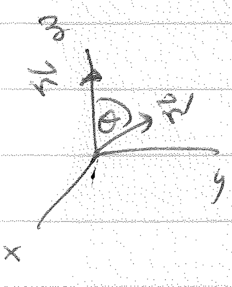
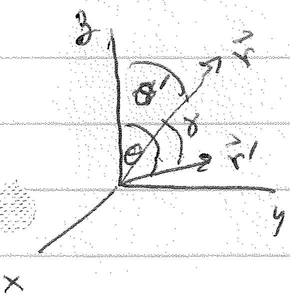
General method

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



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 $\cos\gamma = \hat{r} \cdot \hat{r}'$

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

$\Rightarrow$

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

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, $\vec{p}$, $\overleftrightarrow{Q}$.

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

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

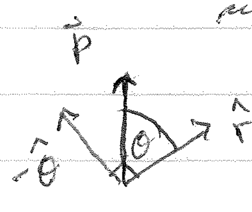
For the monopole term $\vec{E} = \frac{q}{r^2}\hat{r}$

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

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

So

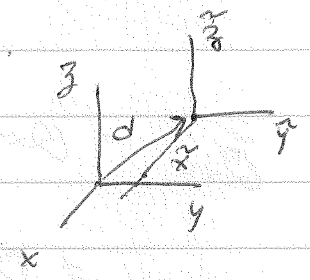
$$\vec{E} = \frac{1}{r^3}\left[2(\vec{p}\cdot\hat{r})\hat{r} + (\vec{p}\cdot\hat{r})\hat{r} - \vec{p}\right]$$

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

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

monopole does not depend on choice of origin.

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

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

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

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

$\Rightarrow$ ~~One coul~~ 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 $\vec{p} = 0$.~~

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

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

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

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

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

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

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

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 _leading_ term in the multipole expansion.

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

We saw that if $q=0$, we can choose an origin for coordinates such that $\vec{p}=0$.

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 $\overleftrightarrow{Q}=0$?

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

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

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

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

Since we have three degrees of freedom d_x, d_y, d_z in translating to a new origin, one might think that we can always choose a ~~new~~ new coordinate system in which $Q_{xx} = Q_{yy} = 0$ and then by traceless condition $Q_{zz} = 0$ also and so $\overleftrightarrow{Q} = 0$ (if all eigenvalues are zero, the matrix must vanish)

Under a shift of coordinates $\tilde{\vec{r}} = \vec{r} - \vec{d}$, the new quadrupole tensor is related to the old by

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

if, as assumed, $q = 0$, then

$$\tilde{\overleftrightarrow{Q}} = \overleftrightarrow{Q} - 3\vec{p}\vec{d} - 3\vec{d}\vec{p} + 2\vec{p}\cdot\vec{d}\,\overline{\overline{I}}$$

Suppose we start in a frame in which $\overleftrightarrow{Q}$ is diagonal, ie only $Q_{xx}, Q_{yy}, Q_{zz} \neq 0$ then we have the transformations

1) $\tilde{Q}_{xx} = Q_{xx} - 4p_x d_x + 2p_y d_y + 2p_z d_z$

2) $\tilde{Q}_{yy} = Q_{yy} + 2p_x d_x - 4p_y d_y + 2p_z d_z$

3) $\tilde{Q}_{zz} = Q_{zz} + 2p_x d_x + 2p_y d_y - 4p_z d_z$

4) $\tilde{Q}_{xy} = -3(p_x d_y + p_y d_x)$

5) $\tilde{Q}_{yz} = -3(p_y d_z + p_z d_y)$

6) $\tilde{Q}_{zx} = -3(p_z d_x + p_x d_z)$

We have 6 linear equations in three unknowns d_x, d_y, d_z

Since we know $\overleftarrow{Q}$ is always traceless then we can eliminate one of equations (1), (2), and (3) since $Q_{zz} = -(Q_{xx} + Q_{yy})$ so (3) is dependent on (1) and (2)

That gives 5 equations.

Can we choose d_x, d_y, d_z so that $\tilde{Q}_{xx} = \tilde{Q}_{yy} = \tilde{Q}_{xy} = \tilde{Q}_{yz} = \tilde{Q}_{zx} = 0$?

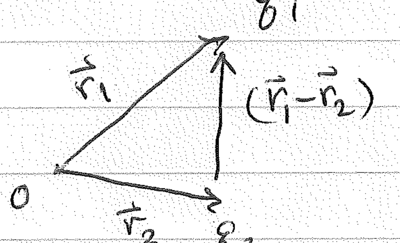
In general NO! That would be 5 equations in 3 unknowns so the system is in general overspecified and there is no solution. Only in special cases might there be a solution.

Note, even though $Q_{xy} = Q_{yz} = Q_{zx} = 0$ in the original coordinate system that does not general remain so in the translated coordinate system

In general we cannot use rotation to rotate a non-zero tensor into a zero tensor. This is why adding the rotational degrees of freedom to our coordinate transformation does not help.

<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

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

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

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

Origin of new coord system is at

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

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

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

In this coord system

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

$$= 0 \quad \text{as it must be!}$$

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

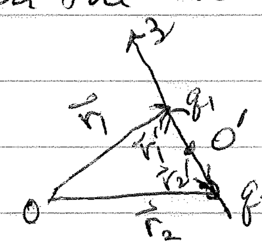
$$\overleftrightarrow{Q}' = \left[3\vec{r}_1\,'\vec{r}_1\,' - (r_1')^2 \overleftrightarrow{I}\right] q_1 + \left[3\vec{r}_2\,'\vec{r}_2\,' - (r_2')^2 \overleftrightarrow{I}\right] q_2$$

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

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

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

(check: $\overleftrightarrow{Q}'$ is traceless: $-1-1+2=0$)

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

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

$$\Phi_{quad} = \frac{s^2}{2r^3}\,\frac{q_1 q_2}{q_1+q_2}\,\underbrace{(2\cos^2\theta - \sin^2\theta)}_{= 2P_2(\cos\theta)}$$

use $\sin^2\theta = 1-\cos^2\theta \Rightarrow 2\cos^2\theta - \sin^2\theta = 3\cos^2\theta - 1$

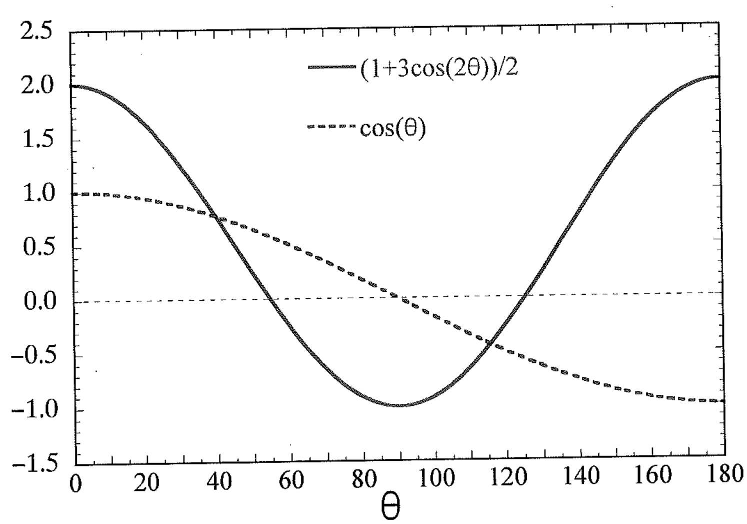
use $\cos^2\theta = \frac{1+\cos 2\theta}{2} \Rightarrow 3\cos^2\theta - 1 = \frac{1+3\cos 2\theta}{2}$

So $$\Phi_{quad} = \frac{s^2}{2r^3}\,\frac{q_1 q_2}{q_1+q_2}\,\frac{1+3\cos 2\theta}{2}$$

compare to
$$\Phi_{dipole} = \frac{p\cos\theta}{r^2}$$

Note, if we average over θ then
$$\int_0^\pi d\theta \sin\theta\ \Phi_{quad} \propto \int_0^\pi d\theta \sin\theta\,(3\cos^2\theta - 1) = \left[-\cos^3\theta + \cos\theta\right]_0^\pi$$
$$= 0$$

similarly $$\int_0^\pi d\theta \sin\theta\ \Phi_{dipole} \propto \int_0^\pi d\theta \sin\theta \cos\theta = \left[-\tfrac{1}{2}\cos^2\theta\right]_0^\pi$$
$$= 0$$



Quadrupole term more generally

$$\phi_{quad} = \frac{\hat{r}\cdot\overleftrightarrow{Q}\cdot\hat{r}}{2r^3}$$

since $\overleftrightarrow{Q}$ is a symmetric tensor, there is always some coordinate system in which it is diagonal. Lets work in that coordinate system. Then

$$\overleftrightarrow{Q} = \begin{pmatrix} Q_1 & 0 & 0 \\ 0 & Q_2 & 0 \\ 0 & 0 & Q_3 \end{pmatrix}$$

let us take $\hat{z}$ axis as the axis with the largest Q_i so $Q_3 \geq Q_1, Q_2$

in this coord system $\hat{r} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$

$$\hat{r}\cdot\overleftrightarrow{Q}\cdot\hat{r} = Q_1\sin^2\theta\cos^2\varphi + Q_2\sin^2\theta\sin^2\varphi + Q_3\cos^2\theta$$

this gives the angular variation of ϕ_{quad} as the direction of the observer varies

let us consider now averaging this over all directions

$$\frac{1}{4\pi}\int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\varphi\left[Q_1\sin^2\theta\cos^2\varphi + Q_2\sin^2\theta\sin^2\varphi + Q_3\cos^2\theta\right]$$

$$= \frac{1}{4\pi}\int_0^\pi d\theta\sin\theta\left[\pi Q_1\sin^2\theta + \pi Q_2\sin^2\theta + 2\pi Q_3\cos^2\theta\right]$$

$$= \frac{1}{4}\int_0^\pi d\theta\sin\theta\left[(Q_1+Q_2)\sin^2\theta + 2Q_3\cos^2\theta\right]$$

$$= \frac{1}{4}(Q_1+Q_2)\int_0^\pi d\theta\sin^3\theta + \frac{1}{2}Q_3\int_0^\pi d\theta\sin\theta\cos^2\theta$$

Now $\int_0^\pi d\theta \sin\theta \cos^2\theta = \left. -\frac{\cos^3\theta}{3} \right|_0^\pi = \frac{2}{3}$

$$\int_0^\pi d\theta \sin^3\theta = \int_0^\pi d\theta \sin\theta (1 - \cos^2\theta)$$

$$= \int_0^\pi d\theta \sin\theta - \frac{2}{3} = \left. -\cos\theta \right|_0^\pi - \frac{2}{3}$$

$$= 2 - \frac{2}{3} = \frac{4}{3}$$

So angular average of $\hat{r} \cdot \overleftrightarrow{Q} \cdot \hat{r}$

$$= \frac{1}{4}(Q_1 + Q_2)\frac{4}{3} + \frac{1}{2} Q_3 \frac{2}{3} = \frac{1}{3}(Q_1 + Q_2 + Q_3)$$

$$= \frac{1}{3} \text{trace}[\overleftrightarrow{Q}]$$

But we know $\text{trace}[\overleftrightarrow{Q}] = 0$

$\Rightarrow$ angular average of Φ_{quad} always vanishes for any charge distribution!