MULTIPOLE EXPANSION

Consider the Coulomb potential of some compact charge system,

$$V(\mathbf{R}) = \frac{1}{4\pi\epsilon_0} \iiint d^3\mathrm{Vol}(\mathbf{r}) \frac{\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|}. \tag{1}$$

Suppose all charges are confined inside a small volume of size D while we are interested in the behavior of the potential at large distances $R \gg D$ from this charge system. In this situation, it's convenient to expand the potential (1) in a series of negative powers of R,

$$V(\mathbf{R}) = \frac{1}{4\pi\epsilon_0} \sum_{\ell=0}^{\infty} \frac{\mathcal{M}_\ell(\widehat{\mathbf{R}})}{R^{\ell+1}}, \tag{2}$$

where $\mathcal{M}_\ell$ is the ℓ^{th} multipole moment of the charge system, or rather $\mathcal{M}_\ell(\widehat{\mathbf{R}})$ is the component of this multipole moment in the direction of $\mathbf{R}$.

A point of notation: In this notes, the upper-case $\mathbf{R}$ is the distant point where we measure the potential $V(\mathbf{R})$, $R = |\mathbf{R}|$, $\widehat{\mathbf{R}} = \mathbf{R}/R$ is the unit vector in the direction of $\mathbf{R}$, and (R, Θ, Φ) are the spherical coordinates of the $\mathbf{R}$. On the other hand, the lower-case $\mathbf{r}$ is a point where some charge is located; likewise, $r = |\mathbf{r}|$, $\hat{\mathbf{r}} = \mathbf{r}/r$ is the unit vector in the direction of $\mathbf{r}$, and (r, θ, ϕ) are the spherical coordinates of the $\mathbf{r}$. Finally, α is the angle between the directions of $\hat{\mathbf{r}}$ and $\widehat{\mathbf{R}}$, thus

$$\cos\alpha = \hat{\mathbf{r}} \cdot \widehat{\mathbf{R}}. \tag{3}$$

Finally, sometimes I shall use the asterisk $*$ to emphasize the product of two scalars or of a scalar and a vector.

The key to the expansion (2) is the mathematical **theorem:** Consider two points with respective radius vectors $\mathbf{R}$ and $\mathbf{r}$. Suppose the second point is closer to the origin than the first point, $r < R$. Then the inverse distance between the two points

$$\frac{1}{|\mathbf{R}-\mathbf{r}|} = \frac{1}{\sqrt{R^2 + r^2 - 2Rr\cos\alpha}} \tag{4}$$

(where α is the angle between the vectors $\mathbf{R}$ and $\mathbf{r}$) can be expanded in powers of the ratio

r/R as

$$\frac{1}{|\mathbf{R}-\mathbf{r}|} = \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(\cos\alpha) \tag{5}$$

where $P_\ell(x)$ is the Legendre polynomial of degree ℓ. Spelling out the first few Legendre polynomials explicitly, the expansion (5) becomes

$$\frac{1}{|\mathbf{R}-\mathbf{r}|} = \frac{1}{R}\times 1 + \frac{r}{R^2}\times\cos\alpha + \frac{r^2}{R^3}\times\frac{3\cos^2\alpha-1}{2} + \frac{r^3}{R^4}\times\frac{5\cos^3\alpha-3\cos\alpha}{2} + \cdots. \tag{6}$$

The proof of the theorem (5) involves complex contour integration — a technique many students have not yet learned, — so I present it at as *optional* reading material in the Appendix to of these notes.

Meanwhile, let me simply verify the first few terms in the expansion (6) for $r \ll R$. For the sake of compactness, let's denote

$$a = \frac{r}{R} \ll 1, \quad x = \cos\alpha, \quad b = 2ax - a^2 \ll 1.$$

In these notations,

$$\frac{1}{\sqrt{R^2+r^2-2Rr\cos\alpha}} = \frac{1}{\sqrt{R^2(1+a^2-2ax)}} = \frac{1}{R}\times\frac{1}{\sqrt{1-b}}. \tag{7}$$

Next, let's expand the $1/\sqrt{1-b}$ into powers of b:

$$S = \frac{1}{\sqrt{1-b}} = 1 + \sum_{n=1}^{\infty}\frac{(2n-1)!!}{2^n\, n!}\times b^n = 1 + \tfrac{1}{2}b + \tfrac{3}{8}b^2 + \tfrac{5}{16}b^3 + \tfrac{35}{128}b^4 + \cdots. \tag{8}$$

Now, remember that $b = 2ax - a^2$, plug that into the above expansion, open up the $(\cdots)$, and rearrange the terms according to the powers of a. For simplicity, let's stop with terms $\sim a^4$

and truncate the higher powers of a, thus

$$
\begin{aligned}
S \;=\;& 1 \;+\; \tfrac{1}{2}(2ax-a^2) \;+\; \tfrac{3}{8}(2ax-a^2)^2 \;+\; \tfrac{5}{16}(2ax-a^2)^3 \;+\; \tfrac{35}{128}(2ax-a^2)^4 \;+\; \cdots \\
=\;& 1 \;+\; ax \quad - \tfrac{1}{2}a^2 \\
& \quad + \tfrac{3}{2}a^2x^2 \quad - \tfrac{3}{2}a^3x \quad + \tfrac{3}{8}a^4 \\
& \quad\quad + \tfrac{5}{2}a^3x^3 \quad - \tfrac{15}{4}a^4x^2 \quad + \cdots \\
& \quad\quad\quad + \tfrac{35}{8}a^4x^4 \quad - \cdots \\
& \quad\quad\quad\quad + \cdots \\
=\;& 1 \;+\; a\times x \;+\; a^2\times\frac{3x^2-1}{2} \;+\; a^3\times\frac{5x^3-3x}{2} \;+\; a^4\times\frac{35x^4-30x^2+3}{8} \;+\; \cdots \\
=\;& 1 \;+\; a\times P_1(x) \;+\; a^2\times P_2(X) \;+\; a^3\times P_3(x) \;+\; a^4\times P_4(x) \;+\; \cdots
\end{aligned}
\tag{9}
$$

where $P_1(x)$, $P_2(x)$, $P_3(x)$ and $P_4(x)$ are the Legendre polynomials of respective degrees 1, 2, 3, and 4. Plugging this result back into eq. (7), we obtain

$$
\begin{aligned}
\frac{1}{\sqrt{R^2+r^2-2Rr\cos\alpha}} \;=\;& \frac{1}{R} \;+\; \frac{r}{R^2}\times P_1(\cos\alpha) \;+\; \frac{r^2}{R^3}\times P_2(\cos\alpha) \\
&+\; \frac{r^3}{R^4}\times P_3(\cos\alpha) \;+\; \frac{r^4}{R^5}\times P_4(\cos\alpha) \;+\; \cdots,
\end{aligned}
\tag{10}
$$

in perfect agreement with eq. (6).

Now let's apply the theorem (5) to the Coulomb potential

$$
V(\mathbf{R}) \;=\; \frac{1}{4\pi\epsilon_0}\iiint d^3\mathrm{Vol}(\mathbf{r})\,\frac{\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|}
\tag{1}
$$

of a compact charge distribution. Since all the charges are located within a small volume of size D, we may limit the integration range here to $|\mathbf{r}|\leq D$, while we are interested in the potential at large distances $|\mathbf{R}|\gg D$. Thus, throughout the integration volume we have $|\mathbf{r}|\ll|\mathbf{R}|$, so we may expand the inverse distance $1/|\mathbf{R}-\mathbf{r}|$ into a power series in r/R

according to eq. (5), thus

$$
\begin{aligned}
V(\mathbf{R}) &= \frac{1}{4\pi\epsilon_0}\iiint d^3\mathrm{Vol}(\mathbf{r})\,\rho(\mathbf{r})\times\sum_{\ell=0}^{\infty}\frac{r^\ell}{R^{\ell+1}}\times P_\ell(\cos\alpha)\\
&= \sum_{\ell=0}^{\infty}\frac{1}{4\pi\epsilon_0\,R^{\ell+1}}\times\iiint d^3\mathrm{Vol}(\mathbf{r})\,\rho(\mathbf{r})\times r^\ell P_\ell(\cos\alpha) \qquad (11)\\
&= \sum_{\ell=0}^{\infty}\frac{1}{4\pi\epsilon_0\,R^{\ell+1}}\times\iiint d^3\mathrm{Vol}(\mathbf{r})\,\rho(\mathbf{r})\times r^\ell P_\ell(\hat{\mathbf{r}}\cdot\widehat{\mathbf{R}}).
\end{aligned}
$$

Or in other words,

$$
V(\mathbf{R}) = \sum_{\ell=0}^{\infty}\frac{\mathcal{M}_\ell(\widehat{\mathbf{R}})}{4\pi\epsilon_0\,R^{\ell+1}}\,, \tag{12}
$$

exactly as in eq. (2), where the multipole moments of the charge distribution $\rho(\mathbf{r})$ — or rather their components in the direction $\widehat{\mathbf{R}}$ — obtain as integrals

$$
\mathcal{M}_\ell(\widehat{\mathbf{R}}) = \iiint r^\ell P_\ell(\hat{\mathbf{r}}\cdot\widehat{\mathbf{R}})\times\rho(\mathbf{r})\,d^3\mathrm{Vol}(\mathbf{r}). \tag{13}
$$

Or for a system of discrete point charges, as sums

$$
\mathcal{M}_\ell(\widehat{\mathbf{R}}) = \sum_i r_i^\ell\times P_\ell(\hat{\mathbf{r}}_i\cdot\widehat{\mathbf{R}})\times Q_i\,. \tag{14}
$$

The $\widehat{\mathbf{R}}$-dependence of the multipole moments can be described of ℓ-index tensors, or alternatively in terms of spherical harmonics $Y_{\ell,m}(\Theta,\Phi)$. To see how this works — especially the tensor description, — let's start with the leading multipole moments for $\ell = 0, 1, 2, 3$.

Monopole and Dipole Moments, $\ell = 0$ and $\ell = 1$

The multipole moment for $\ell = 0$ is simply the net charge of the distribution. Indeed, $P_0(x) = 1$, hence $r^0 \times P_0(\hat{\mathbf{r}} \cdot \widehat{\mathbf{R}}) = 1 \times 1 = 1$ and therefore

$$\mathcal{M}_0 \;=\; \iiint \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \;=\; Q^{\mathrm{net}} \tag{15}$$

regardless of the direction $\widehat{\mathbf{R}}$. Consequently, the $\ell = 0$ term in the potential is the isotropic Coulomb potential

$$V_{\ell=0}(\mathbf{R}) \;=\; \frac{Q^{\mathrm{net}}}{4\pi\epsilon_0\, R} \tag{16}$$

of a point charge Q^{net}, that's why the $\ell = 0$ multipole is called the monopole.

Next, the moment for $\ell = 1$ is the net dipole moment $\mathbf{p}^{\mathrm{net}}$, or rather its projection $\widehat{\mathbf{R}} \cdot \mathbf{p}^{\mathrm{net}}$ onto the direction of $\mathbf{R}$. Indeed, $P_1(x) = x$, hence

$$r * P_1(\widehat{\mathbf{R}} \cdot \hat{\mathbf{r}}) \;=\; r * (\widehat{\mathbf{R}} \cdot \hat{\mathbf{r}}) \;=\; \widehat{\mathbf{R}} \cdot \mathbf{r} \tag{17}$$

and therefore

$$\mathcal{M}_1(\widehat{\mathbf{R}}) \;=\; \iiint (\widehat{\mathbf{R}} \cdot \mathbf{r})\rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \;=\; \widehat{\mathbf{R}} \cdot \iiint \mathbf{r}\, \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) = \; \widehat{\mathbf{R}} \cdot \mathbf{p}^{\mathrm{net}}. \tag{18}$$

Consequently, the potential of the $\ell = 1$ term is the dipole potential

$$V_{\mathrm{dipole}}(\mathbf{R}) \;=\; \frac{\mathbf{p}^{\mathrm{net}} \cdot \widehat{\mathbf{R}}}{4\pi\epsilon_0\, R^2}\,. \tag{19}$$

Note: the net charge is a scalar while the net dipole moment is a vector, and both scalars and vectors are special case of tensors with respectively 0 indices or 1 index.

Quadrupole Moment for $\ell = 2$

The quadrupole moment is a 2-index symmetric tensor

$$\mathcal{Q}_{i,j} \;=\; \iiint \left(\tfrac{3}{2} r_i r_j \;-\; \tfrac{1}{2}\delta_{i,j}\mathbf{r}^2\right)\rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \tag{20}$$

where the indices i, j run over x, y, z, the r_i are the components of the vector $\mathbf{r}$, and $\delta_{i,j}$ is the Kronecker's delta (1 for $i = j$ and 0 for $i \neq j$). The tensor (20) is symmetric WRT permutation of its two indices, $\mathcal{Q}_{i,j} = \mathcal{Q}_{j,i}$, and the component of this tensor in the direction $\widehat{\mathbf{R}}$ is simply the tensor analogue of the dot product with the unit vector $\widehat{\mathbf{R}}$,

$$\mathcal{M}_2(\widehat{\mathbf{R}}) \;=\; \sum_{i,j=x,y,z} \mathcal{Q}_{i,j}\, \widehat{R}_i \widehat{R}_j\,. \tag{21}$$

To see how this works, we start with $P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$, hence

$$r^2 * P_2(\widehat{\mathbf{R}}\cdot\hat{\mathbf{r}}) \;=\; \tfrac{3}{2} r^2 * (\widehat{\mathbf{R}}\cdot\hat{\mathbf{r}})^2 \;-\; \tfrac{1}{2}r^2 \;=\; \tfrac{3}{2}(\widehat{\mathbf{R}}\cdot\mathbf{r})^2 \;-\; \tfrac{1}{2}\mathbf{r}^2 * \widehat{\mathbf{R}}^2 \tag{22}$$
$$\langle\!\langle\, \widehat{\mathbf{R}} \text{ is a unit vector so } \widehat{\mathbf{R}}^2 = 1 \,\rangle\!\rangle,$$

where

$$(\widehat{\mathbf{R}}\cdot\mathbf{r})^2 \;=\; \Bigl(\sum_i \widehat{R}_i r_i\Bigr)^2 \;=\; \Bigl(\sum_i \widehat{R}_i r_i\Bigr)\Bigl(\sum_j \widehat{R}_j r_j\Bigr) \;=\; \sum_{i,j} \widehat{R}_i \widehat{R}_j\, r_i r_j\,, \tag{23}$$

$$\widehat{\mathbf{R}}^2 \;=\; \sum_i \widehat{R}_i \widehat{R}_i \;=\; \sum_{i,j} \widehat{R}_i \widehat{R}_j\, \delta_{i,j}\,, \tag{24}$$

and therefore

$$\begin{aligned} r^2 * P_2(\widehat{\mathbf{R}}\cdot\hat{\mathbf{r}}) \;&=\; \tfrac{3}{2}\sum_{i,j} \widehat{R}_i \widehat{R}_j\, r_i r_j \;-\; \tfrac{1}{2}\mathbf{r}^2 \sum_{i,j} \widehat{R}_i \widehat{R}_j\, \delta_{ij} \\ &=\; \sum_{i,j} \widehat{R}_i \widehat{R}_j * \left(\tfrac{3}{2} r_i r_j \;-\; \tfrac{1}{2}\mathbf{r}^2 \delta_{i,j}\right). \end{aligned} \tag{25}$$

Plugging this formula into the integral for the $\ell = 2$ moment, we get

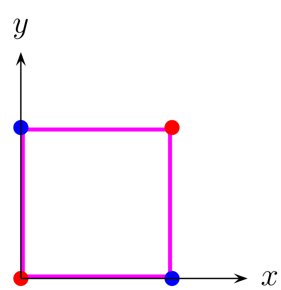
$$\begin{aligned}
\mathcal{M}_2(\widehat{\mathbf{R}}) &= \iiint r^2 * P_2(\widehat{\mathbf{R}} \cdot \hat{\mathbf{r}}) * \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \\
&= \iiint \sum_{i,j} \widehat{R}_i \widehat{R}_j * \left(\tfrac{3}{2} r_i r_j \,-\, \tfrac{1}{2} r^2 \delta_{i,j}\right) * \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \\
&= \sum_{i,j} \widehat{R}_i \widehat{R}_j * \iiint \left(\tfrac{3}{2} r_i r_j \,-\, \tfrac{1}{2} r^2 \delta_{i,j}\right) * \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \\
&= \sum_{i,j} \widehat{R}_i \widehat{R}_j * \mathcal{Q}_{i,j}
\end{aligned} \tag{26}$$

where the quadrupole moment tensor $\mathcal{Q}_{i,j}$ is exactly as in eq. (20). In terms of this tensor, the quadrupole potential is

$$V_{\text{quadrupole}}(\mathbf{R}) \;=\; \frac{\sum_{i,j} \mathcal{Q}_{i,j} \widehat{R}_i \widehat{R}_j}{4\pi\epsilon_0\, R^3}\,. \tag{27}$$

Example 1.

A good example of a quadrupole moment tensor is a simple quadrupole — for alternating charges $\pm Q$ at the corners of a square, hence the name *quadrupole*,



$$\begin{aligned}
&+Q \;@(0,0,0), \\
&-Q \;@(a,0,0), \\
&-Q \;@(0,a,0), \\
&+Q \;@(a,a,0).
\end{aligned} \tag{28}$$

It is easy to see that this 4-charge system has zero net charge as well as zero net dipole moment, so the leading term in its potential at long distances is the quadrupole potential (27). Let's calculate the quadrupole moment tensor

$$\mathcal{Q}_{i,j} \;=\; \sum_{a=1}^{4} Q_\alpha \left(\tfrac{3}{2} r_{a,i} r_{a,j} \,-\, \tfrac{1}{2} \mathbf{r}_a^2 \delta_{i,j}\right) \tag{29}$$

of this simple quadrupole. In matrix notations,

$$Q_1 \left(\tfrac{3}{2} r_i r_j \,-\, \tfrac{1}{2} \mathbf{r}^2 \delta_{i,j}\right)_1 \;=\; +Q \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{30}$$

$$Q_2\left(\tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}\mathbf{r}^2\delta_{i,j}\right)_2 \;=\; -Q\left(\frac{3}{2}\begin{pmatrix} a^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{\mathrm{a}^2}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)$$

$$= -\frac{Qa^2}{2}\begin{pmatrix} +2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{31}$$

$$Q_3\left(\tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}\mathbf{r}^2\delta_{i,j}\right)_3 \;=\; -Q\left(\frac{3}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{\mathrm{a}^2}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)$$

$$= -\frac{Qa^2}{2}\begin{pmatrix} -1 & 0 & 0 \\ 0 & +2 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{32}$$

$$Q_4\left(\tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}\mathbf{r}^2\delta_{i,j}\right)_4 \;=\; +Q\left(\frac{3}{2}\begin{pmatrix} a^2 & a^2 & 0 \\ a^2 & a^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{2\mathrm{a}^2}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)$$

$$= +\frac{Qa^2}{2}\begin{pmatrix} +1 & +3 & 0 \\ +3 & +1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \tag{33}$$

and therefore

$$\mathcal{Q}_{i,j} \;=\; \frac{Qa^2}{2}\begin{pmatrix} 0 & 3 & 0 \\ 3 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{34}$$

For this quadrupole moment tensor

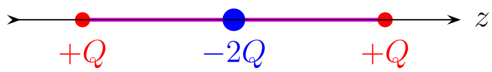
$$\mathcal{M}_2(\widehat{\mathbf{R}}) \;=\; \sum_{i,j}\widehat{R}_i\widehat{R}_j\mathcal{Q}_{i,j} \;=\; 3Qa^2\times\widehat{R}_x\widehat{R}_y \;=\; 3Qa^2\times\sin^2\Theta\cos\Phi\sin\Phi, \tag{35}$$

hence the quadrupole potential

$$V(R,\theta,\phi) \;=\; \frac{3Qa^2}{4\pi\epsilon_0}*\frac{\sin^2\Theta\cos\Phi\sin\Phi}{R^3} \;=\; \frac{3Qa^2}{4\pi\epsilon_0}*\frac{XY}{R^5}\,. \tag{36}$$

Example 2.

Another good example of a quadrupole moment is a linear quadrupole: a charge $-2Q$ in the middle, and two charges $+Q$ at its opposite sides (and at exactly the same distance a):



Again, this charge system has zero net charge and zero net dipole moment, so the leading term in the multipole expansion of its potential is the quadrupole term $\ell = 2$, but this time the quadrupole moment tensor

$$\mathcal{Q}_{i,j} \;=\; \sum_{a=1}^{3} Q_a\left(\tfrac{3}{2} r_{a,i} r_{a,j} \;-\; \tfrac{1}{2}\mathbf{r}_a^2 \delta_{i,j}\right) \tag{37}$$

has a different form. Indeed, for the charges at hand

$$\sum_{\alpha} Q_a r_{a,i} r_{a,j} \;=\; 2Q \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a^2 \end{pmatrix} \tag{38}$$

while

$$\sum Q_a \mathbf{r}_a^2 \;=\; 2Qa^2, \tag{39}$$

hence

$$\mathcal{Q}_{i,j} \;=\; Qa^2 \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +2 \end{pmatrix}. \tag{40}$$

For this quadrupole moment,

$$\begin{aligned} \mathcal{M}_2(\widehat{\mathbf{R}}) \;&=\; Qa^2\left(-\widehat{R}_x^2 - \widehat{R}_y^2 + 2\widehat{R}_z^2\right) \;=\; Qa^2(2\cos^2\Theta - \sin^2\Theta) \\ &=\; Qa^2(3\cos^2\Theta - 1) \;=\; 2Qa^2 * P_2(\cos\Theta), \end{aligned} \tag{41}$$

and the quadrupole potential is

$$V_{\text{quadrupole}} \;=\; \frac{2Qa^2}{4\pi\epsilon_0} * \frac{P_2(\cos\Theta)}{R^3}\,. \tag{42}$$

Tracelessness.

In both of the above examples, the matrices of the quadrupole moment tensors (34) and (40) have zero traces,

$$\mathrm{tr}(\mathcal{Q}) \stackrel{\mathrm{def}}{=} \sum_{i=x,y,z} \mathcal{Q}_{i,i} = 0. \tag{43}$$

Actually, this is a general property of the quadrupole moment tensor of any system. Indeed, by definition of the quadrupole moment tensor,

$$\mathcal{Q}_{i,j} \stackrel{\mathrm{def}}{=} \iiint \left(\tfrac{3}{2} r_i r_j - \tfrac{1}{2}\mathbf{r}^2 \delta_{i,j}\right) \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}), \tag{20}$$

its trace is

$$\begin{aligned} \mathrm{tr}(\mathcal{Q}) &= \sum_{i=x,y,z} \iiint \left(\tfrac{3}{2} r_i r_i - \tfrac{1}{2}\mathbf{r}^2 \delta_{i,i}\right) \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \\ &= \iiint \sum_i \left(\tfrac{3}{2} r_i r_i - \tfrac{1}{2}\mathbf{r}^2 \delta_{i,i}\right) \times \rho(\mathbf{r})\, d^3\mathrm{Vol}(\mathbf{r}) \end{aligned} \tag{44}$$

where

$$\sum_i r_i r_i = \mathbf{r}^2, \qquad \sum_i \delta_{i,i} = \sum_i 1 = 3, \tag{45}$$

hence

$$\sum_i \left(\tfrac{3}{2} r_i r_i - \tfrac{1}{2}\mathbf{r}^2 \delta_{i,i}\right) = \tfrac{3}{2} \times \mathbf{r}^2 - \tfrac{1}{2}\mathbf{r}^2 \times 3 = 0 \tag{46}$$

and therefore $\mathrm{tr}(\mathcal{Q}) = 0$.

Consequently, out of $3^3 = 9$ components of the 2-index quadrupole moment tensor, only 5 components are linearly independent: The symmetry $\mathcal{Q}_{i,j} = \mathcal{Q}_{j,i}$ of the tensor imposes 3 linear relations between the components, and the zero trace condition is another linear constraint, so only $9 - 3 - 1 = 5$ components are linearly independent.

Octupole Moment for $\ell = 3$

For $\ell = 3$ we have $P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$, hence

$$\begin{aligned} r^3 * P_3(\widehat{\mathbf{R}} \cdot \hat{\mathbf{r}}) \;&=\; \tfrac{5}{2}(\widehat{\mathbf{R}} \cdot \mathbf{r})^3 \;-\; \tfrac{3}{2}\widehat{\mathbf{R}}^2\,\mathbf{r}^2\,(\widehat{\mathbf{R}} \cdot \mathbf{r}) \\ &\qquad \langle\!\langle \text{ after a bit of algebra } \rangle\!\rangle \\ &=\; \sum_{i,j,k=x,y,z} \widehat{R}_i\widehat{R}_j\widehat{R}_k \times \Big(\tfrac{5}{2}r_ir_jr_k \;-\; \tfrac{1}{2}\mathbf{r}^2\big(r_i\delta_{j,k} + r_j\delta_{i,k} +\; r_k\delta_{i,j}\big)\Big) \end{aligned} \tag{47}$$

and therefore

$$\begin{aligned} \mathcal{M}_3(\widehat{\mathbf{R}}) \;&=\; \iiint r^3 P_3(\hat{\mathbf{r}} \cdot \widehat{\mathbf{R}})\,\rho(\mathbf{r})\,d^3\mathrm{Vol}(\mathbf{r}) \\ &=\; \sum_{i,j,k=x,y,z} \widehat{R}_i\widehat{R}_j\widehat{R}_k \times \mathcal{O}_{i,j,k} \end{aligned} \tag{48}$$

where

$$\mathcal{O}_{i,j,k} \;\stackrel{\text{def}}{=}\; \iiint\Big(\tfrac{5}{2}r_ir_jr_k \;-\; \tfrac{1}{2}\mathbf{r}^2\big(r_i\delta_{j,k} + r_j\delta_{i,k} +\; r_k\delta_{i,j}\big)\Big)\,\rho(\mathbf{r})\,d^3\mathrm{Vol}(\mathbf{r}) \tag{49}$$

are components of the 3-index *octupole moment tensor*. In terms of this tensor, the $\ell = 3$ term in the multipole expansion of the potential at large distances amounts to

$$V_{\ell=3}(\mathbf{R}) \;=\; \frac{\sum_{i,j,k} \widehat{R}_i\widehat{R}_j\widehat{R}_k \times \mathcal{O}_{i,j,k}}{4\pi\epsilon_0\,R^4}\,. \tag{50}$$

By construction, the octupole moment is a totally symmetric 3-index tensor,

$$\mathcal{O}_{\text{any permutation of } i,j,k} \;=\; \mathcal{O}_{i,j,k}\,. \tag{51}$$

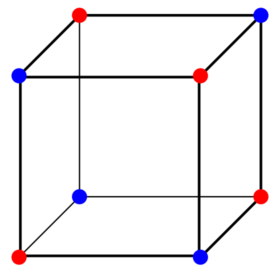
Less obviously, it obeys a generalized zero-trace condition

$$\sum_{i=x,y,z,} \mathcal{O}_{i,i,k} \;=\; 0 \quad \text{for any } k = x,y,z. \tag{52}$$

Consequently, out of $3^3 = 27$ components of the octupole moment tensor, only 7 are linearly independent.

Examples.

A good example of an octupole moment is made from 8 alternating charges $\pm Q$ — hence the name *octupole* — at the vertices of a cube:



(53)

For this cube,

$$\mathcal{O}_{i,j,k} \stackrel{\text{def}}{=} \sum_a Q_a \Big(\tfrac{5}{2} r_i r_j r_k \;-\; \tfrac{1}{2}\mathbf{r}^2 \big(r_i\delta_{j,k} + r_j\delta_{i,k} + \; r_k\delta_{i,j}\big)\Big)_a \tag{54}$$

evaluates to

$$\mathcal{O}_{i,j,k} \;=\begin{cases} \tfrac{5}{2}Qa^3 & \text{for } (i,j,k)=(x,y,z) \text{ in some order,}\\ 0 & \text{otherwise,}\end{cases} \tag{55}$$

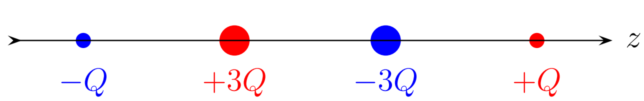
hence

$$\sum_{i,j,k} \widehat{R}_i \widehat{R}_j \widehat{R}_k \times \mathcal{O}_{i,j,k} \;=\; \frac{5Qa^3}{2} \times \frac{6XYZ}{R^3} \tag{56}$$

and therefore octupole potential

$$V_{\text{octupole}} \;=\; \frac{15Qa^3}{4\pi\epsilon_0} * \frac{XYZ}{R^7}\,. \tag{57}$$

Another example of the octupole moment is the linear octupole — 4 equidistant charges $-Q$, $+3Q$, $-3Q$, $+Q$ arranged in a line, say the z axis:



For this system, the octupole moment tensor evaluates to

$$\begin{aligned}
Q_{z,z,z} &= +6Qa^3, \\
Q_{(x,x,z)} &= -3Qa^3, \\
Q_{(y,y,z)} &= -3Qa^3, \\
\text{all other } Q_{i,j,k} &= 0.
\end{aligned} \tag{58}$$

Consequently,

$$\begin{aligned}
\sum_{i,j,k} \widehat{R}_i \widehat{R}_j \widehat{R}_k \times \mathcal{O}_{i,j,k} &= 6Qa^3 \times \frac{Z^3}{R^3} - 3Qa^3 \times \frac{X^2 Z + Y^2 Z}{R^3} \times 3 \\
&= 3Qa^3 \times \bigl(2\cos^3\Theta - 3\cos\Theta\sin^2\Theta\bigr) \\
&= 3Qa^3 \times \bigl(5\cos^3\Theta - 3\cos\Theta\bigr) \\
&= 6Qa^3 \times P_3(\cos\Theta),
\end{aligned} \tag{59}$$

and the octupole potential

$$V_{\text{octupole}}(R,\theta,\phi) = \frac{6Qa^3}{4\pi\epsilon_0} * \frac{P_3(\cos\theta)}{R^4}\,. \tag{60}$$

Higher Multipole Moments

We saw that for $\ell = 0,1,2,3$, the ℓ^{th} term in the multipole expansion is related to an ℓ-index tensor — called the 2^ℓ-pole moment $\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell}$ as

$$\mathcal{M}_\ell(\widehat{\mathbf{R}}) = \sum_{i_i,\ldots,i_\ell} \widehat{R}_{i_1} \cdots \widehat{R}_{i_\ell} \times \mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell}\,,$$

hence

$$V_\ell(\mathbf{R}) = \frac{\sum_{i_i,\ldots,i_\ell} \widehat{R}_{i_1} \cdots \widehat{R}_{i_\ell} \times \mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell}}{4\pi\epsilon_0 R^{\ell+1}}\,. \tag{61}$$

Also, the 2^ℓ-pole moment tensor itself obtains as an integral (or a sum over discrete charges)

$$\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell} = \iiint F^{(\ell)}_{i_i,\ldots,i_\ell}(x,y,z) \times \rho(x,y,z)\, d^3\text{Vol}(x,y,z) \tag{62}$$

or a similar sum over discrete charges

$$\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell} \;=\; \sum_a Q_a \times F^{(\ell)}_{i_i,\ldots,i_\ell}(x_a,y_a,z_a) \tag{63}$$

where each component of the $F^{(\ell)}_{i_i,\ldots,i_\ell}(x,y,z)$ is a homogeneous polynomial of degree ℓ in (x,y,z). Specifically,

$$\begin{aligned} F^{(0)}(x,y,z) &= 1, \\ F^{(1)}_i(x,y,z) &= r_i\,, \\ F^{(2)}_{i,j}(x,y,z) &= \tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}\mathbf{r}^2\delta_{i,j}\,, \\ F^{(3)}_{i,j,k}(x,y,z) &= \tfrac{5}{2}r_ir_jr_k \;-\; \tfrac{1}{2}\mathbf{r}^2\big(r_i\delta_{j,k}+r_j\delta_{i,k}+r_k\delta_{i,j}\big). \end{aligned} \tag{64}$$

At the higher $\ell > 3$ levels of the multipole expansion, we get exactly the same behavior for the higher-rank 2^ℓ-pole moment tensors with ℓ indices: Specifically,

$$V_\ell(\mathbf{R}) \;=\; \frac{\sum_{i_i,\ldots,i_\ell}\widehat{R}_{i_1}\cdots\widehat{R}_{i_\ell}\times\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell}}{4\pi\epsilon_0 R^{\ell+1}} \tag{61}$$

for

$$\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell} \;= \iiint F^{(\ell)}_{i_i,\ldots,i_\ell}(x,y,z)\times\rho(x,y,z)\,d^3\mathrm{Vol} \tag{62}$$

or

$$\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell} \;=\; \sum_a Q_a \times F^{(\ell)}_{i_i,\ldots,i_\ell}(x_a,y_a,z_a), \tag{63}$$

only the polynomials $F^{(\ell)}_{i_i,\ldots,i_\ell}(x,y,z)$ become more complicated for higher ℓ. But fortunately, we are not going to need their explicit form in this class.

Instead, let me simply state that for any ℓ, the 2^ℓ-pole moment tensor $\mathcal{M}^{(\ell)}_{i_i,\ldots,i_\ell}$ is totally symmetric WRT to all permutations of its ℓ indices $i_1,\ldots,i_l$. Also, for any $\ell \geq 2$, it obeys the generalized zero-trace condition:

$$\forall i_3,\ldots,i_\ell: \qquad \sum_{i_1=x,y,z}\mathcal{M}^{(\ell)}_{i_1,i_2=i_1,i_3,\ldots,i_\ell} \;=\; 0. \tag{65}$$

Consequently, out of 3^ℓ components of the 2^ℓ-pole moment tensor, only $2\ell+1$ components are linearly independent. The rest of the components follow from these by the permutation symmetries of the tensor's indices and by the zero-trace conditions (65). Note that $2\ell+1$ is also the number of independent spherical harmonics $Y_{\ell,m}(\theta,\phi)$ for a given ℓ, and this is no coincidence. Instead, this allows us to re-express the angular dependence of all the 2^ℓ-pole terms in the potential in terms of the spherical harmonics, as we shall see in the next section.

Spherical Harmonic Expansion

Instead of describing the angular dependence of the multipoles' components in the direction $\widehat{\mathbf{R}}$ in terms of symmetric multipole tensors, we may expand it in terms of spherical harmonics. The key to this expansion is the following **Lemma:** for any integer $\ell=0,1,2,3,\ldots$ and any two unit vectors $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$, the Legendre polynomial of their dot product (*i.e.*, of the cosine of the angle between these vectors) expands into products of spherical harmonics according to

$$P_\ell(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}}) \;=\; \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\hat{\mathbf{a}})Y^*_{\ell,m}(\hat{\mathbf{b}}). \tag{66}$$

Proving this lemma is best done in the quantum-mechanical language of Dirac brackets and projection operators. Since some students may be unfamiliar with this language, the proof is postponed to the Appendix to these notes as *optional reading*.

Meanwhile, let's apply the Lemma to the vectors $\widehat{\mathbf{R}}$ and $\hat{\mathbf{r}}$ in the context of eq. (13):

$$\begin{aligned}
\mathcal{M}_\ell(\widehat{\mathbf{R}}) &= \iiint r^\ell\times P_\ell(\widehat{\mathbf{R}}\cdot\hat{\mathbf{r}})\times\rho(\mathbf{r})\,d^3\mathrm{Vol}(\mathbf{r})\\
&= \iiint r^\ell\times\frac{4\pi}{2\ell+1}\left(\sum_{m=-\ell}^{+\ell}Y_{\ell,m}(\widehat{\mathbf{R}})Y^*_{\ell,m}(\hat{\mathbf{r}})\right)\times\rho(\mathbf{r})\,d^3\mathrm{Vol}(\mathbf{r})\\
&= \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{+\ell}Y_{\ell,m}(\widehat{\mathbf{R}})\times\iiint r^\ell\times Y^*_{\ell,m}(\hat{\mathbf{r}})\times\rho(\mathbf{r})\,d^3\mathrm{Vol}.
\end{aligned} \tag{67}$$

Hence, let's define the *spherical harmonics of multipoles* according to

$$\mathcal{M}_{\ell,m} \;\stackrel{\text{def}}{=}\; \sqrt{\frac{4\pi}{2\ell+1}}\iiint r^\ell\times Y^*_{\ell,m}(\theta,\phi)\times\rho(r,\theta,\phi)\,d^3\mathrm{Vol}(r,\theta,\phi). \tag{68}$$

Then, the 2^ℓ–pole potential has form

$$V_{2^\ell-\text{pole}}(R,\Theta,\Phi) \;=\; \frac{1}{4\pi\epsilon_0}\sum_{m=-\ell}^{+\ell}\mathcal{M}_{\ell,m}\times\sqrt{\frac{4\pi}{2\ell+1}}\,\frac{Y_{\ell,m}(\Theta,\Phi)}{R^{\ell+1}} \tag{69}$$

and the entire potential expands into

$$V_{\rm net}(R,\Theta,\Phi) \;=\; \frac{1}{4\pi\epsilon_0}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\mathcal{M}_{\ell,m}\times\sqrt{\frac{4\pi}{2\ell+1}}\,\frac{Y_{\ell,m}(\Theta,\Phi)}{R^{\ell+1}}\,. \tag{70}$$

Axial Symmetry

For the axially symmetric charge distributions $\rho(r,\theta,\phi)=\rho(r,\theta$ only), expanding the electric multipoles into spherical harmonics becomes particularly simple: for each ℓ, only the $m=0$ harmonic may have a non-zero coefficient $\mathcal{M}_{\ell,0}\neq 0$; all the other $\mathcal{M}_{\ell,m}$ with $m\neq 0$ must vanish. Indeed, for the axially symmetric charges, the integral (68) becomes

$$\mathcal{M}_{\ell,m} \;=\; \sqrt{\frac{4\pi}{2\ell+1}}\int_0^\infty dr\,r^2\times\int_0^\pi d\theta\,\sin\theta\times r^\ell\rho(r,\theta)\times\int_0^{2\pi}d\phi\,Y^*_{\ell,m}(\theta,\phi), \tag{71}$$

and since $Y_{\ell,m}(\theta,\phi)=e^{im\phi}\times$ a function of θ, the ϕ integral vanishes for $m\neq 0$,

$$\int_0^{2\pi}d\phi\,Y^*_{\ell,m}(\theta,\phi) \;=\; 0 \quad \text{for } m\neq 0. \tag{72}$$

For the remaining $m=0$ components, the spherical harmonics $Y_{\ell,0}(\theta,\phi)$ are proportional to the Legendre polynomials,

$$\sqrt{\frac{4\pi}{2\ell+1}}\times Y_{\ell,0}(\theta,\phi) \;=\; P_\ell(\cos\theta), \tag{73}$$

so the multipole expansion (70) becomes

$$V_{\rm net}(R,\Theta,\not\Phi) \;=\; \frac{1}{4\pi\epsilon_0}\sum_{\ell=0}^{\infty}\mathcal{M}^{(\ell)}_{\rm axial}\times\frac{P_\ell(\cos\Theta)}{R^{\ell+1}} \tag{74}$$

where

$$\begin{aligned}\mathcal{M}^{(\ell)}_{\rm axial} \;\stackrel{\rm def}{=}\; \mathcal{M}_{\ell,0} \;&=\; \sqrt{\frac{4\pi}{2\ell+1}}\iiint r^\ell Y^*_{\ell,0}(\theta)\rho(r,\theta)\,d^3{\rm Vol}\\ &= \iiint r^\ell P_\ell(\cos\theta)\times\rho(r,\theta)\,d^3{\rm Vol}(r,\theta,\phi).\end{aligned} \tag{75}$$

In terms of the multipole moment tensors $\mathcal{M}^{(\ell)}_{i_1,\ldots,i_\ell}$,

$$\mathcal{M}^{(\ell)}_{\text{axial}} \;=\; \mathcal{M}^{(\ell)}_{z,\ldots,z}\,. \tag{76}$$

For example, for a simple dipole, a linear quadrupole, and a linear octupole — which all have axial symmetries —

$$\begin{aligned}
M^{(1)}_{\text{axial}} &= p_z \;=\; Qa, && (77)\\
V_{\text{dipole}}(R,\Theta) &= \frac{Qa}{4\pi\epsilon_0}\,\frac{P_1(\cos\Theta)}{R^2}\,, && (78)\\
M^{(2)}_{\text{axial}} &= \mathcal{Q}_{z,z} \;=\; 2Qa^2, && (79)\\
V_{\text{lin.quadrupole}}(R,\Theta) &= \frac{2Qa^2}{4\pi\epsilon_0}\,\frac{P_2(\cos\Theta)}{R^3}\,, && (80)\\
M^{(3)}_{\text{axial}} &= \mathcal{O}_{z,z,z} \;=\; 6Qa^3, && (81)\\
V_{\text{lin.octupole}}(R,\Theta) &= \frac{6Qa^3}{4\pi\epsilon_0}\,\frac{P_3(\cos\Theta)}{R^3}\,, && (82)\\
&\cdots\cdots\cdots\cdots\cdots\cdots
\end{aligned}$$

And you will see more examples in your homework (set#7).

Appendix: Proving the Theorems

In this Appendix I shall prove the theorem (5) and the lemma (66). This proof is optional reading for the students in my ElectroDynamics class, as it involves complex analysis techniques (for the theorem (5)) or quantum-mechanical techniques (for the lemma (66)) that many students have not yet learned. But please, learn both complex analysis and quantum mechanics before your graduate: All physicists should be familiar with these subjects, just as they should be familiar with the electrodynamics.

Proving the Theorem About Inverse Distance Expansion

Let's start by proving the theorem (5) about expanding the inverse distance $1/|\mathbf{R}-\mathbf{r}|$ into powers of r/R. That is, let's prove that the series on the LHS of

$$\sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(\cos\alpha) \;=\; \frac{1}{\sqrt{R^2 - 2Rr\cos\alpha + r^2}} \;=\; \frac{1}{|\mathbf{R}-\mathbf{r}|}\,. \tag{83}$$

converges for any $r < R$ and that the sum is precisely the expression on the RHS. The key here is the residue method for evaluating contour integrals in the complex plane:

$$\oint\limits_{\Gamma} \frac{dz}{2\pi i}\,\frac{f(z)}{(z-x)^{n+1}} \;=\; \text{Residue}\left[\frac{f(z)}{(z-x)^{n+1}}\right]_{@z=x} \;=\; \frac{1}{n!}\,\frac{d^n f(z)}{dz^n}\bigg|_{@z=x} \tag{84}$$

provided the contour Γ circles x and that the function $f(x)$ is analytic and has no singularities inside the contour Γ.

My starting point is the Rodriguez formula for the Legendre polynomials,

$$P_\ell(x) \;=\; \frac{1}{2^\ell\,\ell!}\,\frac{d^\ell}{dx^\ell}\,(x^2-1)^\ell. \tag{85}$$

In light of the residue-method formula (84), we may turn the ℓ^{th} derivative in this formula into a complex contour integral

$$P_\ell(x) \;=\; \frac{1}{2^\ell}\oint\limits_{\Gamma} \frac{dz}{2\pi i}\,\frac{(z^2-1)^\ell}{(z-x)^{\ell+1}} \tag{86}$$

where Γ is some closed contour which circles x. Now let's plug this formula into the series on the LHS of eq. (83):

$$\begin{aligned}
\text{series} &= \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(x) \\
&= \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times \frac{1}{2^\ell} \oint\limits_\Gamma \frac{dz}{2\pi i} \, \frac{(z^2-1)^\ell}{(z-x)^{\ell+1}} \\
&\qquad \langle\!\langle \text{ putting the sum inside the integral } \rangle\!\rangle \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times \frac{(z^2-1)^\ell}{2^\ell (z-x)^{\ell+1}} \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \, \frac{1}{R(z-x)} \times \sum_{\ell=0}^{\infty} \left(\frac{r(z^2-1)}{2R(z-t)} \right)^\ell \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \, \frac{1}{R(z-x)} \times \frac{1}{1 - \frac{r(z^2-1)}{2R(z-x)}} \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \, \frac{-2}{rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r} \,.
\end{aligned} \tag{87}$$

Note: before the summation, each term on the third line has poles at $z = x$ and at $z = \infty$, but after the summation, both poles have moved to the roots of the quadratic equation

$$rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r \;=\; 0, \tag{88}$$

thus

$$z_{1,2} \;=\; \frac{R \pm \sqrt{R^2 - 2rRx + r^2}}{r}\,; \qquad \text{for } r \ll R, \quad z_1 \;\approx\; \frac{2R}{r} \;\to\; \infty, \quad \text{while} \quad z_2 \;\approx\; x. \tag{89}$$

This tells us how to choose the integration contour Γ: It should circle around x and have enough room to accommodate the shifting of the pole from x to z_2, but it should not include the other pole at z_1 which have moved in from the infinity. Consequently, evaluating the integral on the bottom line of eq. (87) by the residue method, we have

$$\oint\limits_\Gamma \frac{dz}{2\pi i} \, \frac{-2}{rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r} \;=\; \text{Residue} \left[\frac{-2}{rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r} \right]_{@z=z_2} . \tag{90}$$

Specifically,

$$\frac{-2}{rz^2\,-\,2Rz\,+\,2Rx\,-\,r}\;=\;\frac{-2}{r}\times\frac{1}{(z-z_1)(z-z_2)}\,, \tag{91}$$

so the residue of this function at $z=z_2$ is simply

$$\text{Residue}\;=\;\frac{-2}{r}\times\frac{1}{z_2-z_1}\;=\;\frac{-2}{r}\times\frac{r}{-2\sqrt{R^2-2rRx+r^2}}\;=\;+\frac{1}{\sqrt{R^2-2rRx+r^2}}\,. \tag{92}$$

Thus,

$$\text{the series}\;=\sum_{\ell=0}^{\infty}\frac{r^\ell}{R^{\ell+1}}\times P_\ell(x)\;=\;\frac{1}{\sqrt{R^2-2rRx+r^2}}\,, \tag{93}$$

exactly as on the RHS of eq. (83).

To complete the proof, consider the convergence of the multipole expansion (83). For any physical angle α ranging between 0 and π, the $x=\cos\alpha$ ranges between $+1$ and -1, and for all such x, all the Legendre polynomials $P_\ell(x)$ take values between -1 and $+1$. Consequently,

$$\left|\begin{matrix}\ell^{\text{th}}\text{ term in the}\\ \text{multipole expansion}\end{matrix}\right|\;<\;\frac{r^\ell}{R^{\ell+1}}\;=\;\frac{(r/R)^\ell}{R}\,, \tag{94}$$

so the series on the LHS of eq. (83) converges for any $r<R$.

Moreover, if we analytically continue the series to complex r, it would converge for all $|r|<R$; in other words, it has *radius of convergence* $=R$. Indeed, as a function of complex r, the $1/\sqrt{\cdots}$ on the RHS of (83) has singularities at

$$r_{1,2}\;=\;R\cos\alpha\;\pm\;iR\sin\alpha,\qquad |r_{1,2}|\;=\;R,$$

and that's what sets the radius of convergence to $|r|<R$.

For $r>R$ we may no longer expand the inverse distance into powers of r/R. Instead, we may expand it into powers of the inverse ratio R/r:

$$\text{For } r>R,\qquad \frac{1}{\sqrt{R^2+r^2-2Rr\cos\alpha}}\;=\sum_{\ell=0}^{\infty}\frac{R^\ell}{r^{\ell+1}}\times P_\ell(\cos\alpha), \tag{95}$$

which works exactly like eq. (5) once we exchange $r\leftrightarrow R$.

Physically, the expansion (5) is useful for potentials far outside complicated charged bodies, while the inverse expansion (95) is useful for potentials deep inside a cavity.

Proving the Lemma About Spherical Harmonics

Now let's prove the lemma (66): for any $\ell = 0, 1, 2, 3, \ldots$,

$$\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\theta_a,\phi_a)Y^*_{\ell,m}(\theta_b,\phi_b) \;=\; \frac{2\ell+1}{4\pi}\times P_\ell(\cos\Theta_{ab}) \tag{96}$$

where Θ_{ab} is the angle between the directions (θ_a,ϕ_a) and (θ_b,ϕ_b).[⋆] I am going to prove this lemma in two steps: First, I shall prove that the sum on the LHS here depends only on the relative angle Θ_{ab} but remains invariant under simultaneous rotations of both directions. Second, I shall use this invariance to evaluate the sum and show that it agrees with the Legendre polynomial on the RHS.

The first step is best described in the quantum mechanical language of Dirac brackets and operators. Specifically, consider a quantum particle living in 2 curved dimensions, specifically on a sphere of some fixed radius $r = \text{const}$. The position (a) of such a particle can be described by two spherical angles (θ_a,ϕ_a), or equivalently by a unit vector $\mathbf{a}$ pointing towards the particle from the sphere's center. Consequently, the quantum states of such a particle are described by wave-functions $\psi(\mathbf{a}) = \psi(\theta_a,\phi_a)$.

Now consider the Hilbert space of such wave-functions. The spherical harmonics provide a complete orthonormal basis for this Hilbert space:

$$\begin{aligned} \text{any } \psi(\theta,\phi) \;&=\; \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\langle\ell,m|\psi\rangle\times Y_{\ell,m}(\theta,\phi)\\ \text{for } \langle\ell,m|\psi\rangle \;&=\; \iint Y^*_{\ell,m}(\theta,\phi)\psi(\theta,\phi)\,d^2\Omega(\theta,\phi). \end{aligned} \tag{97}$$

Physically, the states $|\ell,m\rangle$ are eigenstates of the angular momentum operators $\hat{\mathbf{L}}^2$ and $\hat{L}_z$,

$$\hat{L}_z\,|\ell,m\rangle \;=\; \hbar m\,|\ell,m\rangle\,, \quad \hat{\mathbf{L}}^2\,|\ell,m\rangle \;=\; \hbar^2\ell(\ell+1)\,|\ell,m\rangle\,. \tag{98}$$

⋆ In the context of the multipole expansion, $(\theta_a,\phi_b) = (\Theta,\Phi)$, $(\theta_b,\phi_b) = (\theta,\phi)$, and $\Theta_{ab} = \alpha$, the angle between $\widehat{\mathbf{R}}$ and $\hat{\mathbf{r}}$.

Consequently, the operators

$$\hat{\Pi}_\ell \;=\; \sum_{m=-\ell}^{+\ell} |\ell,m\rangle\,\langle\ell,m| \tag{99}$$

are projector operators onto all states with a specific value of $\mathbf{L}^2$, namely $\hbar^2\ell(\ell+1)$.

Since the $\hat{\mathbf{L}}^2$ operator is invariant under all 3D rotations of the sphere about its center, the projection operators $\hat{\Pi}_\ell$ must also be invariant under rotations. Consequently, for any two definite-positions states $|\mathbf{a}\rangle = |\theta_a,\phi_a\rangle$ and $|\mathbf{b}\rangle = |\theta_b,\phi_b\rangle$, the Dirac sandwich

$$\langle\mathbf{a}|\,\hat{\Pi}_\ell\,|\mathbf{b}\rangle \tag{100}$$

must be invariant under *simultaneous* rotations of the unit vectors **a** and **b**. Therefore, this Dirac sandwich may depend only on the *relative* angle Θ_{ab} between the unit vectors **a** and **b**, but it cannot depend on where the vectors **a** and **b** point in absolute terms, thus

$$\langle\mathbf{a}|\,\hat{\Pi}_\ell\,|\mathbf{b}\rangle \;=\; F_\ell(\Theta_{ab}\text{ only}). \tag{101}$$

On the other hand, by construction of the operator (99),

$$\langle\mathbf{a}|\,\hat{\Pi}_\ell\,|\mathbf{b}\rangle \;=\; \sum_{m=-\ell}^{+\ell} \langle\mathbf{a}|\ell,m\rangle\,\langle\ell,m|\mathbf{b}\rangle \;=\; \sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\theta_a,\phi_a)\times Y^*_{\ell,m}(\theta_b,\phi_b), \tag{102}$$

hence

$$\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\theta_a,\phi_a)\times Y^*_{\ell,m}(\theta_b,\phi_b) \;=\; F_\ell(\Theta_{ab}\text{ only}). \tag{103}$$

This completes the first step of the proof.

The second step is to find the specific form of the functions $F_\ell(\Theta_{ab})$. To do that, let's evaluate the sums (103) for a particularly simple choice of point **b**, namely the North pole of the sphere, $\theta_b = 0$, ϕ_b undefined. Meanwhile, the point **a** can be anywhere on the sphere. For our choice of point **b**, the angle between the vectors **a** and **b** is simply the latitude of **a**,

$\Theta_{ab} = \theta_a$, so we may evaluate the $F_\ell(\Theta_{ab})$ as

$$F_\ell(\Theta_{ab} = \theta_a) \;=\; \sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\theta_a, \phi_a) Y^*_{\ell,m}(\theta_b = 0). \tag{104}$$

The spherical harmonics $Y_{\ell,m}(\theta, \phi)$ have general form

$$Y_{\ell,m}(\theta, \phi) \;=\; e^{im\phi} \times \bigl(\sin\theta\bigr)^{|m|} \times \text{Polynomial}(\cos\theta), \tag{105}$$

so thanks to the $(\sin\theta)^{|m|}$ factor, all the harmonics with $m \neq 0$ vanish at the poles. Consequently, only the $\ell = 0$ term contributes to the sum (104), thus

$$F(\Theta_{ab} = \theta_a) \;=\; Y_{\ell,0}(\theta_a) \times Y^*_{\ell,0}(\theta_b = 0) \;=\; \frac{2\ell + 1}{4\pi} \times P_\ell(\cos\theta_a) \times P_\ell(1) \tag{106}$$

where the second equality follows from the relation (73) of the $Y_{\ell,0}$ harmonics to the Legendre polynomials. Moreover, the Legendre polynomials are normalized so that $P_\ell(1) = 1$ for all ℓ, hence

$$F(\Theta_{ab} = \theta_a) \;=\; \frac{2\ell + 1}{4\pi} \times P_\ell(\cos\theta_a). \tag{107}$$

This completes the second step of the proof.

Altogether, we have

$$\sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\theta_a, \phi_a) \times Y^*_{\ell,m}(\theta_b, \phi_b) \;=\; \frac{2\ell + 1}{4\pi} \times P_\ell(\cos\Theta_{ab}), \tag{108}$$

quod erat demonstrandum.