Unit 2-4: Electric Multipole Expansion

We want to find the potential ϕ for an arbitrary *localized* distribution of charge ρ , at a distance r far away from the charge. If the charge is distributed over a region of length R, and the observer is at $r \gg R$, we want to find an expansion for the potential in R/r.

$$\phi(\mathbf{r}) = \int d^3 r' \frac{\rho(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|} \qquad \text{from the general Coulomb formula} \quad (2.4.1)$$

We now seek an expansion of $\frac{1}{|\mathbf{r} - \mathbf{r'}|}$ in powers of $\left(\frac{r'}{r}\right)$, where r' integrates over the localized region of charge.

 $\vec{r} = \vec{r}$ View $\frac{1}{|\mathbf{r} - \mathbf{r}'|}$ as the potential at \mathbf{r} due to a unit point charge q = 1 located at position \mathbf{r}' . If we take \mathbf{r}' to lie on the $\hat{\mathbf{z}}$ axis, then this problem has rotational symmetry about the $\hat{\mathbf{z}}$ axis, so ϕ depends only on the spherical coordinates r and θ . symmetry about the $\hat{\mathbf{z}}$ axis, so ϕ depends only on the spherical coordinates r and θ , so we can express it as an expansion in Legendre polynomials.

For $r \gg r'$

$$\phi(r,\theta) = \frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{\ell=0}^{\infty} \left(A_{\ell}^{\ell} + \frac{B_{\ell}}{r^{\ell+1}} \right) \mathcal{P}_{\ell}(\cos\theta) = \frac{1}{r} \sum_{\ell=0}^{\infty} \frac{B_{\ell}}{r^{\ell}} \mathcal{P}_{\ell}(\cos\theta)$$
(2.4.2)

where all the $A_{\ell} = 0$ since we want $\phi \to 0$ as $r \to \infty$.

Now consider the case where **r** is also on the $\hat{\mathbf{z}}$ axis, so $\theta = 0$. We have,

$$\phi(r,\theta=0) = \frac{1}{r-r'} = \frac{1}{r} \frac{1}{(1-r'/r)} = \frac{1}{r} \left(1 + \frac{r'}{r} + \left(\frac{r'}{r}\right)^2 + \left(\frac{r'}{r}\right)^3 + \dots \right)$$
(2.4.3)

where here we can take r and r' as scalar quantities, since when $\theta = 0$, r and r' are collinear vectors, both along $\hat{\mathbf{z}}$. In the last step we used the Taylor expansion, $\frac{1}{1-\epsilon} = 1 + \epsilon + \epsilon^2 + \epsilon^3 + \dots$ for small ϵ .

Compare Eq. (2.4.3) to the Legendre expansion of Eq. (2.4.2) evaluated at $\theta = 0$, where $\mathcal{P}_{\ell}(1) = 1$ for all ℓ . We have

$$\phi(r,\theta=0) = \frac{1}{r} \sum_{\ell=0}^{\infty} \frac{B_{\ell}}{r^{\ell}} \mathcal{P}_{\ell}(1) = \frac{1}{r} \sum_{\ell=0}^{\infty} \frac{B_{\ell}}{r^{\ell}} = \frac{1}{r} \left(B_0 + \frac{B_1}{r} + \frac{B_2}{r^2} + \frac{B_3}{r^3} + \dots \right)$$
(2.4.4)

Comparing Eqs (2.4.3) and (2.4.4) we conclude $B_{\ell} = (r')^{\ell}$

So for a general position \mathbf{r} we then have,

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \frac{1}{r} \sum_{\ell=0}^{\infty} \left(\frac{r'}{r}\right)^{\ell} \mathcal{P}_{\ell}(\cos\theta)$$
(2.4.5)

Note, this was a somewhat different application of the Legendre polynomial expansion than we saw before. Rather that a boundary condition on the surface of a sphere of radius r = R being used to determine the expansion coefficients, here we are using the behavior along the $\hat{\mathbf{z}}$ axis.

With the above result, the potential for an arbitrary distribution $\rho(\mathbf{r})$ is then,

$$\phi(\mathbf{r}) = \int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} = \int d^3r' \frac{\rho(\mathbf{r}')}{r} \sum_{\ell=0}^{\infty} \left(\frac{r'}{r}\right)^{\ell} \mathcal{P}_{\ell}(\cos\theta) = \sum_{\ell=0}^{\infty} \frac{1}{r^{\ell+1}} \int d^3r' \,\rho(\mathbf{r}') \,\left(r'\right)^{\ell} \mathcal{P}_{\ell}(\cos\theta) \tag{2.4.6}$$

where θ is the angle between the fixed observer at position **r** and the integration variable **r'**.

This is the multipole expansion, which expresses the potential far from a localized source as a power series in $(r'/r)^{\ell}$. It is exact, provided one sums up all the infinite number of terms ℓ . In practice, one generally approximates ϕ by summing up only to some finite ℓ .

Note, in doing the integrals $\int d^3 r' \rho(\mathbf{r}')(r')^{\ell} \mathcal{P}_{\ell}(\cos\theta)$, the angle θ is defined as the angle of \mathbf{r}' with respect to the observer at \mathbf{r} . We therefore in principle have to repeat this integration every time we want to change \mathbf{r} .

We can get around this problem two ways:

(i) Looking explicitly at the few lowest order terms, and seeing how to rewrite the integral in a way that moves the \mathbf{r} dependence outside the integral.

(ii) Using a general method involving the spherical harmonics $Y_{\ell m}(\theta, \varphi)$.

We will do (i), and then at the end I will tell you about (ii).

monopole: the $\ell = 0$ term

Using $\mathcal{P}_0(\cos\theta) = 1$, we get,

$$\phi^{(0)}(\mathbf{r}) = \frac{1}{r} \int d^3 r' \,\rho(\mathbf{r}') = \frac{q}{r} \quad \text{where} \quad q \equiv \int d^3 r' \rho(\mathbf{r}') \quad \text{is the total charge in the distribution}$$
(2.4.7)

dipole: the $\ell = 1$ term

$$\phi^{(1)}(\mathbf{r}) = \frac{1}{r^2} \int d^3 r' \,\rho(\mathbf{r}') r' \,\mathcal{P}_1(\cos\theta) = \frac{1}{r^2} \int d^3 r' \,\rho(\mathbf{r}') r' \,\cos\theta \tag{2.4.8}$$

Now use $\mathbf{r} \cdot \mathbf{r}' = rr' \cos \theta \implies \hat{\mathbf{r}} \cdot \mathbf{r}' = r' \cos \theta$. Use that in the integral above to get,

$$\phi^{(1)}(\mathbf{r}) = \frac{1}{r^2} \,\hat{\mathbf{r}} \cdot \int d^3 r' \,\rho(\mathbf{r}') \mathbf{r}' = \frac{\hat{\mathbf{r}} \cdot \mathbf{p}}{r^2} \quad \text{where} \quad \mathbf{p} \equiv \int d^3 r' \,\rho(\mathbf{r}') \mathbf{r}' \quad \text{is the electric dipole moment}$$
(2.4.9)

Note, for a set of point charges q_i at positions \mathbf{r}_i , the dipole moment is $\mathbf{p} = \sum_i q_i \mathbf{r}_i$.

quadrupole: the $\ell = 2$ term

$$\phi^{(2)}(\mathbf{r}) = \frac{1}{r^3} \int d^3 r' \,\rho(\mathbf{r}') \,(r')^2 \mathcal{P}_2(\cos\theta) = \frac{1}{r^3} \int d^3 r' \,\rho(\mathbf{r}') \,(r')^2 \frac{1}{2} \left(3\cos^2\theta - 1\right) \tag{2.4.10}$$

Now use $r' \cos \theta = \mathbf{r}' \cdot \hat{\mathbf{r}}$ to write,

$$\phi^{(2)}(\mathbf{r}) = \frac{1}{r^3} \int d^3 r' \,\rho(\mathbf{r}') \,\frac{1}{2} \left(3(\mathbf{r}' \cdot \hat{\mathbf{r}})^2 - (r')^2 \right) = \frac{1}{r^3} \,\hat{\mathbf{r}} \cdot \left[\int d^3 r' \,\rho(\mathbf{r}') \,\frac{1}{2} \left(\mathbf{r}' \mathbf{r}' - (r')^2 \,\widehat{\mathbf{I}} \right) \right] \cdot \hat{\mathbf{r}}$$
(2.4.11)

Here $\mathbf{\hat{I}}$ is the second rank *identity tensor*, such that for any two vectors \mathbf{v} and \mathbf{u} , we have $\mathbf{u} \cdot \mathbf{\hat{I}} \cdot \mathbf{v} = \mathbf{u} \cdot \mathbf{v}$. And $\mathbf{r'r'}$ is the second rank tensor such that for any two vectors \mathbf{v} and \mathbf{u} , we have $\mathbf{u} \cdot [\mathbf{r'r'}] \cdot \mathbf{v} = (\mathbf{u} \cdot \mathbf{r'})(\mathbf{r' \cdot v})$. A second rank tensor is an object such that one gets a scalar when one takes the dot product on both sides with a vector; one gets a vector if one takes the dot product of only one side with a vector. When writing down in a coordinate system, a second rank tensor can be written as a matrix.

We can now define the quadrupole tensor tensor as,

$$\vec{\mathbf{Q}} \equiv \int d^3 r' \,\rho(\mathbf{r}') \,\left(3\mathbf{r}'\mathbf{r}' - (r')^2 \vec{\mathbf{I}}\right) \tag{2.4.12}$$

and then write,

$$\phi^{(2)}(\mathbf{r}) = \frac{\mathbf{\hat{r}} \cdot \mathbf{\hat{Q}} \cdot \mathbf{\hat{r}}}{2r^3}$$
(2.4.13)

So, to these lowest three terms, the multipole expansion gives, \overleftrightarrow

$$\phi(\mathbf{r}) = \frac{q}{r} + \frac{\mathbf{p} \cdot \hat{\mathbf{r}}}{r^2} + \frac{\hat{\mathbf{r}} \cdot \mathbf{Q} \cdot \hat{\mathbf{r}}}{2r^3} + \dots$$
(2.4.14)

defined in terms of the zeroth, first, and second order moments of the charge distribution, q, \mathbf{p} , and \mathbf{Q} .

Note the important point that q, \mathbf{p} , and $\mathbf{\ddot{Q}}$ do *not* depend on the location of the observation point \mathbf{r} – we can calculate these moments once, and then use them to compute $\phi(\mathbf{r})$ at all values of \mathbf{r} .

<u>monopole</u>: $q = \int d^3 r \,\rho(\mathbf{r})$ is a scalar integral. dipole: $\mathbf{p} = \int d^3 r \,\rho(\mathbf{r})\mathbf{r}$ is a vector integral.

If we pick a coordinate system, we have to do 3 integrations to get the three components of the dipole moment, $p_x = \hat{\mathbf{x}} \cdot \mathbf{p} = \int d^3 r \,\rho(\mathbf{r}) x$, and similarly for p_y and p_z .

<u>quadrupole</u>: $\overleftrightarrow{\mathbf{Q}} = \int d^3 r \,\rho(\mathbf{r}) \left(3\mathbf{r}\mathbf{r} - r^2 \overleftrightarrow{\mathbf{I}}\right)$ is a tensor integral

If we pick a coordinate system, we have in principle to do 9 integrations to get the 9 components of the 3×3 matrix representing the tensor $\overleftrightarrow{\mathbf{Q}}$. For example,

$$Q_{xx} = \hat{\mathbf{x}} \cdot \overleftrightarrow{\mathbf{Q}} \cdot \hat{\mathbf{x}} = \int d^3 r \,\rho(\mathbf{r}) \,\left(3x^2 - r^2\right) \qquad \text{and} \qquad Q_{xy} = \hat{\mathbf{x}} \cdot \overleftrightarrow{\mathbf{Q}} \cdot \hat{\mathbf{y}} = \int d^3 r \,\rho(\mathbf{r}) \,\left(3xy\right) \tag{2.4.15}$$

and similarly for the other components to get the 3×3 matrix

$$\overrightarrow{\mathbf{Q}} = \begin{pmatrix} Q_{xx} & Q_{xy} & Q_{xz} \\ Q_{yx} & Q_{yy} & Q_{yz} \\ Q_{zx} & Q_{zy} & Q_{zz} \end{pmatrix}$$
(2.4.16)

Note, however that $\mathbf{\hat{Q}}$ is a *symmetric* tensor, so that $Q_{xy} = Q_{yx}$ and similarly for other non-diagonal components, and so there are only 6 independent elements of $\mathbf{\hat{Q}}$ that one has to compute.

Note also that the trace of $\overleftrightarrow{\mathbf{Q}}$ vanishes!

$$\operatorname{Tr}[\overleftrightarrow{\mathbf{Q}}] = Q_{xx} + Q_{yy} + Q_{zz} = \int d^3 r \,\rho(\mathbf{r}) \,\left[(3x^2 - r^2) + (3y^2 - r^2) + (3z^2 - r^2) \right] = 0 \tag{2.4.17}$$

since $3x^2 + 3y^2 + 3z^2 = 3r^2$. So really there are only 5 independent components one has to compute. If one has computed Q_{xx} and Q_{yy} , then one knows that $Q_{zz} = -Q_{xx} - Q_{yy}$.

General Method

We will continue the discussion of q, \mathbf{p} , and $\overleftrightarrow{\mathbf{Q}}$ soon. But first we make an aside to discuss the more general method.

In our expression,

$$\phi(\mathbf{r}) = \sum_{\ell=0}^{\infty} \frac{1}{r^{\ell+1}} \int d^3 r' \,\rho(\mathbf{r}')(r')^{\ell} \mathcal{P}_{\ell}(\cos\theta)$$
(2.4.18)





To do this, we can use the *addition theorem* for spherical harmonics (see Jackson section 3.6 for a discussion and proof).

$$\mathcal{P}_{\ell}(\cos\gamma) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\theta',\varphi') Y_{\ell m}(\theta,\varphi)$$
(2.4.19)

where (θ, φ) are the angles of the observer's direction $\hat{\mathbf{r}}$, and (θ', φ') are the angles of the direction of the integration variable $\hat{\mathbf{r}}'$, and γ is the angle between $\hat{\mathbf{r}}$ and $\hat{\mathbf{r}}'$, so $\cos \theta = \hat{\mathbf{z}} \cdot \hat{\mathbf{r}}$, $\cos \theta' = \hat{\mathbf{z}} \cdot \hat{\mathbf{r}}'$, and $\cos \gamma = \hat{\mathbf{r}} \cdot \hat{\mathbf{r}}'$,

We can then write,

$$\phi(\mathbf{r}) = \sum_{\ell=0}^{\infty} \frac{1}{r^{\ell+1}} \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} \int d^3 r' \,\rho(\mathbf{r}')(r')^{\ell} \,Y_{\ell m}^*(\theta',\varphi') Y_{\ell m}(\theta,\varphi)$$
(2.4.20)

Define the moment,

$$q_{\ell m} = \int d^3 r' \,\rho(\mathbf{r}')(r')^{\ell} \,Y_{\ell m}^*(\theta',\varphi') \qquad \text{which is independent of the observation point } \mathbf{r}$$
(2.4.21)

and then,

$$\phi(\mathbf{r}) = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{q_{\ell m} Y_{\ell m}(\theta, \varphi)}{(2\ell+1)r^{\ell+1}}$$
(2.4.22)

see Jackson Eqs. (4.4) – (4.6) to relate the $q_{\ell m}$ to q, \mathbf{p} , and \mathbf{Q} .

Electric Field

Back to the monopole, dipole, and quadrupole moments.

$$\phi(\mathbf{r}) = \frac{q}{r} + \frac{\mathbf{p} \cdot \hat{\mathbf{r}}}{r^2} + \frac{\hat{\mathbf{r}} \cdot \mathbf{Q} \cdot \hat{\mathbf{r}}}{2r^3} + \dots$$
(2.4.23)

The electric field is given by

$$\mathbf{E} = -\nabla\phi = -\frac{\partial\phi}{\partial r}\hat{\mathbf{r}} - \frac{1}{r}\frac{\partial\phi}{\partial\theta}\hat{\boldsymbol{\theta}} - \frac{1}{r\sin\theta}\frac{\partial\phi}{\partial\varphi}\hat{\boldsymbol{\varphi}}$$
(2.4.24)

For the monopole term,

$$\mathbf{E} = \frac{q}{r^2} \,\hat{\mathbf{r}} \tag{2.4.25}$$

For the dipole term, for convenience we choose \mathbf{p} to lie along the $\hat{\mathbf{z}}$ axis. Then,

$$\phi(\mathbf{r}) = \frac{p\cos\theta}{r^2} \tag{2.4.26}$$

$$\mathbf{E} = \frac{2p\cos\theta}{r^3}\,\hat{\mathbf{r}} + \frac{p\sin\theta}{r^3}\,\hat{\boldsymbol{\theta}} = \frac{p}{r^3}\,\left(2\cos\theta\,\hat{\mathbf{r}} + \sin\theta\,\hat{\boldsymbol{\theta}}\right) \tag{2.4.27}$$

Note, the above expressions for ϕ and **E** are the same as we found earlier outside a sphere with surface charge density $\sigma(\theta) = k \cos \theta$, i.e. the uniformly polarized sphere. So now we see that that field is just the same as the electric dipole field.

It would be nice to have an expression for the dipole **E** that does not make reference to any special direction (i.e. does not assume that **p** is along $\hat{\mathbf{z}}$).



To get such an expression, note,

$$p\cos\theta\,\hat{\mathbf{r}} = (\mathbf{p}\cdot\hat{\mathbf{r}})\,\hat{\mathbf{r}}$$
 and $p\sin\theta\,\hat{\boldsymbol{\theta}} = -(\mathbf{p}\cdot\hat{\boldsymbol{\theta}})\,\hat{\boldsymbol{\theta}}$ (2.4.28)

Now,

$$\mathbf{p} = (\mathbf{p} \cdot \hat{\mathbf{r}}) \,\hat{\mathbf{r}} + (\mathbf{p} \cdot \hat{\boldsymbol{\theta}}) \,\hat{\boldsymbol{\theta}} \qquad \text{so} \qquad -(\mathbf{p} \cdot \hat{\boldsymbol{\theta}}) \,\hat{\boldsymbol{\theta}} = (\mathbf{p} \cdot \hat{\mathbf{r}}) \,\hat{\mathbf{r}} - \mathbf{p} \tag{2.4.29}$$

We can now substitute these results into Eq. (2.4.27) to get,

$$\mathbf{E} = \frac{1}{r^3} \left[2(\mathbf{p} \cdot \hat{\mathbf{r}}) \,\hat{\mathbf{r}} + (\mathbf{p} \cdot \hat{\mathbf{r}}) \,\hat{\mathbf{r}} - \mathbf{p} \right] = \frac{1}{r^3} \left[3(\mathbf{p} \cdot \hat{\mathbf{r}}) \,\hat{\mathbf{r}} - \mathbf{p} \right]$$
(2.4.30)

So,

$$\mathbf{E} = \frac{3(\mathbf{p} \cdot \hat{\mathbf{r}}) \hat{\mathbf{r}} - \mathbf{p}}{r^3} \qquad \text{expresses the dipole electric field in a coordinate free form (i.e. no reference to θ) (2.4.31)$$

Origin of the Coordinates

There is one point we have glossed over. The definition of the multipole moments depends on the choice of the origin of the coordinates. Clearly we have in mind to put the origin somewhere in the middle of the charge distribution ρ , but is there a best place to put it?

Suppose we have a coordinate system (x, y, z), and we transform to a new coordinate system $(\tilde{x}, \tilde{y}, \tilde{z})$ by translating the origin of the coordinates by **d**, so that $\tilde{\mathbf{r}} = \mathbf{r} - \mathbf{d}$ (so that the origin $\tilde{0}$ of the $(\tilde{x}, \tilde{y}, \tilde{z})$ coordinate system is at the position **d** in the (x, y, z) coordinate system). How do the multipole moments computed in the $(\tilde{x}, \tilde{y}, \tilde{z})$ system compare with those computed in the (x, y, z) system?



monopole:

$$\tilde{q} = \int d^3 \tilde{r} \, \rho = \int d^3 r \, \rho = q,$$
 so the monopole moment does not depend on the choice of the origin. (2.4.32)

dipole:

$$\tilde{\mathbf{p}} = \int d^3 \tilde{r} \,\rho \,\tilde{\mathbf{r}} = \int d^3 r \,\rho \,(\mathbf{r} - \mathbf{d}) = \int d^3 r \,\rho \,\mathbf{r} - \mathbf{d} \int d^3 r \,\rho = \mathbf{p} - q\mathbf{d} \qquad \text{So } \,\tilde{\mathbf{p}} = \mathbf{p} \text{ only if } q = 0 \,! \tag{2.4.33}$$

If $q \neq 0$, then $\tilde{\mathbf{p}} \neq \mathbf{p}$. In this case, one can always choose an origin of the coordinates for which the dipole moment will vanish! Proof: If one is working in coordinates (x, y, z) in which $\mathbf{p} \neq 0$, then all one has to do is to transform to new coordinates $(\tilde{x}, \tilde{y}, \tilde{z})$ defined by $\tilde{\mathbf{r}} = \mathbf{r} - \mathbf{d}$ where the displacement is given by $\mathbf{d} = \mathbf{p}/q$. In that coordinate system $\tilde{\mathbf{p}} = 0$. This then is the best place to put the origin since, in making the expansion,

$$\phi(\mathbf{r}) = \frac{q}{r} + \frac{\mathbf{p} \cdot \hat{\mathbf{r}}}{r^2} + \frac{\hat{\mathbf{r}} \cdot \overleftrightarrow{\mathbf{Q}} \cdot \hat{\mathbf{r}}}{2r^3} + \dots$$
(2.4.34)

this choice for the origin of the coordinates will make the dipole term vanish. The leading term in ϕ will always be q/r. For a general location of the origin, the next to leading term will be $\sim 1/r^2$. But if we compute the moments about the origin $\tilde{0}$, then the next to leading term will be $\sim 1/r^3$, and our approximation is therefore more accurate!

If q = 0, then it does not matter where we put the coordinate origin, the value of the dipole moment **p** will stay the same.

When $q \neq 0$, how did we accomplish this trick of picking an origin so that **p** vanished? It is because there are 3 components of $\mathbf{p} = (p_x, p_y, p_z)$. When we make a translation of the origin by $\mathbf{d} = (d_x, d_y, d_z)$ we have 3 degrees of freedom that we can adjust, exactly the right number so as to eliminate the 3 components of **p**.

quadrupole:

$$\tilde{\vec{\mathbf{Q}}} = \int d^3 \tilde{r} \,\rho \,\left[3\tilde{\mathbf{r}}\tilde{\mathbf{r}} - \tilde{r}^2 \vec{\mathbf{I}}\right] = \int d^3 r \,\rho \,\left[3(\mathbf{r} - \mathbf{d})(\mathbf{r} - \mathbf{d}) - |\mathbf{r} - \mathbf{d}|^2 \vec{\mathbf{I}}\right]$$
(2.4.35)

$$= \int d^3 r \,\rho \left[3\mathbf{r}\mathbf{r} - 3\mathbf{r}\mathbf{d} - 3\mathbf{d}\mathbf{r} + 3\mathbf{d}\mathbf{d} - (r^2 + d^2 - 2\mathbf{r} \cdot \mathbf{d}) \overleftrightarrow{\mathbf{I}} \right]$$
(2.4.36)

$$= \int d^3 r \,\rho \left[3\mathbf{r}\mathbf{r} - r^2 \overleftrightarrow{\mathbf{I}} \right] - 3 \left[\int d^3 r \,\rho \,\mathbf{r} \right] \mathbf{d} - 3\mathbf{d} \left[\int d^3 r \,\rho \,\mathbf{r} \right]$$
(2.4.37)

$$+ 3\mathbf{d}\mathbf{d}\left[\int d^{3}r\,\rho\right] - d^{2}\overset{\leftrightarrow}{\mathbf{I}}\left[\int d^{3}r\,\rho\right] + 2\left[\int d^{3}r\,\rho\,\mathbf{r}\right] \cdot \mathbf{d}\overset{\leftrightarrow}{\mathbf{I}}$$
(2.4.38)

$$= \overset{\leftrightarrow}{\mathbf{Q}} - 3\mathbf{p}\mathbf{d} - 3\mathbf{d}\mathbf{p} + 3\mathbf{d}\mathbf{d}q - \left[d^2q - 2\mathbf{p}\cdot\mathbf{d}\right] \overset{\leftrightarrow}{\mathbf{I}}$$
(2.4.39)

We see that $\overleftrightarrow{\mathbf{Q}}$ is independent of the choice of the origin of the coordinates only when both q and \mathbf{p} vanish. When this happens, the quadrupole term is the *leading* term in the multipole expansion.

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

Discussion Question 2.4

We saw that when $q \neq 0$, it was possible to choose the coordinate origin so that $\mathbf{p} = 0$. Now suppose q = 0 but $\mathbf{p} \neq 0$, is it possible to choose the coordinate origin so that $\mathbf{Q} = 0$?

We saw that $\vec{\mathbf{Q}}$ is symmetric and traceless, so it has 5 independent elements. If we translate the origin of the coordinate system, that gives 3 degrees of freedom to adjust. It would seem that we can not make 5 elements vanish with only 3 degrees of freedom to adjust. But what if we also consider a rotation of the coordinate system? That is 3 more degrees of freedom to adjust! Put another way, since $\vec{\mathbf{Q}}$ is symmetric, we know that by rotating the coordinate system appropriately we can make $\vec{\mathbf{Q}}$ diagonal – so only Q_{xx}, Q_{yy} , and Q_{zz} are non-zero, and now there are only 3 components of $\vec{\mathbf{Q}}$. Also, if $\vec{\mathbf{Q}}$ is traceless in one coordinate system, it is traceless in all coordinate systems, so $Q_{xx} + Q_{yy} + Q_{zz} = 0$, and now it would appear that there are only 2 independent matrix elements to $\vec{\mathbf{Q}}$. Can one now make these 2 elements vanish by translating the origin, so that $\vec{\mathbf{Q}} = 0$ in the new coordinate system?

Example

Suppose there are two charges, q_1 at \mathbf{r}_1 and q_2 at \mathbf{r}_2 , and $q_1 + q_2 = q \neq 0$. Find the first three multipole moments.

$$\underline{\text{monopole:}} \quad q = q_1 + q_2$$

$$\underline{\text{dipole:}} \quad \mathbf{p} = q_1 \mathbf{r}_1 + q_2 \mathbf{r}_2$$

$$\underline{\text{quadrupole:}} \quad \mathbf{\hat{Q}} = (3\mathbf{r}_1\mathbf{r}_1 - r_1^2\mathbf{\hat{I}})q_1 + (3\mathbf{r}_2\mathbf{r}_2 - r_2^2\mathbf{\hat{I}})q_2$$

We can make the dipole moment vanish by shifting to a new coordinate system $\mathbf{r}' = \mathbf{r} - \mathbf{d}$, where $\mathbf{d} = \mathbf{p}/q$.

$$\Rightarrow \mathbf{r}' = \mathbf{r} - \frac{q_1 \mathbf{r}_1 + q_2 \mathbf{r}_2}{q_1 + q_2} = \frac{q_1 (\mathbf{r} - \mathbf{r}_1) + q_2 (\mathbf{r} - \mathbf{r}_2)}{q_1 + q_2}$$
(2.4.40)

In this new coordinate system, the positions of q_1 and q_2 are,

$$\mathbf{r}_{1}^{\prime} = \frac{q_{2}}{q_{1} + q_{2}} \left(\mathbf{r}_{1} - \mathbf{r}_{2}\right) \text{ and } \mathbf{r}_{2}^{\prime} = \frac{-q_{1}}{q_{1} + q_{2}} \left(\mathbf{r}_{1} - \mathbf{r}_{2}\right)$$

$$(2.4.41)$$

The origin of the new coordinate system is at

$$\mathbf{r}' = 0 \quad \Rightarrow \quad \mathbf{r} = \frac{q_1 \mathbf{r}_1 + q_2 \mathbf{r}_2}{q_1 + q_2}$$
 this is the "center of charge" – it lies along the vector from \mathbf{r}_1 to \mathbf{r}_2 (2.4.42)

For many charges q_i at positions \mathbf{r}_i , the origin that makes the dipole vanish is the center of charge, $\mathbf{r} = \frac{\sum_i q_i \mathbf{r}_i}{\sum_i q_i}$.

In this primed coordinate system,

$$\mathbf{p}' = q_1 \mathbf{r}'_1 + q_2 \mathbf{r}'_2 = \frac{q_1 q_2}{q_1 + q_2} \left(\mathbf{r}_1 - \mathbf{r}_2 \right) - \frac{q_2 q_2}{q_1 + q_2} \left(\mathbf{r}_1 - \mathbf{r}_2 \right) = 0 \qquad \text{as it must be!}$$
(2.4.43)

We now compute the quadrupole moment in the primed coordinate system.

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

$$(2.4.44)$$

Let us choose spherical coordinates with the origin at O' and $\hat{\mathbf{z}}$ axis aligned along $\mathbf{r}_1 - \mathbf{r}_2$ so that $\mathbf{r}_1 - \mathbf{r}_2 = s\hat{\mathbf{z}}$, where $s = |\mathbf{r}_1 - \mathbf{r}_2|$ is the separation between the charges. Then,

$$\mathbf{r}'_1 = \frac{q_2}{q_1 + q_2} \, s \, \hat{\mathbf{z}} \qquad \text{and} \qquad \mathbf{r}'_2 = \frac{-q_1}{q_1 + q_2} \, s \, \hat{\mathbf{z}}$$
 (2.4.45)

and

$$\overrightarrow{\mathbf{Q}}' = \left(\frac{q_2}{q_1 + q_2}\right)^2 q_1 \left[3s^2 \widehat{\mathbf{z}} \widehat{\mathbf{z}} - s^2 \overleftrightarrow{\mathbf{I}}\right] + \left(\frac{-q_1}{q_1 + q_2}\right)^2 q_2 \left[3s^2 \widehat{\mathbf{z}} \widehat{\mathbf{z}} - s^2 \overleftrightarrow{\mathbf{I}}\right]$$
(2.4.46)

$$= \frac{q_2^2 q_1 + q_1^2 q^2}{(q_1 + q_2)^2} s^2 \left[3\hat{\mathbf{z}}\hat{\mathbf{z}} - \stackrel{\leftrightarrow}{\mathbf{I}} \right] = \frac{q_1 q_2}{q_1 + q_2} s^2 \begin{pmatrix} -1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 2 \end{pmatrix}$$
(2.4.47)

The last result in matrix form follows because in the xyz coordinate system, $\hat{\mathbf{z}}\hat{\mathbf{z}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, while $\stackrel{\leftrightarrow}{\mathbf{I}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

To clarify, if we denote $\hat{\mathbf{e}}_1 = \hat{\mathbf{x}}$, $\hat{\mathbf{e}}_2 = \hat{\mathbf{y}}$, and $\hat{\mathbf{e}}_3 = \hat{\mathbf{z}}$, then the *ij* matrix element of any tensor $\overset{\leftrightarrow}{\mathbf{M}}$ is, $M_{ij} = \hat{\mathbf{e}}_i \cdot \overset{\leftrightarrow}{\mathbf{M}} \cdot \hat{\mathbf{e}}_j$.

As a check (it is always good to make checks of one's calculations!) we see that $\overleftrightarrow{\mathbf{Q}}$ is symmetric and that the trace of $\overleftrightarrow{\mathbf{Q}}$ is zero.

The contribution of the quadrupole to the electrostatic potential ϕ is then

$$\phi^{\text{quad}}(\mathbf{r}) = \frac{\mathbf{\hat{r}} \cdot \overleftrightarrow{\mathbf{Q}} \cdot \mathbf{\hat{r}}}{2r^3} \tag{2.4.48}$$

Let us evaluate in spherical coordinates (we will drop the primes from the coordinate variables to make the notation simpler – but we are still talking about the coordinate system in which $\mathbf{p} = 0$). With $\hat{\mathbf{r}} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ in spherical coordinates we have,

$$\phi^{\text{quad}}(\mathbf{r}) = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1 + q_2} \left(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\right) \begin{pmatrix} -1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} \sin\theta\cos\varphi\\ \sin\theta\sin\varphi\\ \cos\theta \end{pmatrix}$$
(2.4.49)

Do the matrix multiplications to get,

$$\phi^{\text{quad}}(\mathbf{r}) = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1 + q_2} \left(2\cos^2\theta - \sin^2\theta \right) \tag{2.4.50}$$

We see that ϕ^{quad} is independent of the azimuthal angle φ , as it must be due to the rotational symmetry about the $\hat{\mathbf{z}}$ axis.

We can rewrite this in a simpler form using $\sin^2 \theta = 1 - \cos^2 \theta \Rightarrow 2\cos^2 \theta - \sin^2 \theta = 3\cos^2 \theta - 1$ and $\cos^2 \theta = (1 + \cos 2\theta)/2 \Rightarrow 3\cos^2 \theta - 1 = (1 + 3\cos 2\theta)/2$. So then,

$$\phi^{\text{quad}} = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1 + q_2} \frac{1 + 3\cos 2\theta}{2} \qquad \text{as compared to the dipole term} \qquad \phi^{\text{dipole}} = \frac{p\cos\theta}{r^2} \tag{2.4.51}$$

We plot these forms vs θ below. We see that the angular distribution of the quadrupole term is more complex than that of the dipole term.



Note, if we compute the average of ϕ , averaging over the angle θ , then we find,

$$[\phi^{\text{dipole}}]_{\text{ave}} \propto \int_0^{\pi} d\theta \sin \theta \, \cos \theta = \left[-\frac{1}{2} \cos^2 \theta \right]_0^{\pi} = 0 \tag{2.4.52}$$

$$[\phi^{\text{quad}}]_{\text{ave}} \propto \int_0^{\pi} d\theta \sin\theta \left(3\cos^2\theta - 1\right) = \left[-\cos^3\theta + \cos\theta\right]_0^{\pi} = 0 \tag{2.4.53}$$

So the moments higher than the monopole vanish when averaging over the orientation of $\hat{\mathbf{r}}$. We will soon see that this holds in general, not just for the specific example considered here.

Quadrupole Term More Generally

Now we consider the quadrupole term more generally,

$$\phi^{\text{quad}}(\mathbf{r}) = \frac{\hat{\mathbf{r}} \cdot \overleftrightarrow{\mathbf{Q}} \cdot \hat{\mathbf{r}}}{2r^3} \tag{2.4.54}$$

Since $\overleftrightarrow{\mathbf{Q}}$ is a symmetric tensor, we can always rotate to a coordinate system in which it is diagonal. Let us work in that coordinate system, where

$$\overrightarrow{\mathbf{Q}} = \begin{pmatrix} Q_x & 0 & 0\\ 0 & Q_y & 0\\ 0 & 0 & Q_z \end{pmatrix}$$
 (2.4.55)

In this coordinate system, $\hat{\mathbf{r}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. Then,

$$\hat{\mathbf{r}} \cdot \overleftrightarrow{\mathbf{Q}} \cdot \hat{\mathbf{r}} = Q_x \sin^2 \theta \cos^2 \varphi + Q_y \sin^2 \theta \sin^2 \varphi + Q_z \cos^2 \theta$$
(2.4.56)

Since $\overleftrightarrow{\mathbf{Q}}$ is traceless, we can also write $Q_z = -(Q_x + Q_y)$. So finally the most general angular distribution from the quadrupole term is,

$$\phi^{\text{quad}} = \frac{1}{2r^3} \left[Q_x \sin^2 \theta \cos^2 \varphi + Q_y \sin^2 \theta \sin^2 \varphi - (Q_x + Q_y) \cos^2 \theta \right]$$
(2.4.57)

$$= \frac{1}{2r^3} \left[Q_x \left(\sin^2 \theta \cos^2 \varphi - \cos^2 \theta \right) + Q_y \left(\sin^2 \theta \sin^2 \varphi - \cos^2 \theta \right) \right]$$
(2.4.58)

In general, ϕ^{quad} can depend on both angles θ and φ . However, if there is rotational symmetry about the $\hat{\mathbf{z}}$ axis, then we will have $Q_x = Q_y$, and then the above angular form simplifies to $(\sin^2 \theta - 2\cos^2 \theta)$, just as we found in our simple example above consisting of two charges.

Angular Averaging

The multipole expansion is,

$$\phi(\mathbf{r}) = \frac{q}{r} + \frac{\mathbf{p} \cdot \hat{\mathbf{r}}}{r^2} + \frac{\hat{\mathbf{r}} \cdot \hat{\mathbf{Q}} \cdot \hat{\mathbf{r}}}{2r^3} + \dots$$
(2.4.59)

Note, in each term the dependence on the distance from the charge source $r = |\mathbf{r}|$ is only in the denominator. The numerators depend on the orientation of \mathbf{r} via $\hat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$. So we can write,

$$\phi(\mathbf{r}) = \frac{q}{r} + \sum_{n=2}^{\infty} \frac{f_n(\theta, \varphi)}{r^n}$$
(2.4.60)

where $f_n(\theta, \varphi)$ gives the dependence of the potential on the orientation $\hat{\mathbf{r}}$.

Now we will show that the angular average of $f_n(\theta, \varphi)$ must always vanish, i.e. $\int_0^{\pi} d\theta \sin \theta \int_0^{2\pi} d\varphi f_n(\theta, \varphi) = 0.$

Consider the corresponding electric field $\mathbf{E} = -\boldsymbol{\nabla}\phi$,

$$\mathbf{E} = \frac{q\hat{\mathbf{r}}}{r^2} - \sum_{n=2}^{\infty} \nabla\left(\frac{f_n(\theta,\varphi)}{r^n}\right)$$
(2.4.61)



Consider a sphere of radius R centered on the charge distribution. Let S be the surface of this sphere. We know from Gauss' Law that,

$$\oint_{S} da \, \hat{\mathbf{n}} \cdot \mathbf{E} = 4\pi Q_{\text{encl}} = 4\pi q \qquad \text{with } q \text{ the monopole moment}$$
(2.4.62)

Since

$$\oint_{S} da \,\hat{\mathbf{n}} \cdot \frac{q\hat{\mathbf{r}}}{r^{2}} = \oint_{S} da \,\frac{q}{r^{2}} \qquad \text{since } \hat{\mathbf{n}} = \hat{\mathbf{r}} \text{ on the surface } S \tag{2.4.63}$$

$$= \int_{0}^{\pi} d\theta R^{2} \sin \theta \int_{0}^{2\pi} d\varphi \frac{q}{R^{2}} = 4\pi q$$
 (2.4.64)

we see that the monopole term gives all the flux of \mathbf{E} flowing through the surface, and so the flux from the sum of the higher terms in the multipole expansion must therefore give zero. Since this must be true for a sphere of *any* radius R, it can only be true if each of the higher terms individually gives zero flux. Thus,

$$-\oint_{S} da \,\hat{\mathbf{r}} \cdot \boldsymbol{\nabla} \left(\frac{f_n(\theta, \varphi)}{r^n} \right) = 0 \tag{2.4.65}$$

But $\hat{\mathbf{r}} \cdot \boldsymbol{\nabla} = \frac{\partial}{\partial r}$ is the radial directional derivative. So the above is,

$$-\oint_{S} da \ \frac{\partial}{\partial r} \left(\frac{f_n(\theta,\varphi)}{r^n} \right) = n \oint_{S} da \ \frac{f_n(\theta,\varphi)}{r^{n+1}} = \frac{n}{R^{n+1}} \oint_{S} da \ f_n(\theta,\varphi)$$
(2.4.66)

$$=\frac{n}{R^{n+1}}\int_0^{\pi} d\theta R^2 \sin\theta \int_0^{2\pi} d\varphi f_n(\theta,\varphi) = 0$$
(2.4.67)

And we have demonstrated that the *n*-th moment contribution to the potential, $\phi^{(n)}(\mathbf{r}) = \frac{f_n(\theta, \varphi)}{r^n}$ vanishes if we take an angular average.

Sample Charge Distributions

We end our discussion of the electric multipole expansion by illustrating some charge configurations that give rise to different terms in the expansion.

 $\begin{array}{c} & g \\ & & & \\ & & & \\ + g \\ & & & \\ + g \\ & & & \\ - g \\ & & & \\ + g \\ & & \\$

 \Rightarrow monopole is the leading term

 \Rightarrow monopole = 0 \Rightarrow **dipole** is the leading term, **p** is independent of the location of the coordinate origin.

 \Rightarrow monopole = 0, the total dipole is the sum of oppositely oriented dipoles and so is zero, the **quadrupole** is the leading term.

 \Rightarrow monopole and dipole both = 0, total quadrupole is the sum of oppositely charged quadrupoles and so sum to zero, the **octapole** is the leading term.