Multipole Expansion of Electrostatic Potential

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Published on July 19, 2023

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1 Cartesian Multipole Expansion

1.1 Direct Derivation from Taylor Expansion

Suppose a localised electric charge distribution $\rho(\mathbf{r})$; $\rho(\mathbf{r}) = 0$ if $|\mathbf{r}| > R$. The electric potential given by Coulomb's law is

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \mathrm{d}^3 r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \tag{1}$$

By rewriting the Green's function with the translation operator $e^{\mathbf{a}\cdot\nabla}$:

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = e^{-\mathbf{r}'\cdot\nabla} \left(\frac{1}{r}\right) = \sum_{l=0}^{\infty} \frac{1}{l!} (-\mathbf{r}' \cdot \nabla)^l \left(\frac{1}{r}\right), \tag{2}$$

we could expand the potential outside of the charge distribution as

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{l=0}^{\infty} \frac{1}{l!} \int \mathrm{d}^3 r' \rho(\mathbf{r}') (-\mathbf{r}' \cdot \nabla)^l \left(\frac{1}{r}\right). \tag{3}$$

We find the lth term of the sum proportional to:

$$\sum_{i_1,\cdots,i_l} Q^l_{i_1\cdots i_l} r_{i_1} \cdots r_{i_l} = \int \mathrm{d}^3 r' \rho(\mathbf{r}') r^{2l+1} (-\mathbf{r}' \cdot \nabla)^l \left(\frac{1}{r}\right), \tag{4}$$

where r_{i_j}s are cartesian coordinates and Q^l is a tensor of rank l. Note that the tensor Q^ls are independent of $\mathbf{r}$ and determined by only the charge distribution. Generally, components of Q^l are determined as well as to be symmetric and trace-less over any pair of indices. Those of components of Q^l are called the **cartesian multipole moments**—to be more precise, 2^l-pole moments.

The potential expanded in terms of the cartesian multipole moments

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\left(\frac{Q^0}{r} + \frac{\mathbf{Q}^1\cdot\mathbf{r}}{r^3} + \frac{1}{2}\frac{\mathbf{r}\cdot\mathbf{Q}^2\cdot\mathbf{r}}{r^5} + \cdots + \frac{1}{l!}\frac{\sum_{i_1,\cdots i_l} Q^l_{i_1\cdots i_l} r_{i_1}\cdots r_{i_l}}{r^{2l+1}} + \cdots\right) \tag{5}$$

is called the **cartesian multipole expansion**.

The components of the first three multipole moments are

$$\begin{aligned} Q^0 &= \int \mathrm{d}^3 r \rho(\mathbf{r}) \\ Q^1_i &= \int \mathrm{d}^3 r \rho(\mathbf{r}) r_i \\ Q^2_{ij} &= \int \mathrm{d}^3 r \rho(\mathbf{r}) \left(3 r_i r_j - r^2 \delta_{ij}\right). \end{aligned}$$

It is easy to check whether they depend on the choice of origin; Q^0 is always independent, $\mathbf{Q}^1$ is independent only if $Q^0 = 0$, and generally higher order multipole moments depend on the choice of origin.

1.2 Using Generating Function of the Legendre Polynomials

Since the Green's function for electrostatics takes the form

$$G(\mathbf{r},\mathbf{r}') = \frac{1}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{r}'|} \tag{6}$$

satisfies the Laplace equation, and possesses azimuthal symmetry. Thus we might try to expand $1/|\mathbf{r}-\mathbf{r}'|$ in a series using the Legendre polynomials:

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos\gamma) \tag{7}$$

where γ is the angle between $\mathbf{r}$ and $\mathbf{r}'$. B_l can be determined by substituting 0 into γ, thus we obtain

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^l P_l(\cos\gamma) \tag{8}$$

where we assumed $r > r'$. Substituting into eq. (1), we conclude that

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{\infty}\frac{1}{r^{2l+1}}\int \mathrm{d}^3 r' \rho(\mathbf{r}') r^l {r'}^l P_l(\cos\gamma), \tag{9}$$

thus we can rewrite eq. (4) in more explicit form:

$$\sum_{i_1,\cdots,i_l} Q^l_{i_1\cdots i_l} r_{i_1}\cdots r_{i_l} = l!\int \mathrm{d}^3 r' \rho(\mathbf{r}') r^l {r'}^l P_l(\cos\gamma). \tag{10}$$

2 Spherical Multipole Expansion

2.1 Spherical Harmonics

Spherical harmonics are a complete set of orthonormal functions on the surface of a sphere defined as:

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi} \tag{11}$$

where $P_l^m : [-1,1] \to \mathbb{R}$ is the associated Legendre polynomials with the Condon–Shortley phase. The orthogonality relation

$$\int_0^{2\pi} d\varphi \int_{-1}^{1} \mathrm{d}(\cos\theta)\, Y_{l'}^{m'*}(\theta,\varphi)Y_l^m(\theta,\varphi) = \delta_{ll'}\delta_{mm'} \tag{12}$$

and the completeness relation

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_l^{m*}(\theta',\varphi')Y_l^m(\theta,\varphi) = \delta(\varphi'-\varphi)\delta(\cos\theta'-\cos\theta) \tag{13}$$

holds.

The spherical harmonics form an orthonormal basis, so that every function $f(\theta,\varphi)$ defined over the surface of a sphere can be expanded in a series of spherical harmonics:

$$f(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_l^m Y_l^m(\theta,\varphi). \tag{14}$$

In the sense of separation of variables, the solution of the Laplace equation can be expanded in the form

$$\phi(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[A_l^m r^l + B_l^m r^{-(l+1)}\right]Y_l^m(\theta,\varphi). \tag{15}$$

2.2 Addition Theorem

Consider two vectors $\mathbf{r}(r,\theta,\varphi)$, $\mathbf{r}'(r',\theta',\varphi')$ have an angle γ between them. The spherical harmonics addition theorem states that

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_l^{m*}(\theta',\varphi')Y_l^m(\theta,\varphi). \tag{16}$$

Substituting into eq. (8), we obtain

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\frac{r'^l}{r^{l+1}}Y_l^{m*}(\theta',\varphi')Y_l^m(\theta,\varphi). \tag{17}$$

2.3 Spherical Multipole Expansion

The electric potential outside of the charge distribution can be written as an expansion in spherical harmonics:

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sqrt{\frac{4\pi}{2l+1}} \frac{q_l^m}{r^{l+1}} Y_l^m(\theta, \varphi). \tag{18}$$

Together with eq. (1) and eq. (17), we find

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{Y_l^m(\theta, \varphi)}{r^{l+1}} \int \mathrm{d}^3 r' \rho(\mathbf{r}') r'^l Y_l^{m*}(\theta', \varphi'). \tag{19}$$

The coefficients

$$q_l^m = \sqrt{\frac{4\pi}{2l+1}} \int \mathrm{d}^3 r' \rho(\mathbf{r}') r'^l Y_l^{m*}(\theta', \varphi') \tag{20}$$

are called the **spherical multipole moments**.

The spherical multipole moments are closely related to the cartesian multipole moments:

$$\begin{aligned}
q_0^0 &= \int \mathrm{d}^3 r \rho(\mathbf{r}) = Q^0 \\
q_1^0 &= \int \mathrm{d}^3 r \rho(\mathbf{r}) z = Q_z^1 \\
q_1^{\pm 1} &= \mp \sqrt{\frac{1}{2}} \int \mathrm{d}^3 r \rho(\mathbf{r})(x \mp iy) = \mp \sqrt{\frac{1}{2}} (Q_x^1 \mp i Q_y^1) \\
q_2^0 &= \frac{1}{2} \int \mathrm{d}^3 r \rho(\mathbf{r})(3z^2 - r^2) = \frac{1}{2} Q_{zz}^2 \\
q_2^{\pm 1} &= \mp \sqrt{\frac{3}{2}} \int \mathrm{d}^3 r \rho(\mathbf{r})(x \mp iy) z = \mp \sqrt{\frac{1}{6}} (Q_{xz}^2 \mp i Q_{yz}^2) \\
q_2^{\pm 2} &= \sqrt{\frac{3}{8}} \int \mathrm{d}^3 r \rho(\mathbf{r})(x \mp iy)^2 = \sqrt{\frac{1}{2}} (Q_{xx}^2 \mp 2i Q_{xy}^2 - Q_{yy}^2) \\
&\;\;\vdots
\end{aligned}$$

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