Math of Multipole Expansion

In this note I explain how to expand

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

into a power series in (r/R) for $r < R$, and then apply this expansion to the Coulomb potential.

Let's start with the few leading terms in this expansion for $r \ll R$. For the sake of compactness, let's denote

$$\alpha = \frac{r}{R} \ll 1, \quad x = \cos\theta, \quad \beta = 2\alpha x - \alpha^2 \ll 1.$$

In these notations,

$$\frac{1}{\sqrt{R^2+r^2-2Rr\cos\theta}} = \frac{1}{\sqrt{R^2(1+\alpha^2-2\alpha x)}} = \frac{1}{R}\times\frac{1}{\sqrt{1-\beta}}. \tag{2}$$

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

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

Now, remember that $\beta = 2\alpha x - \alpha^2$, plug that into the above expansion, then truncate it to powers of α no larger than 3:

$$\begin{aligned}
S &= 1 + \tfrac{1}{2}(2\alpha x - \alpha^2) + \tfrac{3}{8}(2\alpha x-\alpha^2)^2 + \tfrac{5}{16}(2\alpha x-\alpha^2)^3 + \cdots \\
&= 1 + \alpha x \qquad - \tfrac{1}{2}\alpha^2 \\
&\qquad\qquad\qquad + \tfrac{3}{2}\alpha^2x^2 \qquad - \tfrac{3}{2}\alpha^3 x \qquad + \cdots \\
&\qquad\qquad\qquad\qquad\qquad\qquad + \tfrac{5}{2}\alpha^3x^3 \qquad + \cdots \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + \cdots \\
&= 1 + \alpha\times x + \alpha^2\times\frac{3x^2-1}{2} + \alpha^3\times\frac{5x^3-3x}{2} + \cdots \\
&= 1 + \alpha\times P_1(x) + \alpha^2\times P_2(X) + \alpha^3\times P_3(x) + \cdots
\end{aligned} \tag{4}$$

where $P_1(x)$, $P_2(x)$, and $P_3(x)$ are the Legendre polynomials of respective degrees 1, 2, 3.

Plugging this result back into eq. (2), we obtain

$$\frac{1}{\sqrt{R^2 + r^2 - 2Rr\cos\theta}} = \frac{1}{R} + \frac{r}{R^2}\times P_1(\cos\theta) + \frac{r^2}{R^3}\times P_2(\cos\theta) + \frac{r^3}{R^4}\times P_3(\cos\theta) + \cdots. \quad (5)$$

The expansion (5) clearly suggests similar terms for the higher powers of r/R, and indeed there is a **theorem:**

$$\text{For } r < R, \quad \frac{1}{\sqrt{R^2 + r^2 - 2Rr\cos\theta}} = \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(\cos\theta). \quad (6)$$

Proof: Let's start with the Rodrigues formula for the Legendre polynomials,

$$P_\ell(x) = \frac{1}{2^\ell\,\ell!}\,\frac{d^\ell}{dx^\ell}\,(x^2-1)^\ell, \quad (7)$$

and the residue method for taking contour integrals in the complex plane,

$$\oint\limits_{\Gamma} \frac{dz}{2\pi i}\,\frac{f(z)}{(z-x)^{n+1}} = \text{Residue}\left[\frac{f(z)}{(z-x)^{n+1}}\right]_{@z=x} = \frac{1}{n!}\,\frac{d^n f(z)}{dz^n}\bigg|_{@z=x} \quad (8)$$

provided the contour Γ circles x and that the function $f(x)$ is analytic and has no singularities inside the contour Γ. Applying this method *in reverse* — *i.e.*, turning n^{th} into a contour integral — to the Rodrigues formula, we obtain

$$P_\ell(x) = \frac{1}{2^\ell}\oint\limits_{\Gamma} \frac{dz}{2\pi i}\,\frac{(z^2-1)^\ell}{(z-x)^{\ell+1}} \quad (9)$$

where the contour Γ circles x. Now let's plug this formula into the series on the RHS of eq. (6):

$$\begin{aligned}
\text{series} &= \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(x) \\
&= \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times \frac{1}{2^\ell} \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{(z^2-1)^\ell}{(z-x)^{\ell+1}} \\
&\qquad \langle\!\langle \text{ putting the sum inside the integral } \rangle\!\rangle \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times \frac{(z^2-1)^\ell}{2^\ell(z-x)^{\ell+1}} \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{1}{R(z-x)} \times \sum_{\ell=0}^{\infty} \left(\frac{r(z^2-1)}{2R(z-t)}\right)^\ell \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{1}{R(z-x)} \times \frac{1}{1-\frac{r(z^2-1)}{2R(z-x)}} \\
&= \oint\limits_\Gamma \frac{dz}{2\pi i} \frac{-2}{rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r} \,.
\end{aligned} \tag{10}$$

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

$$rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r \;=\; 0, \tag{11}$$

thus

$$z_{1,2} \;=\; \frac{R \pm \sqrt{R^2 - 2rRx + r^2}}{r}\,; \qquad \text{for } r \ll R, \quad z_1 \;\approx\; \frac{2R}{r} \;\to\; \infty, \quad \text{while} \quad z_2 \;\approx\; x. \tag{12}$$

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. (10) by the residue method, we have

$$\oint\limits_\Gamma \frac{dz}{2\pi i} \frac{-2}{rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r} \;=\; \text{Residue}\left[\frac{-2}{rz^2 \,-\, 2Rz \,+\, 2Rx \,-\, r}\right]_{@z=z_2} . \tag{13}$$

Specifically,

$$\frac{-2}{rz^2 \;-\; 2Rz \;+\; 2Rx \;-\; r} \;=\; \frac{-2}{r} \times \frac{1}{(z-z_1)(z-z_2)}\,, \tag{14}$$

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

$$\text{Residue} \;=\; \frac{-2}{r} \times \frac{1}{z_2 - z_1} \;=\; \frac{-2}{r} \times \frac{r}{-2\sqrt{R^2 - 2rRx + r^2}} \;=\; +\frac{1}{\sqrt{R^2 - 2rRx + r^2}}\,. \tag{15}$$

Thus,

$$\text{the series} \;=\; \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(x) \;=\; \frac{1}{\sqrt{R^2 - 2rRx + r^2}}\,, \tag{16}$$

which proves the theorem (6), *quod erat demonstrandum.*

ASIDE: A few words about the convergence of the expansion (6). For $x = \cos\theta$ ranging between -1 and $+1$, all the Legendre polynomials take values between -1 and $+1$. Consequently, the series (6) converges for any $r < R$. If we analytically continue it to the complex r, it would converge for $|r| < R$; in other words, it has *radius of convergence* $= R$. Indeed, as a function of complex r, the $1/\sqrt{\cdots}$ on the LHS of (6) has singularities at

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

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

For $r > R$ we may longer expand the inverse distance into powers of r/R. Instead, we may expand it into powers of the inverse ratio R/r:

$$\text{For } r > R, \quad \frac{1}{\sqrt{R^2 + r^2 - 2Rr\cos\theta}} \;=\; \sum_{\ell=0}^{\infty} \frac{R^\ell}{r^{\ell+1}} \times P_\ell(\cos\theta), \tag{17}$$

which works exactly like eq. (6) once we exchange $r \leftrightarrow R$.

Physically, the expansion (6) is useful for potentials far outside complicated charged bodies, while the inverse expansion (17) is useful for potentials deep inside a cavity.

Multipole Expansion of the Electric Potential

Now consider the Coulomb potential of some continuous charge distribution $\rho(\vec{r})$,

$$V(\vec{R}) = \frac{1}{4\pi\epsilon_0} \iiint \frac{\rho(\mathbf{r})\, d^3\mathrm{Vol}}{|\mathbf{R}-\mathbf{r}|}\,. \tag{18}$$

Suppose all the charges are limited to some compact volume, while we want to know the potential far away from that volume, so in the integral (18) we always have $r \ll R$. Consequently, we may expand the denominator in the Coulomb potential according to the Theorem (6), thus

$$\begin{aligned} V(\mathbf{R}) &= \frac{1}{4\pi\epsilon_0} \iiint d^3\mathrm{Vol}\, \rho(\mathbf{r}) \times \sum_{\ell=0}^{\infty} \frac{r^\ell}{R^{\ell+1}} \times P_\ell(\cos\theta) \\ &= \sum_{\ell=0}^{\infty} \frac{1}{4\pi\epsilon_0\, R^{\ell+1}} \times \iiint d^3\mathrm{Vol}\, \rho(\mathbf{r}) \times r^\ell P_\ell(\cos\theta) \end{aligned} \tag{19}$$

where θ is the angle between the radius-vectors $\mathbf{R}$ and $\mathbf{r}$. In terms of the unit vectors $\widehat{\mathbf{R}}$ and $\widehat{\mathbf{r}}$ in the directions of $\mathbf{R}$ and $\mathbf{r}$,

$$\cos\theta = \widehat{\mathbf{R}} \cdot \widehat{\mathbf{r}}. \tag{20}$$

Consequently, we may decompose the potential $V(\mathbf{R})$ of the charges $\rho(\mathbf{r})$ into a series of multipole potentials,

$$V(\mathbf{R}) = \sum_{\ell=0}^{\infty} \frac{\mathcal{M}_\ell(\widehat{\mathbf{R}})}{4\pi\epsilon_0\, R^{\ell+1}} \tag{21}$$

where

$$\mathcal{M}_\ell(\widehat{\mathbf{R}}) = \iiint r^\ell P_\ell(\widehat{\mathbf{r}} \cdot \widehat{\mathbf{R}}) \times \rho(\mathbf{r})\, d^3\mathrm{Vol}. \tag{22}$$

is the 2^ℓ–pole moment of the charge distribution $\rho(\mathbf{r})$. Or rather, it's the *component of the 2^ℓ–pole moment in the direction* $\widehat{\mathbf{R}}$.

Let's take a closer look at these components:

• $\ell = 0$ • The monopole moment $\mathcal{M}_0$ is simply the net charge of the distribution,

$$\mathcal{M}_0 \;=\; \iiint \rho(\mathbf{r})\, d^3\mathrm{Vol} \;=\; Q^{\mathrm{net}}, \tag{23}$$

and it obviously does not depend on the direction $\widehat{\mathbf{R}}$, hence isotropic monopole potential,

$$V_{\mathrm{monopole}} \;=\; \frac{Q^{\mathrm{net}}}{4\pi\epsilon_0\, R}\,. \tag{24}$$

• $\ell = 1$ • The dipole moment is a vector

$$\mathbf{p} \;=\; \iiint \mathbf{r}\,\rho(\mathbf{r})\, d^3\mathrm{Vol} \tag{25}$$

and the $\mathcal{M}_1(\widehat{\mathbf{R}})$ in the series (21) is simply

$$\mathcal{M}_1(\widehat{\mathbf{R}}) \;=\; \widehat{\mathbf{R}}\cdot\mathbf{p}, \tag{26}$$

hence the dipole's potential

$$V_{\mathrm{dipole}} \;=\; \frac{\mathbf{p}\cdot\widehat{\mathbf{R}}}{4\pi\epsilon_0\, R^2}\,. \tag{27}$$

To see how this works, note that $r^1 \times P_1(\widehat{\mathbf{R}}\cdot\hat{\mathbf{r}}) \;=\; r(\widehat{\mathbf{R}}\cdot\hat{\mathbf{r}}) = \widehat{\mathbf{R}}\cdot\mathbf{r}$, hence

$$\mathcal{M}_1(\widehat{\mathbf{R}}) \;=\; \iiint (\widehat{\mathbf{R}}\cdot\mathbf{r})\rho(\mathbf{r})\, d^3\mathrm{Vol} \;=\; \widehat{\mathbf{R}}\cdot \iiint \mathbf{r}\,\rho(\mathbf{r})\, d^3\mathrm{Vol} = \;\widehat{\mathbf{R}}\cdot\mathbf{p}. \tag{28}$$

• $\ell = 2$ • The quadrupole moment is a 2-index symmetric tensor

$$\mathcal{Q}_{i,j} \;=\; \iiint \left(\tfrac{3}{2} r_i r_j \;-\; \tfrac{1}{2}\delta_{i,j} r^2\right)\rho(\mathbf{r})\, d^3\mathrm{Vol} \tag{29}$$

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 $i \neq j$).

To see the relation between this tensor and the $\mathcal{M}_2(\widehat{\mathbf{R}})$ in the series (21), let's expand the second Legendre polynomial $P_2(\cos\theta) = P_2(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}})$:

$$P_2(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}}) \;=\; \tfrac{3}{2}(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}})^2 \;-\; \tfrac{1}{2}, \tag{30}$$

$$\begin{aligned}\tfrac{3}{2}(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}})^2 \;&=\; \frac{3}{2}\left(\sum_i \widehat{R}_i\widehat{r}_i\right)^2 \;=\; \frac{3}{2}\left(\sum_i \widehat{R}_i\widehat{r}_i\right)\times\left(\sum_j \widehat{R}_j\widehat{r}_j\right)\\ &=\; \frac{3}{2}\sum_{i,j}\widehat{R}_i\widehat{R}_j\widehat{r}_i\widehat{r}_j\,,\end{aligned} \tag{31}$$

$$\begin{aligned}\tfrac{1}{2} \;&=\; \tfrac{1}{2}\widehat{\mathbf{R}}\cdot\widehat{\mathbf{R}} \quad \langle\!\langle\,\text{since } \widehat{\mathbf{R}} \text{ is a unit vector}\,\rangle\!\rangle\\ &=\; \frac{1}{2}\sum_i \widehat{R}_i\widehat{R}_i \;=\; \frac{1}{2}\sum_{i,j}\delta_{i,j}\times\widehat{R}_i\widehat{R}_j\,,\end{aligned} \tag{32}$$

$$\text{hence } P_2(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}}) \;=\; \sum_{i,j}\widehat{R}_i\widehat{R}_j\Bigl(\tfrac{3}{2}\widehat{r}_i\widehat{r}_j \;-\; \tfrac{1}{2}\delta_{ij}\Bigr), \tag{33}$$

$$\text{and } r^2\times P_2(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}}) \;=\; \sum_{i,j}\widehat{R}_i\widehat{R}_j\Bigl(\tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}r^2\delta_{ij}\Bigr). \tag{34}$$

Plugging the last line here into eq. (22) for $\ell = 2$, we obtain

$$\begin{aligned}\mathcal{M}_2(\widehat{\mathbf{R}}) \;&=\; \iiint\sum_{i,j}\widehat{R}_i\widehat{R}_j\Bigl(\tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}r^2\delta_{ij}\Bigr)\times\rho(\mathbf{r})\,d^3\mathrm{Vol}\\ &=\; \sum_{i,j}\widehat{R}_i\widehat{R}_j\times\iiint\Bigl(\tfrac{3}{2}r_ir_j \;-\; \tfrac{1}{2}r^2\delta_{ij}\Bigr)\times\rho(\mathbf{r})\,d^3\mathrm{Vol}\\ &=\; \sum_{i,j}\widehat{R}_i\widehat{R}_j\times\mathcal{Q}_{i,j}\,,\end{aligned} \tag{35}$$

hence the quadrupole potential

$$V_{\text{quadrupole}}(\mathbf{R}) \;=\; \frac{\sum_{i,j}\mathcal{Q}_{i,j}\widehat{R}_i\widehat{R}_j}{4\pi\epsilon_0\,R^3}\,. \tag{36}$$

• $\ell \geq 3$ • The higher multipoles are ℓ–index symmetric tensors. For example, the octupole moment is the 3-index tensor

$$\mathcal{O}_{i,j,k} \;=\; \iiint \left(\tfrac{5}{2} r_i r_j r_k \;-\; \tfrac{1}{2}\delta_{i,j} r_k \;-\; \tfrac{1}{2}\delta_{i,k} r_j \;-\; \tfrac{1}{2}\delta_{j,k} r_i\right) \times \rho(\mathbf{r})\, d^3\mathrm{Vol} \tag{37}$$

whose potential is

$$V_{\text{octupole}}(\mathbf{R}) \;=\; \frac{\sum_{i,j,k} \mathcal{O}_{i,j,k} \widehat{R}_i \widehat{R}_j \widehat{R}_k}{4\pi\epsilon_0\, R^4}\,. \tag{38}$$

Likewise, for higher ℓ the potential has form

$$V_{2^\ell-\text{pole}}(\mathbf{R}) \;=\; \frac{\sum_{i,j,\ldots,n} \mathcal{M}^{(\ell)}_{i,j,\ldots,n} \widehat{R}_i \widehat{R}_j \cdots \widehat{R}_n}{4\pi\epsilon_0\, R^{\ell+1}} \tag{39}$$

where

$$\mathcal{M}^{(\ell)}_{i,j,\ldots,n} \;=\; \iiint \begin{pmatrix} \text{homogeneous polynomial} \\ \text{of degree } \ell \text{ in } x,y,z \end{pmatrix} \times \rho(\mathbf{r})\, d^3\mathrm{Vol} \tag{40}$$

where the specific form of the degree–ℓ polynomial follows from the $P_\ell(\cos\theta)$.

Axial Symmetry

For the axially symmetric charge distributions $\rho(r,\theta,\phi) = \rho(r,\theta$ only), we may re-express the angular dependence of the multipole expansion using the following

Lemma: Let (θ,ϕ) be the spherical angles of the direction $\widehat{\mathbf{R}}$ while (θ',ϕ') are spherical angles of the direction $\widehat{\mathbf{r}}$, then

$$\int_0^{2\pi} \frac{d\phi'}{2\pi}\, P_\ell(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}}) \;=\; P_\ell(\cos\theta) \times P_\ell(\cos\theta'). \tag{41}$$

Consequently, for an axially symmetric charge distribution

$$\begin{aligned}\mathcal{M}_\ell(\widehat{\mathbf{R}}) &= \iiint r^\ell P_\ell(\widehat{\mathbf{R}}\cdot\widehat{\mathbf{r}}) \times \rho(r,\theta') \times r^2 \sin\theta'\, dr\, d\theta'\, d\phi' \\ &= P_\ell(\cos\theta) \times \mathcal{M}^{(\ell)}_{z\cdots z}\end{aligned} \tag{42}$$

$$\text{where } \mathcal{M}^{(\ell)}_{z\cdots z} \;=\; \iiint r^\ell P_\ell(\cos\theta') \times \rho(r,\theta') \times r^2 \sin\theta'\, dr\, d\theta'\, d\phi' \tag{43}$$

is the $z,\ldots,z$ component of the 2^ℓ–pole vector or tensor, for example p_z, $\mathcal{Q}_{z,z}$, or $\mathcal{O}_{z,z,z}$. For the axially symmetric charge distribution it's the only independent component, and it's also the only component we need for expanding the potential:

$$V(R,\theta) \;=\; \frac{\mathcal{M}^{(\ell)}_{z\cdots z}}{4\pi\epsilon_0} \times \frac{P_\ell(\cos\theta)}{R^{\ell+1}}\,. \tag{44}$$

You should see examples of such expansion in your homework.