x}$, $\hat{e}_2 \equiv \hat{y}$, $\hat{e}_3 \equiv \hat{z}$

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

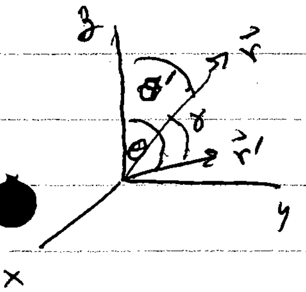
There are 9 elements of the 3×3 matrix Q_{ij}, but $Q_{ij} = Q_{ji}$ is symmetric so there are only 6 independent elements to compute.

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

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

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

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

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 $\vec{E} = \frac{q}{r^2}\hat{r}$

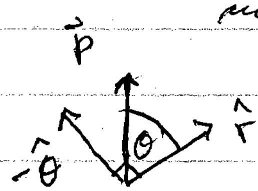
For the dipole term, choose $\vec{p}$ along $\hat{z}$ axis so

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

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

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

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

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

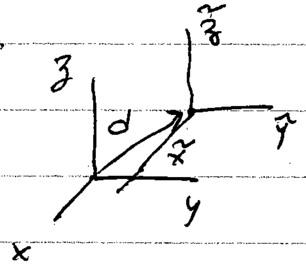
So

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

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

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

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

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

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

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

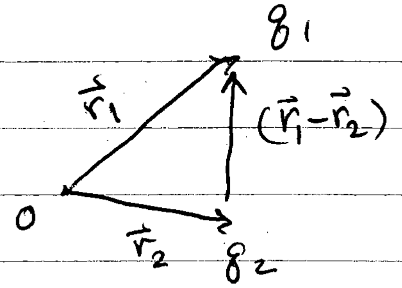
if $q \neq 0$, then $\tilde{\vec{p}} \neq \vec{p}$

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

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

<u>Example</u> 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 <u>dipole moment</u> 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 $\vec{r}_1{}' = \dfrac{q_2}{q_1+q_2} s\,\hat{z}$

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

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

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

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

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

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

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

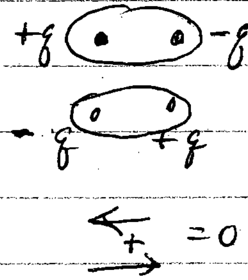
Example

sample charge config's

$\bullet\ q$ $\Rightarrow$ monopole is leading term

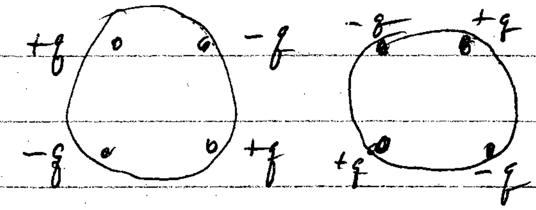
$+q \quad -q$ $\Rightarrow$ monopole $=0$ $\Rightarrow$ dipole is leading term

$\vec{p}$ is indep of origin



$\Rightarrow$ monopole $=0$ $\Rightarrow$ total dipole is sum of dipoles of individual neutral pairs

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 $\vec{p}=0$

$\mathbb{Q} = \mathbb{Q}_1 + \mathbb{Q}_2$

with $\mathbb{Q}_2 = -\mathbb{Q}_1$

$\Rightarrow \mathbb{Q} = 0$ leading term is <u>octopole</u>