Multipole Expansion Generalized [lam19]

In [lln5] we considered the the multipole expansion for the electrostatic field generated by two point charges by elementary means, specifically the leading terms, which are associated with the monopole, dipole and quadrupole.

Here we consider a continuous charge distribution $\rho(\mathbf{x})$ and aim to calculate the electric potential $\Phi(\mathbf{x})$, which is the solution of the Poisson equation,

$$\nabla^2\Phi(\mathbf{x}) = -\frac{\rho(\mathbf{x})}{\epsilon_0}. \tag{1}$$

For that purpose we construct a multipole expansion (in spherical coordinates about the field point) for the Green's function,

$$G(\mathbf{x},\mathbf{x}') = \frac{1}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}-\mathbf{x}'|}, \tag{2}$$

which allows us to write

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int d^3x'\,\frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} = \int d^3x' G(\mathbf{x},\mathbf{x}')\rho(\mathbf{x}'). \tag{3}$$

The function (2) is a solution of

$$\nabla^2 G(\mathbf{x},\mathbf{x}') = -\frac{1}{\epsilon_0}\delta(\mathbf{x}-\mathbf{x}'). \tag{4}$$

which is verified by using the mathematical identity,

$$\nabla^2\frac{1}{|\mathbf{x}-\mathbf{x}'|} = -4\pi\delta(\mathbf{x}-\mathbf{x}'). \tag{5}$$

The delta function expressed in Cartesian and spherical coordinates reads,

$$\begin{aligned}\delta(\mathbf{x}-\mathbf{x}') &= \delta(x-x')\delta(y-y')\delta(z-z')\\ &= \frac{1}{r^2\sin\theta}\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi').\end{aligned} \tag{6}$$

The Laplacian operator expressed in spherical coordinates reads,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]}_{\mathcal{D}^2}, \tag{7}$$

where the operator $\mathcal{D}^2$ is the Laplacian on the unit sphere.

The eigenvalues equation associated with $\mathcal{D}^2$ is solved by spherical harmonics:

$$\mathcal{D}^2 Y_{lm}(\theta,\phi) = -l(l+1)Y_{lm}(\theta,\phi), \tag{8}$$

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{l+m)!}}P_l^m(\cos\theta)e^{\imath m\phi}, \tag{9}$$

where $P_l^m(\cos\theta)$ are associated Legendre functions [lam17].

The Green's function (2) expanded in spherical harmonics for its angular coordinates becomes

$$G(r,\theta,\phi,\mathbf{x}') = \sum_{lm} G_{lm}(r,\mathbf{x}')Y_{lm}(\theta,\phi), \tag{10}$$

Equation (4) for the expansion (10) with use of (8) acquires the form

$$\sum_{lm}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}G_{lm}(r,r',\theta',\phi')\right) - \frac{l(l+1)}{r^2}G_{lm}(r,r',\theta',\phi')\right]Y_{lm}(\theta,\phi)$$
$$= -\frac{1}{\epsilon_0 r^2\sin\theta}\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi'). \tag{11}$$

The angular coordinates θ,ϕ can be integrated out by taking advantage of two of the delta functions and the orthonormality of spherical harmonics:

$$\Rightarrow \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}G_{lm}(r,r',\theta',\phi')\right) - \frac{l(l+1)}{r^2}G_{lm}(r,r',\theta',\phi')$$
$$= -\frac{1}{\epsilon_0 r^2\sin\theta}\delta(r-r')Y^*_{lm}(\theta',\phi'). \tag{12}$$

Next we set $G_{lm}(r,r',\theta',\phi') = g_{lm}(r,r')Y^*_{lm}(\theta',\phi')$:

$$\Rightarrow \frac{d}{dr}\left(r^2\frac{d}{dr}g_{lm}(r,r')\right) - l(l+1)g_{lm}(r,r') = -\frac{1}{\epsilon_0}\delta(r-r'). \tag{13}$$

Solutions of (13) for $r \neq r'$, where the right-hand side vanishes, are readily obtained as a combination of power laws:

$$g_{lm}(r,r') = a_{lm}(r')r^{-(l+1)} + b_{lm}(r')r^l. \tag{14}$$

The Green's function must be non-divergent at the field point ($r=0$) and at infinity ($r\to\infty$) which restricts non-vanishing functions $a_{lm}(r')$ and $b_{lm}(r')$ to two mutually exclusive regions:

$$g_{lm}(r,r') = \begin{cases} b_{lm}(r')r^l, & : \; r < r' \\ a_{lm}(r')r^{-(l+1)} & : \; r > r'. \end{cases} \tag{15}$$

The functions $a_{lm}(r')$ and $b_{lm}(r')$ are determined by the boundary conditions at $r=r'$ encoded in the (13):

▷ The function $g_{lm}(r,r')$ is continuous across the boundary:

$$a_{lm}(r')r'^{(-l-1)} = b_{lm}(r')r'^{(l)}. \tag{16}$$

$\triangleright$ The function $g_{lm}(r,r')$ has a discontinuity in its derivative associated with the weight factor of the delta function:

$$r'^2\left[g'_{lm}(r')_+ - g'_{lm}(r')_-\right] = -\frac{1}{\epsilon_0}$$
$$\Rightarrow\ (l+1)a_{lm}(r')r'^{(-l)} + lb_{lm}(r')r'^{(l+1)} = \frac{1}{\epsilon_0}. \qquad (17)$$

The linear equations (16) and (17) have the solution,

$$a_{lm}(r') = \frac{1}{(2l+1)\epsilon_0}r'^l, \quad b_{lm}(r') = \frac{1}{(2l+1)\epsilon_0}r'^{(-l-1)}. \qquad (18)$$

This solution determines the Green's function in spherical coordinates uniquely:

$$G(\mathbf{x},\mathbf{x}') = \begin{cases} \dfrac{1}{\epsilon_0}\displaystyle\sum_{lm}\frac{1}{2l+1}\frac{r^l}{r'^{(l+1)}}Y^*_{lm}(\theta',\phi')Y_{lm}(\theta,\phi) & : \ r < r', \\ \dfrac{1}{\epsilon_0}\displaystyle\sum_{lm}\frac{1}{2l+1}\frac{r'^l}{r^{l+1}}Y^*_{lm}(\theta',\phi')Y_{lm}(\theta,\phi) & : \ r > r'. \end{cases} \qquad (19)$$

The electric potential of an arbitrary charge distribution in the multipole expansion thus becomes

$$\Phi(\mathbf{x}) = \int d^3x' G(\mathbf{x},\mathbf{x}')\rho(\mathbf{x}') = \frac{1}{\epsilon_0}\sum_{lm}\frac{1}{2l+1}\left[\alpha_{lm}(r)r^l + \frac{\beta_{lm}(r)}{r^{l+1}}\right]Y_{lm}(\theta,\phi), \qquad (20)$$

with coefficients determined by the charge density $\rho(\mathbf{x}')$ as follows:

$$\alpha_{lm}(r) = \int_r^\infty dr' r'^2\int_0^{2\pi}d\phi'\int_0^\pi d\theta'\sin\theta'\rho(r',\theta',\phi')r'^{(-l-1)}Y^*_{lm}(\theta',\phi'),$$
$$\beta_{lm}(r) = \int_0^r dr' r'^2\int_0^{2\pi}d\phi'\int_0^\pi d\theta'\sin\theta'\rho(r',\theta',\phi')r'^l Y^*_{lm}(\theta',\phi'). \qquad (21)$$

For a charge distribution confined to a region near $\mathbf{x}' = 0$ and a field point $\mathbf{x}$ outside that region only the second term of (20) comes into play:

$$\Phi(\mathbf{x}) = \frac{1}{\epsilon_0}\sum_{lm}\frac{1}{2l+1}\frac{q_{lm}}{r^{l+1}}Y_{lm}(\theta,\phi),$$
$$q_{lm} = \int_0^\infty dr' r'^2\int_0^{2\pi}d\phi'\int_0^\pi d\theta'\sin\theta'\rho(r',\theta',\phi')r'^l Y^*_{lm}(\theta',\phi'). \qquad (22)$$

The value of q_{00} determines the net charge (monopole), the the three values q_{1m} the components of the dipole moment, and the five independent values of q_{2m} the elements of the (symmetric and traceless) quadrupole tensor [lln5].