Multipole Expansion

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(Scanned class notes – S. F. Hassan)

Multipole Expansion

We will first treat the problem of multipole expansion in full generality and then explain how to make sense of this expansion physically.

Consider a localized charge distribution $\rho(\vec{x}')$ and the potential $\Phi(x)$ outside it. Since $\nabla^2\Phi = 0$, it has an expansion,

$$\Phi(\vec{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} B_{lm} \frac{Y_{lm}(\theta, \phi)}{r^{l+1}}$$

The A_{lm} terms vanish by the requirement that $\Phi(x)$ does not blow up at infinity. So far we have studied methods that allow us to determine B_{ml} in terms of boundary conditions on some surface. The multipole expansion, on the other hand, determines B_{lm} in terms of the charge distribution $\rho(\vec{x}')$. This can be very easily worked out.

Since the charge distribution is localized, the potential $\Phi(x)$ is given by the generalized Coulomb law,

$$\Phi(\vec{x}) = \int_V \frac{\rho(\vec{x}')}{|\vec{x} - \vec{x}'|} d^3x' .$$

Using the expansion of $\frac{1}{|\vec{x}-\vec{x}'|}$ in terms of spherical harmonics, for $|\vec{x}|>|\vec{x}'|$,

$$\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r'^{l}}{r^{l+1}} Y^{*}_{lm}(\theta',\phi') Y_{lm}(\theta,\phi)$$

one obtains,

$$\boxed{\Phi(\vec{x}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{4\pi}{2l+1} q_{lm} \frac{Y_{lm}(\theta,\phi)}{r^{l+1}}}$$

with

$$\boxed{q_{lm} = \int_V d^3x' \, \rho(r',\theta',\phi') r'^{l} Y^{*}_{lm}(\theta',\phi')}$$

$$\left(\int d^3x' = \int r'^2 dr' \sin\theta' d\theta' d\phi' \right)$$

This is the multipole expansion for $\Phi(\vec{x})$ and q_{lm} are multipole moments of the charge distribution $\rho(\vec{x}')$ in polar coordinates. As such, this expression is equivalent to the generalized coulomb's law. However it is more useful beause very ~~often~~ often, at large distances, charge distributions are characterized by few dominant multipole moments and the remaining terms in the series can be neglected, or treated as corrections. Bellow, we explain the physical meaning of this expansion.

Let us first consider multipoles made up of discrete charges in cartesian coordinates.

Monopole Fields :

A monopole is a point charge q at some point $\vec{x}'$. We know that this is associated with fields

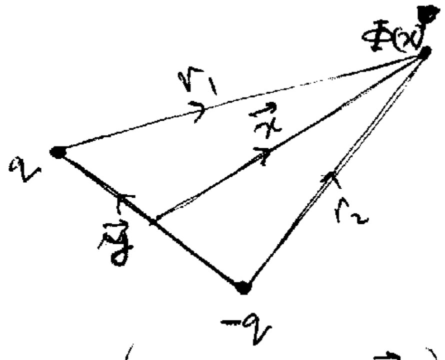
$$\Phi(\vec{x}) = \frac{q}{|\vec{x}-\vec{x}'|} \quad , \qquad \vec{E}(\vec{x}) = \frac{q(\vec{x}-\vec{x}')}{|\vec{x}-\vec{x}'|^3}$$

The "moment" of a monopole is simply its charge q.

Dipole Fields :

Consider charges q and $-q$, a distance $\vec{y}$ apart, and define $\vec{p} = q\vec{y}$. Usually, this system is called a dipole. However, we will define an idealized dipole in terms of this system but not as this system itself (as we will see, for finite y this system does not have a pure dipole moment)

Let us evaluate the potential at $\vec{x}$ for $|\vec{x}| \gg |\vec{y}|$:



$$\Phi(\vec{x}) = \frac{q}{|\vec{r}_1|} - \frac{q}{|\vec{r}_2|} \quad ,$$

$$\left(\begin{aligned} \vec{r}_1 &= \vec{x} - \frac{\vec{y}}{2} \\ \vec{r}_2 &= \vec{x} + \frac{\vec{y}}{2} \end{aligned} \right)$$

$$|\vec{r}_1|^{-1} = \left|\vec{x} - \frac{\vec{y}}{2}\right|^{-1} = x^{-1}\left(1 - \frac{y^2}{4x^2} - \frac{\vec{x}\cdot\vec{y}}{x^2}\right)^{-1/2}$$

$$\Phi(\vec{x}) = \frac{q}{x}\left[\left(1+\frac{y^2}{4x^2}-\frac{\vec{x}\cdot\vec{y}}{x^2}\right)^{-1/2} - \quad (\vec{y}\to-\vec{y})\right]$$

$$= \frac{q}{x}\left[\left(\cancel{1}-\cancel{\frac{y^2}{8x^2}}+\frac{\vec{x}\cdot\vec{y}}{2x^2}+\cdots\right)-\left(\cancel{1}-\cancel{\frac{y^2}{8x^2}}-\frac{\vec{x}\cdot\vec{y}}{2x^2}+\cdots\right)\right]$$

$$= \frac{q\vec{y}\cdot\vec{x}}{x^3} + \cdots$$

In the limit $\frac{\vec{y}}{\vec{x}} \to 0$,

$$\boxed{\Phi(\vec{x}) = \frac{\vec{p}\cdot\vec{x}}{x^3}}$$

The limit in which this expression holds can also be defined independent of $\vec{x}$ as,

$$\boxed{y \to 0 \quad , \quad p = qy = \text{fixed.}}$$

(All higher terms vanish since they contain powers of y and not qy). We define this system as an ideal dipole of moment $\vec{p}$. Hence, in the same way that an ideal charge is a point charge q at some $\vec{x}'$, an ideal dipole also is a dipole moment $\vec{p}$ localized at some $\vec{x}'$ (at one point).

(Problem: show that for finite y, Φ is not a pure dipole potential by computing the next order term.)

It should be emphasized that for finite y, the system does have a dipole moment $\vec{p}=q\vec{y}$, though it is not all that is there.

The electric field can be worked out from Φ as

$$\vec{E} = -\vec{\nabla}\Phi = -p_i\,\vec{\nabla}\left(\frac{x^i}{x^3}\right)$$

For $\vec{x} \neq 0$, $\quad \vec{\nabla}(x^i) = \frac{\partial x^i}{\partial x^j}\,\hat{1}_j\,, \quad \vec{\nabla}\left(\frac{1}{x^3}\right) = \frac{-3\vec{x}}{x^5}$

$$\Rightarrow \boxed{\vec{E} = \frac{3(\vec{p}\cdot\vec{x})\,\vec{x}}{x^5} - \frac{\vec{p}}{x^3} \equiv \frac{3(\hat{n}\cdot\vec{p})\,\hat{n} - \vec{p}}{x^3}}$$

$$\left(\hat{n} = \frac{\vec{x}}{|x|}\right)$$

At $\vec{x} = 0$, there is a further contribution similar to the one in $\nabla^2\left(\frac{1}{x}\right) = -\nabla\cdot\left(\frac{\vec{x}}{x^3}\right)$ [Note the similarity between the two expressions]. Due to the similarities, the proof there can be adapted to the present problem, although now it is somewhat more involved. The outcome is (after shifting the origin to some $\vec{x}_0$):

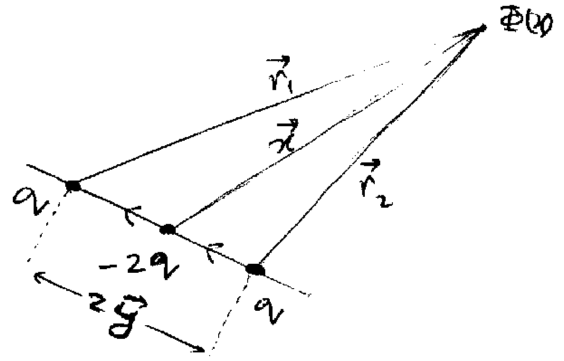
$$\boxed{\vec{E}(\vec{x}) = \frac{3(\hat{n}\cdot\vec{p})\,\hat{n} - \vec{p}}{|\vec{x} - \vec{x}_0|^3} - \frac{4\pi}{3}\,\vec{p}\,\delta(\vec{x} - \vec{x}_0)}$$

In writing this expression it is assumed that at $\vec{x} = \vec{x}_0$ only the second term contributes.

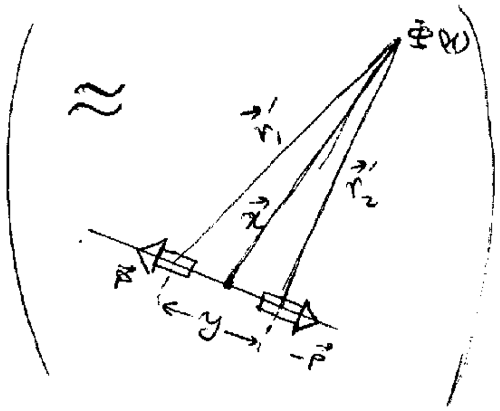
(__Problem__ : Evaluate the extra term.)

Quadrupole Fields

Now consider two equal charges of strength q a distance $2\vec{y}$ apart and a charge $-2q$ placed at the centre of the line joining the two. We will define an ideal quadrupole in terms of this system, which will also capture its leading behaviour (the system can also be approximated by two opposite dipoles of strength $\pm\vec{p} = \pm q\vec{y}$ a distance $\vec{y}$ appart)



Evaluate the potential at $\vec{x}$ for $|\vec{x}| >> |\vec{y}|$:



$$\Phi(x) = \frac{q}{|\vec{r}_1|} + \frac{q}{|\vec{r}_2|} - \frac{2q}{|\vec{x}|}$$

$$= \frac{q}{|\vec{x}-\vec{y}|} + \frac{q}{|\vec{x}+\vec{y}|} - \frac{2q}{|\vec{x}|}$$

$$= \frac{q}{x}\left[\left(1 + \frac{y^2}{x^2} - \frac{2\vec{x}\cdot\vec{y}}{x^2}\right)^{-1/2} + \left(y \to -y \right)^{-1/2} - 2 \right]$$

$$= \frac{q}{x}\left[\left(1 - \frac{1}{2}\left(\frac{y^2}{x^2} - \frac{2\vec{x}\cdot\vec{y}}{x^2}\right) + \frac{1}{2}\frac{1}{2}\frac{3}{2}\left(\frac{y^2}{x^2} - \frac{2\vec{x}\cdot\vec{y}}{x^2}\right)^2 - \cdots\right) + \left(y \to -y \right) - 2 \right]$$

$$\Phi(\vec{x}) = \Big[\Big(1 - \frac{1}{2}\frac{y^2}{x^2} + \cancel{\frac{\vec{x}\cdot\vec{y}}{x^2}} + \frac{3}{8}\frac{y^4}{x^4} + \frac{3}{2}\frac{(\vec{x}\cdot\vec{y})^2}{x^4} \cancel{+\frac{3}{2}}$$

$$- \frac{3}{2}\cancel{\frac{y^2(\vec{x}\cdot\vec{y})}{x^4}} + \cdots\Big) + (y \to -y) - 2\Big]\frac{q}{x}.$$

$$= \frac{q}{x}\Big[\cancel{2} - \frac{y^2}{x^2} + \underbrace{\cancel{\frac{3}{4}\frac{y^4}{x^4}}}_{\sim\frac{1}{x^4}} + 3\frac{(\vec{x}\cdot\vec{y})^2}{x^4} + \cdots - \cancel{2}\Big]$$

$$= \frac{q}{x^5}\left(3(\vec{y}\cdot\vec{x})^2 - y^2x^2\right) = q\left(3y_iy_j - y^2\delta_{ij}\right)\frac{x^ix^j}{x^5}$$

$$+ \cdots$$

$\therefore$

$$\boxed{\Phi(\vec{x}) = Q_{ij}\,\frac{x^ix^j}{x^5}, \qquad Q_{ij} = q\left(3y_iy_j - y^2\delta_{ij}\right)}$$

$(i, j = 1, 2, 3)$

This expression is exact in the limit $y_i \to 0$, $q\,y_i\,y_j$ = fixed, for any value of $\vec{x}$. It then defines an ideal quadrupole of moment Q_{ij} placed at $\vec{x} = 0$. Q is traceless.

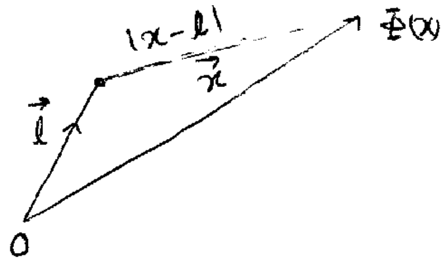
For finite $\vec{y}$, this is the leading contribution to the potential at $|\vec{x}| >> |\vec{y}|$.

In analogy with this, one can define higher ideal multipoles localized at a point. Obviously, in nature there are no ideal multipoles and multipole moments are always associated with charge distributions (like $\vec{p} = q\vec{y}$ for finite $\vec{y}$).

To appreciate the usefulness of the notion of idealized multipoles, we look at the multipole expansion of the potential due to a point charge placed off center.

Multipole Expansion for a Point Charge in Rectangular Coordinates :

Consider a point charge q located off-center at some position $\vec{l}$. The potential at some point $\vec{x}$ $|\vec{x}| \gg |\vec{l}|$ can be expanded about the center as,



$$\Phi(x) = \frac{q}{|\vec{x}-\vec{l}|}$$

$$= \frac{q}{x}\left(1 + \frac{l^2}{x^2} - \frac{2\vec{l}\cdot\vec{x}}{x^2}\right)^{-1/2}$$

$$= \frac{q}{x}\left(1 - \frac{1}{2}\left(\frac{l^2}{x^2} - \frac{2\vec{l}\cdot\vec{x}}{x^2}\right) + \frac{3}{8}\left(\frac{l^2}{x^2} - \frac{2\vec{l}\cdot\vec{x}}{x^2}\right)^2 \cdots\right)$$

$$= \frac{q}{x}\left[1 + \frac{\vec{l}\cdot\vec{x}}{x^2} + \frac{1}{2}\frac{1}{x^4}\left(3(\vec{l}\cdot\vec{x})^2 - l^2x^2\right) + \cdots\right]$$

$$= \frac{q}{x} + \frac{q\vec{l}\cdot\vec{x}}{x^3} + \frac{1}{2}\frac{x^i x^j}{x^5}\, q(3l_il_j - l^2\delta_{ij})$$

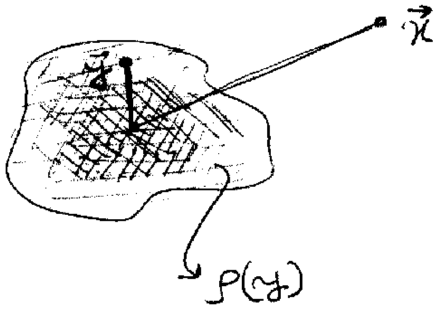
$$\therefore \quad \boxed{\Phi(\vec{x}) = \frac{q}{x} + \frac{\vec{p}\cdot\vec{x}}{x^3} + \frac{1}{2}\sum_{i,j} Q_{ij}\frac{x^i x^j}{x^5} + \cdots}$$

$\vec{p} = q\vec{l}$, $\quad Q_{ij} = q(3l_il_j - l^2\delta_{ij})$, ...

This means that the potential at $\vec{x}$ due to a point charge at $\vec{l}$ can be regarded as arising due to an infinite series of ideal multipoles of moments q, $\vec{p}$, $\frac{1}{2}Q_{ij}$, ... all placed at the center. The moments are given in terms of q and its location $\vec{l}$. Note that it is important to treat the multipoles at the center as ideal. For example, if the dipole at the center is really associated with an extension l, then its potential will have contribution beyond $\vec{p}\cdot\vec{x}/x^3$ which will be of the same order as the higher idealized multipole contributions.

Multipole Expansion for a Continuous Charge Distribution in Rectangular Coordinates:

For a continuous charge distribution the potential at $\vec{x}$ can again be expanded as above,



$$\Phi(\vec{x}) = \int d^3y \; \frac{\rho(\vec{y})}{|\vec{x}-\vec{y}|}$$

$$= \int d^3y \; \frac{\rho(\vec{y})}{x} \left(1 + \frac{y^2}{x^2} - \frac{2\vec{x}\cdot\vec{y}}{x^2}\right)^{-1/2}$$

$$= \int d^3y \; \frac{\rho(\vec{y})}{x} \left(1 + \frac{\vec{y}\cdot\vec{x}}{x^2} + \frac{1}{2}q\left(y_i y_j - y^2\delta_{ij}\right)\frac{x^i x^j}{x^4} + \cdots\right)$$

In analogy with a point charge we can also define multipole moments associated with a charge distribution:

$$\Phi(x) = \frac{1}{x}\underbrace{\int d^3y\, \rho(\vec{y})}_{q} + \frac{\vec{x}}{x^3}\cdot\underbrace{\int d^3y\, \rho(\vec{y})\,\vec{y}}_{\vec{p}}$$

$$+ \frac{1}{2}\frac{x^i x^j}{x^5}\underbrace{\int d^3y\, \rho(\vec{y})\left(3y_i y_j - y^2\delta_{ij}\right)}_{Q_{ij}}$$

$$+ \cdots$$

$$= \frac{q}{x} + \frac{\vec{p}\cdot\vec{x}}{x^3} + \frac{1}{2}\sum_{ij} Q_{ij}\,\frac{x^i x^j}{x^5} + \cdots$$

Thus a continuous charge distribution is also characterized by its multipole moments,

$$q = \int d^3y\, \rho(\vec{y}), \quad \vec{p} = \int d^3y\, \rho(y)\,\vec{y},$$

$$Q_{ij} = \int d^3y\, \rho(y)\left(3y_i y_j - y^2\delta_{ij}\right), \ \ldots$$

The monopole moment is the total charge. A ~~uniform~~ spherically symmetric charge distribution only has a monopole moment. Thus higher moments measure deviations from sphericity. For example, the quadrupole moment is used to study the shape of ~~natu~~ nuclei and hence the nature of the nuclear force.

Multipole Moments in Rectangular and Spherical-Polar Coordinates :

It becomes more and more cumbersom to write higher multipole moments in rectangular coordinates. However, as we have seen, it is possible to write a general expression for moments of any order in spherical coordinates. In fact, we found that

$$\Phi(\vec{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} q_{lm} \frac{Y_{lm}(\theta,\phi)}{r^{l+1}},$$

where,

$$q_{lm} = \int d^3y' \rho(r',\theta',\phi') r'^{l} Y^*_{lm}(\theta',\phi')$$

are the multipole moments in spherical coordinates. By comparing the powers of r in the two coordinate systems one can see that $l=0$ corresponds to the monopole moment, $l=1$ to dipole moment and $l=2$ to quadrupole moment. More explicitly, for example,

$$\frac{1}{2} Q_{ij} \frac{x^i x^j}{x^5} = \frac{1}{2}\int d^3y' \rho(y',\theta',\phi')\left(3y_i' y_j' - \delta_{ij} y'^2\right)\frac{x^i x^j}{x^5}$$

$$= \int d^3y' \rho(y',\theta',\phi')\left(\frac{3\cos^2\gamma - 1}{2}\right) y'^2 x^2/x^5$$

$$= \int d^3y' \rho(y',\theta',\phi') P_2(\cos\gamma) y'^2/x^3$$

$$= \frac{4\pi}{2(2)+1}\int d^3y' \rho(y',\theta',\phi') \sum_{m=-2}^{2} Y^*_{2m}(\theta',\phi') Y_{2m}(\theta,\phi) y'^2/x^3$$

$$\frac{1}{2} Q_{ij} \frac{x^i x^j}{x^5} = \frac{4\pi}{2(2)+1} \sum_{m=-2}^{2} \underbrace{\left[\int d^3y' \, \rho(y', \theta', \varphi') \, y'^2 \, Y^*_{2m}(\theta', \varphi') \right]}_{q_{2m}} \frac{Y_{2m}(\theta, \varphi)}{x^3}$$

$$= \frac{4\pi}{2(2)+1} \sum_{m=-2}^{2} q_{2m} \frac{Y_{2m}(\theta, \varphi)}{x^3}$$

The explicit relationship between the components of Q_{ij} and q_{2m} can be written down by using the explicit form of $Y_{2m}(\theta, \varphi)$.

For the dipole part,

$$\frac{p \cdot x}{x^3} = \frac{px}{x^3} P_1(\cos\gamma) = \frac{p}{x^2}\left(\frac{4\pi}{2+1}\right) \sum_{m=-1}^{1} Y^*_{1m}(\theta', \varphi') Y_{1m}(\theta, \varphi)$$

$$= \frac{4\pi}{2+1} \sum_{m=-1}^{1} \left[p \, Y^*_{1m}(\theta', \varphi') \right] \frac{Y_{1m}(\theta, \varphi)}{r^2}$$

$$\Rightarrow \quad q_{1m} = p \, Y^*_{1m}(\theta', \varphi')$$

$q_{10} =$

$q_{11} =$

Multipole Expansion of the Energy of a charge Distribution in an External Field.

Consider a localized charge distribution $\rho(\vec{x})$ in an external potential $\Phi(\vec{x})$. The system has electrostatic energy,

$$W = \int d^3x \; \rho(\vec{x}) \; \Phi(\vec{x}).$$

If $\Phi(x)$ varies slowly over the charge distribution then we can expand it around a suitably chosen origin,

$$\Phi(\vec{x}) = \Phi(0) + \vec{x}.\vec{\nabla}\Phi(0) + \frac{1}{2}\sum_{i,j} x_i x_j \frac{\partial^2 \Phi(0)}{\partial x_i \partial x_j} \cdots$$

$$= \Phi(0) - \vec{x}.\vec{E}(0) - \frac{1}{2}\sum_{i,j} x_i x_j \frac{\partial}{\partial x^i} E^j(0) + \cdots$$

$$= \Phi(0) - \vec{x}.\vec{E}(0) - \frac{1}{6}\sum_{i,j}\left(3x_i x_j - \delta_{ij}x^2\right)\partial_i E^j(0) + \cdots$$

$$(\text{since } \nabla\cdot E = 0)$$

Then, for the energy W one gets,

$$\boxed{W = q\,\Phi(0) - \vec{P}.\vec{E}(0) - \frac{1}{6}\sum_{i,j} Q_{ij}\frac{\partial E_j}{\partial x^i}(0) + \cdots}$$

This shows the characteristic way in which various multipoles interact with the external field.