

Section 3: Electrostatics

Laplace Equation in Spherical Coordinates

Cartesian coordinates are appropriate for objects with plane boundaries. For round objects, however, it is more appropriate to use the spherical coordinates. In spherical coordinates we use independent variables are (r, θ, ϕ) and the Laplace equation reads

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0. \quad (3.1)$$

Here we will limit our considerations by problems which have *azimuthal symmetry*, i.e. assume that the potential is independent of ϕ . In this case eq.(3.1) takes a simplified form

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial \Phi}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Phi}{\partial \theta} \right) = 0. \quad (3.2)$$

As before we are looking for solution that are products:

$$\Phi(r, \theta) = R(r)P(\theta). \quad (3.3)$$

Substituting this into eq.(3.2) and dividing by Φ we obtain

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{P \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial P}{\partial \theta} \right) = 0. \quad (3.4)$$

Since the first terms depends only on r , and the second term depends only on θ , it follows that each must be a constant:

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = l(l+1); \quad \frac{1}{P \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{dP}{d\theta} \right) = -l(l+1). \quad (3.5)$$

Here, as we will see in a minute, $l(l+1)$ is just a convenient way of writing the constant.

As always, separation of variables has converted a partial differential equation (3.2) into ordinary differential equations (3.5). The equation for the radial function

$$\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = l(l+1)R. \quad (3.6)$$

Has the general solution

$$R(r) = Ar^l + Br^{-l-1} \quad (3.7)$$

as one can easily check. Here A and B are the two arbitrary constants to be expected in the solution of a second order differential equation. The angular equation is more complicated:

$$\frac{d}{d\theta} \left(\sin \theta \frac{dP}{d\theta} \right) = -l(l+1)P \sin \theta. \quad (3.8)$$

This equation is customarily expressed in terms of $x = \cos \theta$, instead of θ itself. Then it takes the form

$$\frac{d}{dx} \left[(1-x^2) \frac{dP}{dx} \right] + l(l+1)P = 0. \quad (3.9)$$

The deseeded solution should be finite and continuous on the interval $-1 \leq x \leq 1$ in order to represent a physical potential. The solutions are *Legendre polynomials* $P_l(x)$ of order l . $P_l(x)$ is most conveniently

defined by the *Rodrigues formula* :

$$P_l(x) = \frac{1}{2^l l!} \left(\frac{d}{dx} \right)^l (x^2 - 1)^l. \quad (3.10)$$

The first few Legendre polynomials are

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= (3x^2 - 1)/2 \\ P_3(x) &= (5x^3 - 3x)/2 \\ P_4(x) &= (35x^4 - 30x^2 + 3)/8 \end{aligned} \quad (3.11)$$

The Legendre polynomials form a complete orthogonal set of functions on the interval $-1 \leq x \leq 1$. The orthogonality condition can be written as follows

$$\int_{-1}^1 P_l(x) P_r(x) dx = \frac{2}{(2l+1)} \delta_{lr} \quad (3.12)$$

or

$$\int_0^\pi P_l(\cos \theta) P_r(\cos \theta) \sin \theta d\theta = \frac{2}{(2l+1)} \delta_{lr} \quad (3.13)$$

Thus, in case of azimuthal symmetry of the problem, separation of variables yields an infinite set of solutions, one for each l . The general solution of the Laplace equation is the linear combination of these solutions:

$$\Phi(r, \theta) = \sum_{l=0}^{\infty} (A_l r^l + B_l r^{-l-1}) P_l(\cos \theta). \quad (3.14)$$

The coefficients A_l and B_l are to be determined from the boundary conditions. Now we consider a few examples which illustrate the power of this important result.

Potential inside a Sphere

Here we find the potential *inside* a hollow sphere of radius R assuming that the potential on the surface of the sphere is given and equal to $\Phi_0(\theta)$. In that case all B_l in the expansion (3.14) are equal to zero – otherwise the potential would diverge at the origin which is an unphysical result. Therefore,

$$\Phi(r, \theta) = \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta). \quad (3.15)$$

At $r = R$ this must match the potential on the surface so that

$$\Phi_0(\theta) = \sum_{l=0}^{\infty} A_l R^l P_l(\cos \theta). \quad (3.16)$$

Since the Legendre polynomials form a complete set of functions, this condition *can* be satisfied for an appropriate choice of coefficients A_l . In order to determine the constants we use the orthogonality condition (3.12). We multiply eq. (3.16) by $P_r(\cos \theta) = P_r(x)$ and integrate over interval $-1 \leq x \leq 1$:

$$\int_0^\pi \Phi_0(\theta) P_r(\cos \theta) \sin \theta d\theta = A_r R^r \frac{2}{(2r+1)} \quad (3.17)$$

or

$$A_l = \frac{(2l+1)}{2R^l} \int_0^\pi \Phi_0(\theta) P_l(\cos \theta) \sin \theta d\theta. \quad (3.18)$$

Equation (3.16) with coefficients (3.18) is the solution of the problem.

In practical situations, in order to evaluate the integral (3.18) it is convenient to represent the potential $\Phi_0(\theta)$ in terms of Legendre polynomials and then to use the orthogonality condition (3.12) to evaluate the integral (3.18). For example, let us assume that the potential on the sphere is

$$\Phi_0(\theta) = 2k \sin^2(\theta/2), \quad (3.19)$$

where k is a constant. We can rewrite it as follows

$$\Phi_0(\theta) = k(1 - \cos \theta) = k[P_0(\cos \theta) - P_1(\cos \theta)]. \quad (3.20)$$

Substitution this to (3.18) we find

$$\begin{aligned} A_0 &= k \\ A_1 &= -k/R \\ A_l &= 0, \quad l > 1 \end{aligned} \quad (3.21)$$

Therefore, the solution for the potential is

$$\Phi(r, \theta) = k \left(1 - \frac{r}{R} \cos \theta \right). \quad (3.22)$$

Potential outside a Sphere

Here we find the potential *outside* a hollow sphere of radius R assuming that the potential on the surface of the sphere is given and equal to $\Phi_0(\theta)$. In that case it is the A_l that are equal to zero in the expansion (3.14) are equal to zero – otherwise the potential would not go to zero at infinity. Therefore,

$$\Phi(r, \theta) = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos \theta). \quad (3.23)$$

At the surface of the sphere ($r = R$) we require that

$$\Phi_0(\theta) = \sum_{l=0}^{\infty} \frac{B_l}{R^{l+1}} P_l(\cos \theta). \quad (3.24)$$

Multiplying by $P_l(\cos \theta) = P_l(x)$, integrating and exploiting the orthogonality condition we find

$$\int_0^\pi \Phi_0(\theta) P_l(\cos \theta) \sin \theta d\theta = \frac{B_l}{R^{l+1}} \frac{2}{(2l+1)} \quad (3.25)$$

or

$$B_l = \frac{(2l+1)}{2} R^{l+1} \int_0^\pi \Phi_0(\theta) P_l(\cos \theta) \sin \theta d\theta. \quad (3.26)$$

Equation (3.16) with coefficients (3.26) is the solution of the problem.

A Metal Sphere in a Homogeneous Electric Field

We have already solved this problem using method of images. Now we solve the problem using the solution of Laplace equation in the spherical coordinate system.

Assume that an uncharged metal sphere of radius R is placed in a homogeneous electric field $\mathbf{E} = E_0 \hat{\mathbf{z}}$. The problem has axial symmetry and hence we can use the approach discussed in the preceding sections. We need to define boundary conditions. Since the sphere is equipotential it is convenient to assume that the potential is zero on the sphere. At infinity the potential is that of a homogeneous electric field, i.e. $\Phi = -E_0 z = -E_0 r \cos \theta$. Therefore the boundary conditions are

$$\begin{aligned}\Phi &= 0, & r &= R \\ \Phi &\rightarrow -E_0 r \cos \theta, & r &\gg R\end{aligned}\quad (3.27)$$

We need to fit these boundary condition to the general solution of the problem (3.14). The first boundary condition yields

$$A_l R^l + B_l R^{-l-1} = 0, \quad (3.28)$$

or

$$B_l = -A_l R^{2l+1}, \quad (3.29)$$

and therefore

$$\Phi(r, \theta) = \sum_{l=0}^{\infty} A_l \left(r^l - \frac{R^{2l+1}}{r^{l+1}} \right) P_l(\cos \theta). \quad (3.30)$$

For $r \gg R$ the second term in parenthesis is negligible, and therefore the second boundary condition requires that

$$\sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta) = -E_0 r \cos \theta. \quad (3.31)$$

Evidently only one term in the expansion is present: $l = 1$. In fact since $P_1(\cos \theta) = \cos \theta$, we can read off immediately

$$\begin{aligned}A_1 &= -E_0, \\ A_l &= 0, \quad l \neq 1.\end{aligned}\quad (3.32)$$

Finally we find that

$$\Phi(r, \theta) = -E_0 \left(r - \frac{R^3}{r^2} \right) \cos \theta. \quad (3.33)$$

This is exactly the same result we have obtained using the method of images.

A Sphere with a Given Surface Charge Density

Here we consider a problem of finding the potential assuming that a specified charge density $\sigma(\theta)$ is glued over the surface of a spherical shell of radius R . We need to find the resulting potential inside and outside the sphere.

For the interior region $B_l = 0$ and we have

$$\Phi_{in}(r, \theta) = \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta), \quad r \leq R. \quad (3.34)$$

In the exterior region $A_l = 0$ and we have

$$\Phi_{out}(r, \theta) = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos \theta), \quad r \geq R. \quad (3.35)$$

These two functions must be joined together by the appropriate boundary conditions at the surface itself.

First, we know that the potential is *continuous* and therefore $\Phi_{in}(R, \theta) = \Phi_{out}(R, \theta)$ so that

$$\sum_{l=0}^{\infty} A_l R^l P_l(\cos \theta) = \sum_{l=0}^{\infty} \frac{B_l}{R^{l+1}} P_l(\cos \theta). \quad (3.36)$$

We have the equation for any arbitrary θ we have to assume that coefficients of the Legendre polynomials of like orders are equal, i.e.

$$B_l = A_l R^{2l+1}. \quad (3.37)$$

Second, we know that the normal derivative of the potential suffers a discontinuity at the surface so that

$$\left(\frac{\partial \Phi_{out}}{\partial r} - \frac{\partial \Phi_{in}}{\partial r} \right)_{r=R} = -\frac{\sigma(\theta)}{\epsilon_0}. \quad (3.38)$$

Thus

$$-\sum_{l=0}^{\infty} (l+1) \frac{B_l}{R^{l+2}} P_l(\cos \theta) - \sum_{l=0}^{\infty} l A_l R^{l-1} P_l(\cos \theta) = -\frac{\sigma(\theta)}{\epsilon_0}, \quad (3.39)$$

or using eq.(3.37):

$$\sum_{l=0}^{\infty} (2l+1) A_l R^{l-1} P_l(\cos \theta) = \frac{\sigma(\theta)}{\epsilon_0}. \quad (3.40)$$

From here the coefficients can be found by multiplying by $P_l(\cos \theta)$, integrating over θ and using the orthogonally condition (3.12)

$$2A_l R^{l-1} = \int_0^{\pi} \frac{\sigma(\theta)}{\epsilon_0} P_l(\cos \theta) \sin \theta d\theta, \quad (3.41)$$

which gives

$$A_l = \frac{1}{2\epsilon_0 R^{l-1}} \int_0^{\pi} \sigma(\theta) P_l(\cos \theta) \sin \theta d\theta. \quad (3.42)$$

Equations (3.34) and (3.35) constitute the solution of the problem, with the coefficients given by eqs. (3.37) and (3.42).

Laplace Equation in Cylindrical Coordinates

Now we consider the solution of the Laplace equation in cylindrical coordinates. In cylindrical coordinates we use independent variables are (s, ϕ, z) and the Laplace equation reads

$$\frac{1}{s} \frac{\partial}{\partial s} \left(s \frac{\partial \Phi}{\partial s} \right) + \frac{1}{s^2} \frac{\partial^2 \Phi}{\partial \phi^2} + \frac{\partial^2 \Phi}{\partial z^2} = 0. \quad (3.43)$$

For simplicity we assume that the system under consideration has such symmetry that there is no dependence on z , i.e. $\Phi = \Phi(s, \phi)$ In this case eq.(3.43) takes a simplified form

$$\frac{1}{s} \frac{\partial}{\partial s} \left(s \frac{\partial \Phi}{\partial s} \right) + \frac{1}{s^2} \frac{\partial^2 \Phi}{\partial \phi^2} = 0. \quad (3.44)$$

As before, we are looking for a solution that separates variables:

$$\Phi(s, \phi) = R(s)\Psi(\phi). \quad (3.45)$$

Substituting this into eq.(3.44), multiplying by s^2 and dividing by Φ we obtain

$$\frac{s}{R} \frac{d}{ds} \left(s \frac{dR}{ds} \right) + \frac{1}{\Psi} \frac{d^2 \Psi}{d\phi^2} = 0. \quad (3.46)$$

Since the first term involves s only and the second term ϕ only, each is a constant:

$$\frac{s}{R} \frac{d}{ds} \left(s \frac{dR}{ds} \right) = C_1; \quad \frac{1}{\Psi} \frac{d^2 \Psi}{d\phi^2} = C_2; \quad C_1 + C_2 = 0. \quad (3.47)$$

The constant C_2 must be negative. Otherwise the solution would represent exponentials which are not periodic with respect to ϕ , and therefore the angular component of the potential Ψ do not return to its original value (as it must by symmetry) when ϕ is increased by 2π . Therefore, we can define $C_2 = -k^2$, which gives

$$\frac{1}{\Psi} \frac{d^2 \Psi}{d\phi^2} = -k^2, \quad (3.48)$$

and therefore

$$\Psi(\phi) = A \cos(k\phi) + B \sin(k\phi) \quad (3.49)$$

Moreover, since $\Psi(\phi) = \Psi(2\pi + \phi)$, k must be an integer: $k = 0, 1, 2, \dots$. The radial equation is

$$s \frac{d}{ds} \left(s \frac{dR}{ds} \right) = k^2 R. \quad (3.50)$$

Assuming that $R \propto s^n$, we find

$$s \frac{d}{ds} (s n s^{n-1}) = n^2 s^n = k^2 s^n \rightarrow n = \pm k. \quad (3.51)$$

Evidently the general solution is

$$R(s) = C s^k + D s^{-k}, \quad (3.52)$$

unless $k = 0$, in which case we have only *one* solution to a *second-order* equation – a constant. Therefore, we must treat $k = 0$ separately, to find another solution. Going back to the differential equation for S , and putting in $k = 0$ we find

$$s \frac{d}{ds} \left(s \frac{dR}{ds} \right) = 0 \rightarrow s \frac{dR}{ds} = c, \quad (3.53)$$

where c is some constant. This leads to

$$\frac{dR}{ds} = \frac{c}{s} \rightarrow R(s) = c \ln s + d, \quad (3.54)$$

where d is another constant. We also need to treat the $k = 0$ case separately for Ψ . Eq.(3.48) leads to the differential equation

$$\frac{1}{\Psi} \frac{d^2 \Psi}{d\phi^2} = 0, \quad (3.55)$$

the solution of which is a linear function of ϕ

$$\Psi(\phi) = b\phi + a, \quad (3.56)$$

where a and b are some constants. But a term in the form $b\phi$ is not acceptable, since it does not return to its initial value when ϕ is augmented by 2π . Finally, we find the general solution for the potential with cylindrical symmetry

$$\Phi(s, \phi) = A_0 + B_0 \ln s + \sum_{k=1}^{\infty} [A_k \cos(k\phi) + B_k \sin(k\phi)] [C_k s^k + D_k s^{-k}] \quad (3.57)$$

Example: As an example of the application of this method we find the potential outside an infinitely long metal pipe, of radius R , placed in a uniform electric field \mathbf{E} such that the uniform field is normal to the axis of the pipe (Fig.3.1). Since the resulting potential does not depend on z direction we can use the approach described above.

We assume that the pipe axis is the z axis and the electric field is $\mathbf{E} = E_0 \hat{\mathbf{x}}$. Since the pipe is equipotential it is convenient to assume that the potential is zero on the pipe. At infinity the potential is that of a homogeneous electric field, i.e. $\Phi = -E_0 x = -E_0 s \cos \phi$. Therefore the boundary conditions are

$$\begin{aligned} \Phi &= 0, \quad s = R \\ \Phi &\rightarrow -E_0 s \cos \phi, \quad s \gg R \end{aligned} \quad (3.58)$$

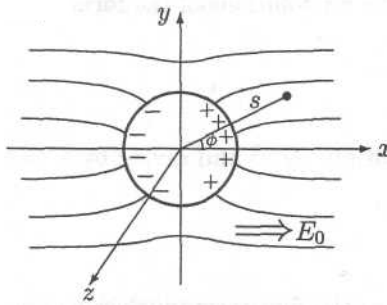


Fig.3.1

To have the right boundary condition at infinity we have to assume in eq.(3.57) that $A_0 = 0, B_0 = 0, B_k = 0$ and the only non-zero terms in the sum which have $k = 1$:

$$\Phi(s, \phi) = (Cs^1 + Ds^{-1}) \cos \phi \quad (3.59)$$

Taking into account the boundary conditions (3.58) we find that

$$\begin{aligned} CR + DR^{-1} &= 0 \\ C &= -E_0 \end{aligned} \quad (3.60)$$

Therefore,

$$\Phi(s, \phi) = \left(-E_0 s + \frac{E_0 R^2}{s} \right) \cos \phi \quad (3.61)$$

or

$$\Phi(s, \phi) = -E_0 s \left(1 - \frac{R^2}{s^2} \right) \cos \phi \quad (3.62)$$

The surface charge density induced by the electric field on the pipe is given by

$$\sigma = -\epsilon_0 \left. \frac{\partial \Phi}{\partial s} \right|_{s=R} = \epsilon_0 E_0 \left(1 + \frac{R^2}{s^2} \right) \cos \phi \Big|_{s=R} = 2\epsilon_0 E_0 \cos \phi. \quad (3.63)$$

Fields and Potentials on Edges

In many practical applications conducting surfaces come together creating edges. Suppose then that one is very close to such an edge where the boundary may be considered to consist of two infinite intersecting planes (Fig.3.2). Two conducting planes intersect at an angle β . The planes are assumed to be held at potential constant Φ_0 . Since the potential is independent on the z direction parallel to the planes, the problem may be solved using the method described in the preceding section.

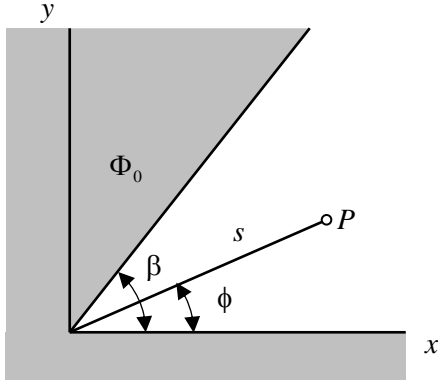


Fig.3.2 Intersection of two conducting planes defining a corner in two dimensions with opening angle β .

In a similar way we can construct a general solution of the Laplace equation using a superposition of the solution for the radial and angular functions:

$$R(s) = Cs^\nu + Ds^{-\nu}, \quad (3.64)$$

$$\Psi(\phi) = A\sin(\nu\phi) + B\cos(\nu\phi) \quad (3.65)$$

Similarly, a separate set of solutions should be included for $\nu = 0$:

$$R(s) = c \ln s + d, \quad (3.66)$$

$$\Psi(\phi) = b\phi + a. \quad (3.67)$$

These are building blocks from which we construct the potential by a linear superposition. There is a difference, though, between the allowed values of ν in this problem and the allowed values of k in the problem considered above. Here it is not acceptable to use the condition $\Phi(\phi) = \Phi(2\pi + \phi)$ (leading to integer k) because this condition assumes a continuous rotation of the coordinate system with respect to the z axis which is not allowed for this problem since we are looking at the solution only for a certain range of angles $0 < \phi < \beta$. Here the restriction to possible values of ν comes from the boundary conditions for the potential.

In our case the azimuthal angle ϕ is restricted to the range $0 < \phi < \beta$. The boundary conditions are that $\Phi = \Phi_0$ for all $s > 0$ when $\phi = 0$ and $\phi = \beta$. This requires that $B = 0$ in (3.65) and $b = 0$ in (3.67). In addition in order to avoid unphysical discontinuity in the potential at $s = 0$ we have to have $D = 0$ in (3.64) and $c = 0$ in (3.66). Furthermore, the boundary conditions require that ν be chosen to make $\sin(\nu\beta) = 0$. Hence

$$\nu = \frac{m\pi}{\beta}, \quad m = 1, 2, \dots \quad (3.68)$$

and the general solution becomes

$$\Phi(s, \phi) = \Phi_0 + \sum_{m=1}^{\infty} a_m s^{\frac{m\pi}{\beta}} \sin\left(\frac{m\pi}{\beta} \phi\right). \quad (3.69)$$

The still undetermined coefficients a_m depend on the potential remote from the corner at $s = 0$. Since the series involves positive powers of $s^{\pi/\beta}$, for small enough s only the first term in the series will be important. Thus, near $s = 0$, the potential is approximately

$$\Phi(s, \phi) \approx \Phi_0 + a_1 s^{\pi/\beta} \sin(\pi\phi / \beta). \quad (3.70)$$

The electric field components are

$$\begin{aligned} E_s(s, \phi) &= -\frac{\partial \Phi}{\partial s} \approx -\frac{\pi a_1}{\beta} s^{\pi/\beta-1} \sin(\pi\phi/\beta) \\ E_\phi(s, \phi) &= -\frac{1}{s} \frac{\partial \Phi}{\partial \phi} \approx -\frac{\pi a_1}{\beta} s^{\pi/\beta-1} \cos(\pi\phi/\beta) \end{aligned} \quad (3.71)$$

The surface-charge densities $\phi=0$ and $\phi=\beta$ are equal and are approximately

$$\sigma(s, 0) = \sigma(s, \beta) = \varepsilon_0 E_\phi(s, 0) \approx -\frac{\varepsilon_0 \pi a_1}{\beta} s^{\pi/\beta-1}. \quad (3.72)$$

The components of the field and the surface-charge density near $s=0$ all vary with distance as $s^{\pi/\beta-1}$. For a very deep corner (small β) the power of s becomes very large. Essentially no charge accumulates in such a corner. For $\beta=\pi$ (a flat surface), the field quantities become independent of s , as is intuitively obvious. When $\beta>\pi$, the two-dimensional corner becomes an edge and the field and the surface-charge density become singular as $s \rightarrow 0$. For $\beta=2\pi$ (the edge of a thin sheet) the singularity is as $s^{-1/2}$. This is still integrable so that the charge within a finite distance from the edge is finite, but it implies that field strengths become very large at the edges of conducting sheets (or, in fact, for any configuration where $\beta>\pi$).

Multipole expansion

In this section we will develop the multipole expansion for a charge distribution. This expression is useful for analyzing the potential and the electric field at distances large compared to that of the localized charge distribution. We start from the general expression for the potential due to a localized charge distribution $\rho(\mathbf{r})$

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r'. \quad (3.73)$$

We assume that the origin lies within the charge distribution and consider the situation when the distance to the point of consideration is large compared to the size of the charge distribution. In this case we may expand the denominator in the integrand,

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{\sqrt{r^2 - 2\mathbf{r}\cdot\mathbf{r}' + r'^2}} = \frac{1}{r\sqrt{1 - 2\mathbf{r}\cdot\mathbf{r}'/r^2 + r'^2/r^2}}. \quad (3.74)$$

in series assuming that r'/r is a small parameter. Using the Taylor expansion

$$(1-x)^{-1/2} = 1 + \frac{1}{2}x + \frac{3}{8}x^2 + \dots \quad (3.75)$$

we find

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r} \left[1 + \frac{1}{2} \left(2 \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2} - \frac{r'^2}{r^2} \right) + \frac{3}{8} \left(\frac{2\mathbf{r}\cdot\mathbf{r}'}{r^2} \right)^2 \right] + O \left[\left(\frac{r'}{r} \right)^3 \right]. \quad (3.76)$$

We can rewrite eq.(3.76) as follows

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r} + \frac{\mathbf{r}\cdot\mathbf{r}'}{r^3} + \frac{1}{2r^5} \left[3(\mathbf{r}\cdot\mathbf{r}')^2 - r^2 r'^2 \right] + \dots \quad (3.77)$$

Using this expansion we can rewrite the potential (3.73) as follows:

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{1}{r} \int \rho(\mathbf{r}') d^3 r' + \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{r}') \frac{\mathbf{r} \cdot \mathbf{r}'}{r^3} d^3 r' + \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{r}') \frac{1}{2r^5} [3(\mathbf{r} \cdot \mathbf{r}')^2 - r^2 r'^2] d^3 r'. \quad (3.78)$$

The equation (3.78) can be written as

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{1}{r} \int \rho(\mathbf{r}') d^3 r' + \frac{1}{4\pi\epsilon_0} \frac{\mathbf{r}}{r^3} \cdot \int \rho(\mathbf{r}') \mathbf{r}' d^3 r' + \frac{1}{4\pi\epsilon_0} \sum_{ij} \frac{x_i x_j}{2r^5} \int \rho(\mathbf{r}') [3x'_i x'_j - r'^2 \delta_{ij}] d^3 r', \quad (3.79)$$

where x_i and x'_i are Cartesian components of vectors \mathbf{r} and \mathbf{r}' respectively. The first term gives monopole contribution the second term – the dipole contribution and the third term – the quadrupole contribution to the potential at large distances. The conventional form to write expression (3.79) is

$$\Phi(\mathbf{r}) = \frac{q}{4\pi\epsilon_0 r} + \frac{1}{4\pi\epsilon_0} \frac{\mathbf{r} \cdot \mathbf{p}}{r^3} + \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{ij} Q_{ij} \frac{x_i x_j}{r^5}, \quad (3.80)$$

where

$$q = \int \rho(\mathbf{r}') d^3 r' \quad (3.81)$$

is the monopole moment or charge,

$$\mathbf{p} = \int \rho(\mathbf{r}') \mathbf{r}' d^3 r' \quad (3.82)$$

is the dipole moment, and

$$Q_{ij} = \int \rho(\mathbf{r}') [3x'_i x'_j - r'^2 \delta_{ij}] d^3 r' \quad (3.83)$$

is the quadrupole moment. The quadrupole moment is represented by a second rank tensor matrix. Note that matrix Q_{ij} is real and symmetric so that $Q_{ij} = Q_{ji}$. Thus, only six components are independent. In fact, only five are, because there is an additional constraint that $\text{Tr}(Q)=0$. Indeed,

$$\text{Tr}(Q) \equiv \sum_i Q_{ii} = \sum_i \int \rho(\mathbf{r}') [3x'_i x'_i - r'^2 \delta_{ii}] d^3 r' = 0, \quad (3.84)$$

and therefore only two diagonal components are independent.

Interpretation of the Moments

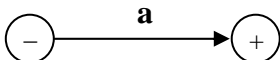
What is the interpretation of these terms? The monopole moment is just the total charge of the distribution. Thus the monopole term gives the potential due to the charge as a whole. Since the monopole term in the potential falls as $1/r$ at large r , it will dominate the far field potential whenever q is finite. The dipole moment is the first moment of the charge distribution; and refers to how the charge is distributed in space. Similarly, the quadrupole moment is a second moment of the distribution. Notice that the dipole potential falls off with the distance as the $1/r^2$, the quadrupole potential and $1/r^3$ and so on. Therefore, at large distance from the charge distribution the lowest moment will dominate the potential and the field.

In general the moments depend upon the origin of the coordinate system. This is not the case, however, for a dipole moment provided that the total charge of the system is zero. Indeed, it easy to see that is we move the origin from zero to \mathbf{R} the dipole moment transforms from \mathbf{p} to

$$\int \rho(\mathbf{r})(\mathbf{r} - \mathbf{R}) d^3 r = \int \rho(\mathbf{r}) \mathbf{r} d^3 r - \mathbf{R} \int \rho(\mathbf{r}) d^3 r = \mathbf{p} - q\mathbf{R}. \quad (3.85)$$

If $q = 0$ the dipole moment does not change.

A simplest dipole represents two charges q and $-q$ separated by a distance a :



The total charge is zero, and therefore at a large distance the potential is dominated by a dipole term

$$\Phi(\mathbf{r}) \approx \frac{1}{4\pi\epsilon_0} \frac{\mathbf{r} \cdot \mathbf{p}}{r^3}, \quad (3.86)$$

where in this case $\mathbf{p} = q\mathbf{a}$. When $a \rightarrow 0$ such that $\mathbf{p} = q\mathbf{a} = \text{const}$, then the higher terms vanish and the result becomes exact. In such a limit we obtain an ideal point dipole.

The potential and the electric field due to a dipole $\mathbf{p} = p\hat{\mathbf{z}}$ can be expressed in spherical coordinates

$$\begin{aligned} \Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \frac{p \cos \theta}{r^2}; \\ E_r(r, \theta) &= -\frac{\partial \Phi}{\partial r} = \frac{1}{4\pi\epsilon_0} \frac{2p \cos \theta}{r^3}; \\ E_\theta(r, \theta) &= -\frac{1}{r} \frac{\partial \Phi}{\partial \theta} = \frac{1}{4\pi\epsilon_0} \frac{p \sin \theta}{r^3}. \end{aligned} \quad (3.87)$$

In Cartesian coordinates:

$$\mathbf{E}(\mathbf{r}) = -\nabla \left(\frac{1}{4\pi\epsilon_0} \frac{\mathbf{r} \cdot \mathbf{p}}{r^3} \right) = \frac{1}{4\pi\epsilon_0} \frac{3\mathbf{r}(\mathbf{p} \cdot \mathbf{r}) - r^2 \mathbf{p}}{r^5}, \quad (3.88)$$

It is interesting to ask what happens on at the origin, where our expansion fails. Let's look at the particular case of the dipole field, assuming a point dipole at $\mathbf{r} = 0$. For any $r > 0$, we know that the potential is as given in Eq.(3.86). Once before we found such a potential when we solved the problem of a conducting sphere of radius a in a uniform external applied field \mathbf{E}_0 along the z direction.

What we found was that the potential outside of the sphere is

$$\Phi(\mathbf{r}) = -E_0 r \cos \theta + E_0 \frac{a^3}{r^2} \cos \theta, \quad (3.89)$$

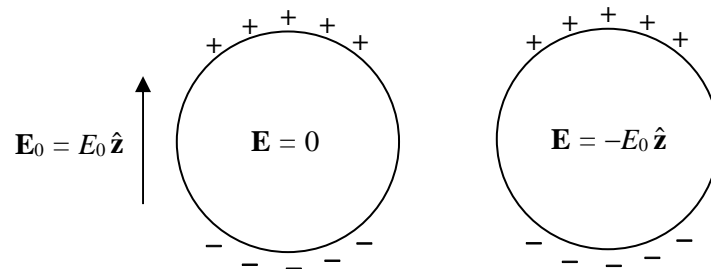
where a is the sphere radius. The first term is simply the potential of the homogeneous external field and the second term is the potential produced by the induced surface charges. By introducing a dipole moment linked to the applied field

$$\mathbf{p} = 4\pi\epsilon_0 E_0 a^3 \hat{\mathbf{z}}, \quad (3.90)$$

this expression can be rewritten as follows

$$\Phi(\mathbf{r}) = -\frac{1}{4\pi\epsilon_0} \frac{\mathbf{p} \cdot \mathbf{r}}{a^3} + \frac{1}{4\pi\epsilon_0} \frac{\mathbf{p} \cdot \mathbf{r}}{r^3}. \quad (3.91)$$

This means that the surface charge on the sphere has a dipole moment and, remarkably, no other multipole moments. The potential inside the sphere is constant and hence the electric field is zero because the sphere is assumed to be metallic.



Now we consider what happens if we remove the applied field but retain the field produced by the charges on the surface of the sphere. In this case the potential outside the sphere is simply

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{p} \cdot \mathbf{r}}{r^3}, \quad r > a. \quad (3.92)$$

By the superposition principle, the potential inside the sphere is now

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{p} \cdot \mathbf{r}}{a^3} = \frac{1}{4\pi\epsilon_0} \frac{pz}{a^3}, \quad r < a, \quad (3.93)$$

and the corresponding electric field is

$$\mathbf{E} = -\frac{1}{4\pi\epsilon_0} \frac{\mathbf{p}}{a^3} = -\mathbf{E}_0. \quad (3.94)$$

Now let us fix the dipole moment \mathbf{p} while letting $a \rightarrow 0$. The region $r < a$ shrinks, while the electric field inside gets bigger. As the region shrinks to zero, the field strength at the origin diverges. The integral of the field over the spherical domain $r < a$ is, however, a constant and is equal to

$$\int \mathbf{E} d^3r = -\frac{1}{4\pi\epsilon_0} \frac{\mathbf{p}}{a^3} \int_0^a r^2 dr \int d\Omega = -\frac{\mathbf{p}}{3\epsilon_0}. \quad (3.95)$$

Consequently, in the limit of vanishing a , this field may be represented by a delta function,

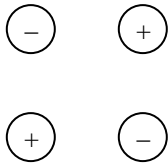
$$\mathbf{E} = -\frac{\mathbf{p}}{3\epsilon_0} \delta^3(\mathbf{r}). \quad (3.96)$$

Thus, the total field of a point dipole of moment \mathbf{p} is thus the dipolar field given by eq.(3.88) for $r > 0$ plus a delta-function piece at the origin,

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{3\mathbf{r}(\mathbf{p} \cdot \mathbf{r}) - r^2\mathbf{p}}{r^5} - \frac{\mathbf{p}}{3\epsilon_0} \delta^3(\mathbf{r}), \quad (3.97)$$

Our derivation of this result is not completely general since it is based on the limiting form of the solution to one particular problem involving a sphere; the result is, however, quite correct for any point dipole.

In a similar fashion the potential term involving the quadrupole moment may be interpreted as due to an assembly of four charges (hence the name):



It is easy to see that the monopole and the dipole moments are zero and the first non-zero contribution is given by the quadrupole moment. Note that the dipole moment is always zero if the charge density has space inversion symmetry, i.e. $\rho(\mathbf{r}) = \rho(-\mathbf{r})$, as follows from Eq. (3.82). If the charge and the dipole moment are zero the quadrupole moment does not depend on choice of coordinate system.

Higher-order moments (octapole, hexadecapole, etc.) may be generated in a similar way.

Energy of the Charge Distribution

Now we consider the energy of a localized charge distribution $\rho(\mathbf{r})$ in an external applied electric field which may be described through its potential $\Phi(\mathbf{r})$. This energy is given by

$$U = \int \rho(\mathbf{r})\Phi(\mathbf{r})d^3r . \quad (3.98)$$

Notice that there is no factor of $1/2$ which has entered the expression for the electrostatic energy of charge distribution. The reason is that we are finding the interaction energy of a charge distribution with a field which is not produced by the same charge distribution and so we must ignore the self-field and hence double counting.

We assume that the potential changes slowly over the region where the charge density is appreciable, then we can expand the potential $\Phi(\mathbf{r})$ around the origin of coordinates using a Taylor series:

$$\Phi(\mathbf{r}) = \Phi(0) + \nabla\Phi(\mathbf{r})\Big|_{\mathbf{r}=0} \cdot \mathbf{r} + \frac{1}{2} \sum_{ij} x_i x_j \frac{\partial^2\Phi(\mathbf{r})}{\partial x_i \partial x_j} \Big|_{\mathbf{r}=0} + \dots , \quad (3.99)$$

where x_i are Cartesian components of vectors \mathbf{r} . It is convenient to rewrite this expression in terms of external electric field $\mathbf{E}(\mathbf{r})$:

$$\Phi(\mathbf{r}) = \Phi(0) - \mathbf{E}(0) \cdot \mathbf{r} - \frac{1}{2} \sum_{ij} x_i x_j \frac{\partial E_j(\mathbf{r})}{\partial x_i} \Big|_{\mathbf{r}=0} + \dots \quad (3.100)$$

Since the electric field is produced by source charges located away from the region of consideration, the divergence of \mathbf{E} must be zero in this region. Therefore, we can add a term proportional to $\nabla \cdot \mathbf{E}(\mathbf{r})$ to the potential without changing the result for the integral in Eq.(3.98). We choose this to be

$$0 = \frac{1}{6} r^2 \nabla \cdot \mathbf{E}(\mathbf{r})\Big|_{\mathbf{r}=0} = \frac{1}{6} \sum_{ij} r^2 \delta_{ij} \frac{\partial E_j(\mathbf{r})}{\partial x_i} \Big|_{\mathbf{r}=0} . \quad (3.101)$$

Hence we have

$$\Phi(\mathbf{r}) = \Phi(0) - \mathbf{E}(0) \cdot \mathbf{r} - \frac{1}{6} \sum_{ij} (3x_i x_j - r^2 \delta_{ij}) \frac{\partial E_j(\mathbf{r})}{\partial x_i} \Big|_{\mathbf{r}=0} + \dots \quad (3.102)$$

If we substitute this expansion to the expression for the energy we find:

$$U = \left[\int \rho(\mathbf{r})d^3r \right] \Phi(0) - \left[\int \rho(\mathbf{r})\mathbf{r}d^3r \right] \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left[\int (3x_i x_j - r^2 \delta_{ij}) \rho(\mathbf{r})d^3r \right] \frac{\partial E_j(\mathbf{r})}{\partial x_i} \Big|_{\mathbf{r}=0} = \\ q\Phi(0) - \mathbf{p} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} Q_{ij} \frac{\partial E_j(\mathbf{r})}{\partial x_i} \Big|_{\mathbf{r}=0} + \dots \quad (3.103)$$

This expansion shows the characteristic way in which various multipole moments interacts with an external field – the charge with the potential, the dipole with the electric field, the quadrupole with the field gradient, and so on...

Example 1: Dipole Energies

As an example making use of this result, suppose that we have a dipole of moment \mathbf{p}_1 at point \mathbf{r}_1 in the presence of a second dipole of moment \mathbf{p}_2 at \mathbf{r}_2 . Then the energy of interaction is

$$U = -\mathbf{p}_1 \cdot \mathbf{E}_2(\mathbf{r}_1) = -\frac{1}{4\pi\epsilon_0} \frac{3(\mathbf{p}_1 \cdot \mathbf{r})(\mathbf{p}_2 \cdot \mathbf{r}) - r^2 \mathbf{p}_1 \cdot \mathbf{p}_2}{r^5} = \frac{1}{4\pi\epsilon_0} \frac{-3(\mathbf{p}_1 \cdot \mathbf{n})(\mathbf{p}_2 \cdot \mathbf{n}) + \mathbf{p}_1 \cdot \mathbf{p}_2}{r^3}, \quad (3.104)$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{n} = (\mathbf{r}_1 - \mathbf{r}_2)/|\mathbf{r}_1 - \mathbf{r}_2|$ is a unit vector pointing from the second dipole to the first one (or vice versa).

Example 2: Quadrupole Energies

A second example is the coupling of a nucleus' electric quadrupole moment to an external field produced by the electronic shell. This coupling lifts the degeneracy of an angular momentum eigenstate $|J, M\rangle$.

By choosing the origin in an appropriate fashion, one can guarantee that any nucleus (any object with a non-zero net charge, in fact) has no dipole moment. Hence the first non-vanishing term in the nucleus' interaction with an external field is the electric quadrupole interaction. Note that here we do not consider a monopole interaction which gives a constant energy shift of the energy levels.

Further, a nucleus in an angular momentum eigenstate $|J, M\rangle$ will have a charge density that is invariant under rotation around the z -axis. This leads to a diagonal electric quadrupole moment tensor. The axial symmetry also implies that $Q_{xx} = Q_{yy}$. Since the trace of the quadrupole tensor is zero, this means that $Q_{xx} = Q_{yy} = -Q_{zz}/2$. Therefore, the interaction of the nuclear quadrupole with the applied field is

$$U = -\frac{1}{6} \sum_{ij} Q_{ij} \left. \frac{\partial E_j(\mathbf{r})}{\partial x_i} \right|_{\mathbf{r}=0} = \frac{Q_{zz}}{12} \left(\left. \frac{\partial E_x}{\partial x} \right|_{\mathbf{r}=0} + \left. \frac{\partial E_y}{\partial y} \right|_{\mathbf{r}=0} - 2 \left. \frac{\partial E_z}{\partial z} \right|_{\mathbf{r}=0} \right). \quad (3.105)$$

Taking into account that the electric field is produced by charges outside the region of consideration so that the divergence of this field is zero it is easy to see that

$$U = -\frac{Q_{zz}}{4} \left. \frac{\partial E_z}{\partial z} \right|_{\mathbf{r}=0}. \quad (3.106)$$

The moment Q_{zz} is a function of the internal state of the nucleus and in particular of its angular momentum projection M . Thus, the quadrupole coupling provides a way to lift the degeneracy associated with the different quantum numbers M for the z -component of angular momentum.