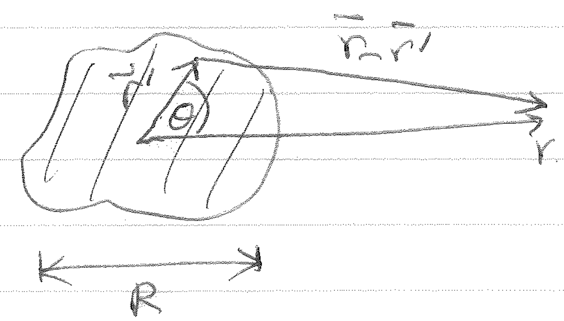
Multipole Expansion

region with $\rho \neq 0$

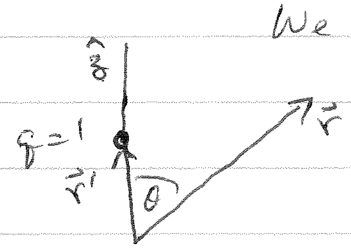


We want to find the potential ϕ for an arbitrary localized distribution of charge ρ, at distances far away $r \gg R$.

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

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

$\frac{1}{|\vec{r}-\vec{r}'|}$ 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

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

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

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

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

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

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

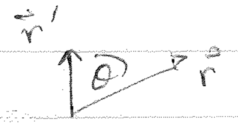
monopole: $l=0$ term

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

$$= \frac{q}{r} \quad \text{where } q \equiv \int d^3r'\,\rho(r') \text{ is}$$
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 $\vec{r}\cdot\vec{r}' = rr'\cos\theta \Rightarrow \hat{r}\cdot\vec{r}' = r'\cos\theta$

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

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

is the dipole moment

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

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

quadrapole: $\ell = 2$ 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 tensor 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 tensor 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 moments 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 components 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

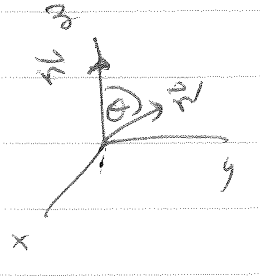
if we pick a coord system $x\,y\,z$ then $\overleftrightarrow{Q}$ is a matrix with components $\hat{e}_1 \equiv \hat{x}$, $\hat{e}_2 \equiv \hat{y}$, $\hat{e}_3 \equiv \hat{z}$

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

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.

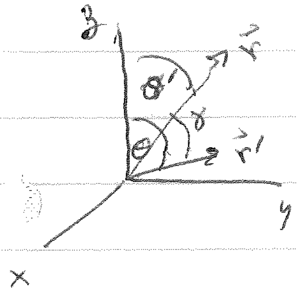
General method

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



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 <u>addition theorem for spherical harmonics</u> - 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 $\cos\gamma = \hat{r} \cdot \hat{r}'$

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

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

$\Rightarrow$

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

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

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

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

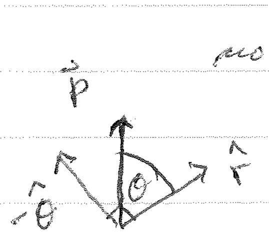
For the monopole term $\vec E = \frac{q}{r^2}\hat r$

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

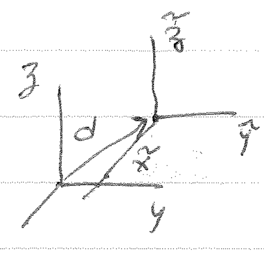
$$\vec E = \frac{1}{r^3}\left[2(\vec p\cdot\hat r)\hat r + (\vec p\cdot\hat r)\hat r - \vec p\right]$$

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

Origin of coordinates

The definition of the multipole moments depends 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

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

monopole does not depend on choice of origin

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

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

$$\tilde{\vec{p}} = \vec{p} - \vec{d}q$$ $\tilde{\vec{p}} = \vec{p}$ 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 $\tilde{Q} = Q$ only if both $q = 0$ and $\vec{p} = 0$~~

Quadrupole moment in new coordinates

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

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

substitute in above

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

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

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

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

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

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

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.

Supposed for some distribution ρ we have the monopole moment $q=0$. $\Rightarrow$ dipole moment $\vec{p}$ is independent of the choice of the coordinate system.

Can we then choose coordinates such that $\overleftrightarrow{Q}=0$?

$$Q_{ij}=\int d^3r\,\rho(\vec{r})\left(3r_ir_j-r^2\delta_{ij}\right)$$

$\overleftrightarrow{Q}$ is not only symmetric, ie $Q_{ij}=Q_{ji}$, but it is traceless $\sum_i Q_{ii}=Q_{xx}+Q_{yy}+Q_{zz}=0$

proof: $\sum_i Q_{ii}=\int d^3r\,\rho(\vec{r})\left[3\sum_i r_ir_i-r^2\sum_i\delta_{ii}\right]$

$$=\int d^3r\,\rho(\vec{r})\left[3r^2-r^2(3)\right]=0$$

So there are really only 5 independent components to $\overleftrightarrow{Q}$.

But since $\overleftrightarrow{Q}$ is symmetric, we know that we can always diagonalize the matrix Q_{ij} and its eigenvalues are real. Or equivalently, we can always rotate our orthonormal coordinate system so that $\overleftrightarrow{Q}$ is diagonal in that coordinate system

$$\begin{pmatrix} Q_{xx} & 0 & 0 \\ 0 & Q_{yy} & 0 \\ 0 & 0 & Q_{zz} \end{pmatrix}$$

and if $\overleftrightarrow{Q}$ is traceless in one coord system, it is traceless in all coordinate systems $\Rightarrow$ $Q_{xx}+Q_{yy}+Q_{zz}=0$
$\longrightarrow$ only two independent components in the diagonalizing frame