PHY481 - Lecture 14: Multipole expansion

Griffiths: Chapter 3

Expansion of $1/|\vec{r}-\vec{r}'|$ (Legendre's original derivation)

Consider a charge distribution $\rho(\vec{r}')$ that is confined to a finite volume τ. For positions $\vec{r}$ that are outside the volume τ, we can find the potential using either superposition, or Laplace's equation, i.e.,

$$V(\vec{r}) = k\int_\tau \frac{\rho(\vec{r}')d\vec{r}'}{|\vec{r}-\vec{r}'|} \quad \text{or} \quad \nabla^2 V = 0 \tag{1}$$

In cases where there is no ϕ dependence the Laplace solution in polar co-ordinates is,

$$\sum_l (A_l r^l + \frac{B_l}{r^{l+1}})P_l(cos\theta) \tag{2}$$

How are these two approaches related? The multipole expansion of $1/|\vec{r}-\vec{r}'|$ shows the relation and demonstrates that at long distances $r >> r'$, we can expand the potential as a multipole, i.e. Eq. (2), with $A_l = 0$. More than that, we can actually get general expressions for the coefficients B_l in terms of $\rho(\vec{r}')$. First lets see Eq. (1) and (2) are related, but doing a systematic expansion of $1/|\vec{r}-\vec{r}'|$, in the case where $r'/r < 1$. We write,

$$\frac{1}{|\vec{r}-\vec{r}'|} = \frac{1}{[r^2 + r'^2 - 2\vec{r}\cdot\vec{r}']^{1/2}} = \frac{1}{r}\frac{1}{[1+(\frac{r'}{r})^2 - \frac{2\vec{r}\cdot\vec{r}'}{r^2}]^{1/2}} \tag{3}$$

We use $x = (\frac{r'}{r})^2 - \frac{2\vec{r}\cdot\vec{r}'}{r^2} = a - b$, where $a = (\frac{r'}{r})^2$ and $b = \frac{2\vec{r}\cdot\vec{r}'}{r^2} = 2(r'/r)cos\theta$, and make a Taylor expansion of $1/(1+x)^{1/2}$, i.e. use

$$f(y) = f(y_0) + (y-y_0)f')y_0) + \frac{1}{2!}(y-y_0)^2 f''(y_0) + \frac{1}{3!}(y-y_0)^3 f'''(y_0) + ... \tag{4}$$

with f(y) $= 1/(1+y)^{1/2}$, $y_0 = 0$ and $y = x$. Then $f(y_0) = 1$, $f'(y_0) = -1/2$; $f''(y_0) = 3/4$, $f'''(y_0) = -15/8$, so that,

$$\frac{1}{(1+x)^{1/2}} = 1 - \frac{x}{2} + \frac{3x^2}{8} - \frac{5x^3}{16} + ... \tag{5}$$

Substituting $x = a - b$ gives,

$$\frac{1}{(1+x)^{1/2}} = 1 - \frac{a-b}{2} + \frac{3(a^2 - 2ab + b^2)}{8} - \frac{5(a^3 - 3a^2 b + 3ab^2 - b^3)}{16} + ..$$

$$= 1 - \frac{a-b}{2} + \frac{3(-2ab + b^2)}{8} - \frac{5(-b^3)}{16} + O((\frac{r}{r'})^4 \tag{6}$$

where we kept terms to octapole order (i.e. keeping terms up to $(r'/r)^3$). Now collecting terms according to their order in the expansion we get;

$$\frac{1}{|\vec{r}-\vec{r}'|} = \frac{1}{r}[1 + \frac{b}{2} + (\frac{3b^2}{8} - \frac{a}{2}) + (\frac{5b^3}{16} - \frac{3ab}{4}) + O((\frac{r}{r'})^3 \tag{7}$$

Finally we use $b = \frac{2\vec{r}\cdot\vec{r}'}{r^2} = 2(r'/r)cos\theta$, $a = (r'/r)^2$ to find,

$$\frac{1}{|\vec{r}-\vec{r}'|} = \frac{1}{r}[1 + \frac{r'}{r}cos\theta + (\frac{r'}{r})^2(\frac{3cos^2\theta}{2} - \frac{1}{2}) + (\frac{r'}{r})^3(\frac{5cos^3\theta}{2} - \frac{3cos\theta}{2}) + O((\frac{r}{r'})^4 \tag{8}$$

Recall Bonnet's recursion formula for Legendre polynomials,

$$(l+1)P_{l+1}(u) = (2l+1)uP_l(u) - lP_{l-1}(u) \tag{9}$$

With $P_0 = 1$ and $P_1 = u$, we find $P_2 = (3u^2-1)/2$, $P_3 = (5u^3 - 3u)/2$, and with $u = cos\theta$ demonstrates that,

$$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_{l=0} \frac{r'^l}{r^{l+1}} P_l(cos\theta) \quad r > r' \tag{10}$$

This expansion is for the case where $r'/r < 1$ and is called the exterior solution. A similar expansion may be carried out for $r'/r > 1$ and this is called the interior expansion

$$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_{l=0} \frac{r^l}{r'^{l+1}} P_l(cos\theta) \qquad r < r' \tag{11}$$

Using the exterior expansion (10) for a dipole charge configuration, we have,

$$V(r,\theta) = \frac{kq}{r}\sum_{l}(\frac{d}{2r})^l P_l(cos\theta) - \frac{kq}{r}\sum_{l=0}(\frac{-d}{2r})^l P_l(cos\theta) \tag{12}$$

The even terms in the sum cancel, while the odd terms add so that,

$$V(r,\theta) = \frac{kq}{r}\sum_{l\ odd} 2(\frac{d}{2r})^l P_1(cos\theta) = \frac{kq}{r}[\frac{d}{r}cos\theta + 2(\frac{d}{2r})^3 P_3(cos\theta) + ...]. \tag{13}$$

The leading term is the dipole potential, though higher order terms do exist and are important for smaller distances.

Monopole and dipole terms for a general localized charge distribution

First consider a discrete charge distribution consisting of charges q_i at positions $\vec{r_i}$. The potential at position $\vec{r}$ is then expanded as,

$$V(\vec{r_i}) = \sum_i \frac{kq_i}{|\vec{r}-\vec{r}_i|} = \sum_i \frac{kq_i}{r} + \sum_i \frac{kq_i r_i cos\theta_i}{r^2} + \sum_i \frac{kq_i r_i^2}{2r^3}[3cos^2\theta_i - 1] + O(\frac{1}{r^4}) \tag{14}$$

It is then natural to define the quantities,

$$Q = \sum_i q_i; \quad \vec{p} = \sum_i q_i \vec{r}_i \tag{15}$$

which are the total charge and the total dipole moment of the charge distribution. The definition of the quadrupole term is more subtle, however a matrix form is convenient so that, we finally have,

$$\sum_i \frac{kq_i}{|\vec{r}-\vec{r}_i|} = \frac{kQ}{r} + \frac{k\vec{p}\cdot\hat{r}}{r^2} + \frac{k\hat{r}\cdot\tilde{Q}_2\cdot\hat{r}}{r^3} + O(1/r^4) \tag{16}$$

where the quadrupole matrix is given by,

$$\tilde{Q}_2 = \sum_i \frac{1}{2} q_i (3\vec{r}_i \bigotimes \vec{r}_i - r_i^2 \tilde{I}) \tag{17}$$

where $\bigotimes$ is the outer product and $\tilde{I}$ is a 3×3 identity matrix. The continuum version of the monopole and dipole terms are,

$$Q = \int \rho(\vec{r}')d\vec{r}' \quad \text{and} \quad \vec{p} = \int \vec{r}'\rho(\vec{r}')d\vec{r}'. \tag{18}$$

In general the dipole and higher order terms depend on the choice of origin for the co-ordinate system. However if the monopole term is zero it is easy to show that the dipole term is independent of the co-ordinate system. To prove this substitute $\vec{r}' + \vec{a}$ for $\vec{r}'$ in the dipole expression and show that the dipole moment is unaltered provided that $Q = 0$.

An example - Cartesian co-ordinates

Consider a square region of space, centered at the origin and with dimensions $a \times a$. The sides of the square are parallel to the x and y axes. The sides at $y = \pm a/2$ are held at a fixed potential V_0, while the sides at $x = \pm a/2$ are grounded, ie $V = 0$ there. Find an expression for the potential everywhere on the interior of the square domain.

Solution The first observation is that the boundary conditions in the x direction are symmetric about the origin so we choose functions of the form $X(x)$ $cos(kx)$. Similarly the boundary conditions in the y-direction are symmetric so we choose $Y(y)$ $cosh(ky)$. Since there is dependence on both x and y directions, we expect the one dimensional solutions will not be useful, so we do not include them. We then have,

$$V(x,y) = \sum_k A(k)cos(kx)cosh(ky) \tag{19}$$

At this point we don't know what values of k are needed. We can find a set of values of k by imposing the boundary conditions in the x-direction where $V(a/2, y) = V(-a/2, y) = 0$. These boundary conditions can be satisfied by choosing,

$$cos(ka/2) = 0 \quad \text{or} \quad k = \frac{(2n+1)\pi}{a}, \quad \text{with} \quad n = 0, 1, 2.... \tag{20}$$

Notice that we don't need to include negative values of n due to the fact that the cosine function is even. The electrostatic potential is then given by

$$V(x, y) = \sum_{n=0}^{\infty} A(n) cos((2n+1)\frac{\pi x}{a}) cosh((2n+1)\frac{\pi y}{a}) \tag{21}$$

Our remaining task is to satisfy the boundary conditions in the y-direction, $V(x, \pm a/2) = V_0$, so we need,

$$V_0 = \sum_{n=0}^{\infty} A(n) cos((2n+1)\frac{\pi x}{a}) cosh((2n+1)\frac{\pi}{2}) = \sum_{n=0}^{\infty} A'(n) cos((2n+1)\frac{\pi x}{a}) \tag{22}$$

where $A'(n) = A(n) cosh((2n+1)\pi/2)$. Our problem reduces to finding the Fourier cosine series for a constant function. Due to the orthogonality of the basis functions, we can extract the coefficient $A'(n)$, by multiplying both sides by $cos[(2n'+1)(\pi x/a)]$ and then integrating both sides over the interval $[-a/2, a/2]$,

$$\int_{-a/2}^{a/2} V_0 cos[(2n'+1)\frac{\pi x}{a}] dx = \sum_{n=0}^{\infty} A'(n) \int_{-a/2}^{a/2} cos((2n+1)\frac{\pi x}{a}) cos((2n'+1)\frac{\pi x}{a}) dx \tag{23}$$

Carrying out the integrals, we find that,

$$\frac{2V_0 a}{(2n'+1)\pi} sin((2n'+1)\frac{\pi}{2}) = \sum_n A'(n) \delta_{nn'} \int_{-a/2}^{a/2} [cos((2n+1)\frac{\pi x}{a})]^2 dx = \frac{aA'(n')}{2} \tag{24}$$

Solving we find that $A'(n) = 4V_0(-1)^n/[(2n+1)\pi]$, so the solution to our problem is,

$$V(x, y) = \sum_{n=0}^{\infty} \frac{4V_0(-1)^n}{(2n+1)\pi} \frac{cos((2n+1)\frac{\pi x}{a}) cosh((2n+1)\frac{\pi y}{a})}{cosh((2n+1)\frac{\pi}{2})} \tag{25}$$