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MULTIPOLE EXPANSION

The potential of an arbitrary charge distribution of finite extent at a large distance can always be expressed as the sum of multiple potentials where the coefficients are certain integrals (moments) of charge distribution.

Let us choose the origin of coordinates in or near the charge distribution. Let $\vec{R}(x_\alpha)$ be the position vector of point 'P' (field point) with respect to 'O'. [Note that, components of $\vec{R}$ be x_α(where α=1, 2, 3)]

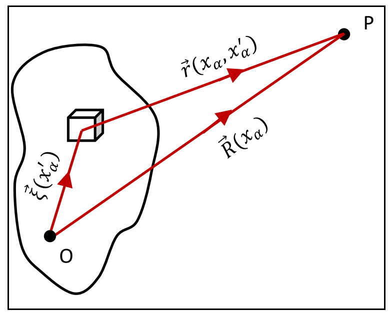
The position vector of source point w.r.t is $\vec{\xi}(x'_\alpha)$, [where components of $\vec{\xi}$ be x'_α (where α=1, 2, 3)]. Now the position vector of field point w.r.t source point be $\vec{r}$. [Where components $\vec{r}$ be $x_\alpha - x'_\alpha$, as $\vec{r} = \vec{R} - \vec{\xi}$]

Now potential at 'P' due to charge distribution is, $\phi_P = \frac{1}{4\pi\epsilon_0}\iiint \frac{\rho(x'_\alpha)}{r(x_\alpha, x'_\alpha)}dV'$

Now if 'a' be limiting dimension of the bounded charge distribution region then we assume $\frac{a}{R} \ll 1$, then we can expand $\frac{1}{r}$ in powers of x'_α about O by Taylor's theorem-

$$\frac{1}{r} = \frac{1}{r} + \sum x'_\alpha\left[\frac{\partial}{\partial x'_\alpha}\left(\frac{1}{r}\right)\right]_{r=R} + \frac{1}{2!}\sum x'_\alpha x'_\beta\left[\frac{\partial^2}{\partial x'_\alpha \partial x'_\beta}\left(\frac{1}{r}\right)\right]_{r=R} + \cdots$$

Now again as, the components of $\vec{r}$ be $x_\alpha - x'_\alpha$ then, $|\vec{r}| = \sqrt{(x_\alpha - x'_\alpha)^2}$ where α=1, 2, 3. Then, $\frac{\partial}{\partial x'_\alpha}f(r) = -\frac{\partial}{\partial x_\alpha}f(r)$.



Then, $\frac{1}{r} = \frac{1}{R} - \sum x'_\alpha\left[\frac{\partial}{\partial x_\alpha}\left(\frac{1}{r}\right)\right]_{r=R} + \frac{1}{2!}\sum x'_\alpha x'_\beta\left[\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{r}\right)\right]_{r=R} + \cdots$

Then, $\phi_P = \frac{1}{4\pi\epsilon_0}\left\{\frac{1}{R}\iiint \rho dV' - \sum\left[\frac{\partial}{\partial x_\alpha}\left(\frac{1}{r}\right)\right]_{r=R}\iiint x'_\alpha \rho dV' + \frac{1}{2!}\sum_{\alpha,\beta}\left[\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{r}\right)\right]_{r=R}\iiint x'_\alpha x'_\beta \rho dV' - \cdots\right\}$

The first term is just the potential that would result if total charge $q = \iiint \rho dV'$ where located at the origin.

The second term is the potential due a dipole of α-component of dipole moment $P_\alpha = \iiint x'_\alpha \rho dV'$.

The third term is the potential due a quadrupole having α-component of quadrupole having α-component of quadrupole moment as $\iiint x'_\alpha x'_\beta \rho dV'$ and so on.

Then $\phi_P = \phi^{2^0} + \phi^{2^1} + \phi^{2^2} + \phi^{2^3} + \cdots + \phi^{2^n} + \cdots$ where general term ϕ^{2^n} is called 2^n multipole potential.

Monopole Term: As total charge $q = \iiint \rho dV'$ then monopole potential, $\phi^{2^0} = \frac{q}{4\pi\epsilon_0 R}$, then monopole potential can be used to calculate the monopole electric field $\vec{E}^{2^0} = -\vec{\nabla}\phi^{2^0} = -\frac{q}{4\pi\epsilon_0}\vec{\nabla}\left(\frac{1}{R}\right) = \frac{q\vec{R}}{4\pi\epsilon_0 R^3}$ [As $\vec{\nabla}\left(\frac{1}{R}\right) = -\frac{\vec{R}}{R^3}$]

Dipole Term: $\phi^{2^1} = -\frac{1}{4\pi\epsilon_0}\sum\left[\frac{\partial}{\partial x'_\alpha}\left(\frac{1}{r}\right)\right]_{r=R}\iiint x'_\alpha \rho dV'$. If we choose $P_\alpha = \iiint x'_\alpha \rho dV'$ as α-component of dipole moment then,

$$\phi^{2^1} = -\frac{1}{4\pi\epsilon_0}\sum\left[\frac{\partial}{\partial x_\alpha}\left(\frac{1}{R}\right)\right]P_\alpha = -\frac{1}{4\pi\epsilon_0}\vec{\nabla}\left(\frac{1}{R}\right)\cdot\vec{P} = -\frac{\vec{P}\cdot\vec{\nabla}\left(\frac{1}{R}\right)}{4\pi\epsilon_0} = \frac{\vec{P}\cdot\vec{R}}{4\pi\epsilon_0 R^3} \quad \left[\text{As } \vec{\nabla}\left(\frac{1}{R}\right) = -\frac{\vec{R}}{R^3}\right]$$

The electric field due to dipole, $\vec{E}^{2^1} = -\vec{\nabla}\phi^{2^1} = -\vec{\nabla}\left(\frac{\vec{P}\cdot\vec{R}}{4\pi\epsilon_0 R^3}\right)$

$$\therefore \vec{E}^{2^1} = -\frac{1}{4\pi\epsilon_0}\left[\frac{1}{R^3}\vec{\nabla}(\vec{P}\cdot\vec{R}) + (\vec{P}\cdot\vec{R})\vec{\nabla}\left(\frac{1}{R^3}\right)\right] = -\frac{1}{4\pi\epsilon_0}\left[\frac{\vec{P}}{R^3} - \frac{3\vec{R}}{R^5}(\vec{P}\cdot\vec{R})\right] = \frac{1}{4\pi\epsilon_0}\left[\frac{3(\vec{P}\cdot\vec{R})\vec{R}}{R^5} - \frac{\vec{P}}{R^3}\right]$$

Quadrupole Term: $\phi^{2^2} = \frac{1}{4\pi\epsilon_0}\frac{1}{2!}\sum\left[\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{r}\right)\right]_{r=R}\iiint x'_\alpha x'_\beta \rho dV' = \frac{1}{4\pi\epsilon_0}\frac{1}{2!}\sum\left[\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right)\right]\iiint x'_\alpha x'_\beta \rho dV'$……….(i)

Now as $\frac{1}{R}$ is a solution of Laplace's equation, except at $R = 0$ then for $R > 0$,

$\nabla^2\left(\frac{1}{R}\right) = 0$ i.e. $\sum\frac{\partial^2}{\partial x_\alpha'^2}\left(\frac{1}{R}\right) = 0$ as $\sum\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right)\delta_{\alpha\beta} = 0$ for $R > 0$…………..(ii)

Then also $-\frac{1}{4\pi\epsilon_0}\frac{1}{6}\iiint \rho\xi^2 dV'\sum\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right)\delta_{\alpha\beta} = 0$…………(iii) [As $-\frac{1}{4\pi\epsilon_0}\frac{1}{6}\iiint \rho\xi^2 dV'$ is a constant]

Then from equation (i) & (iii) we have, $\phi^{2^2} = \frac{1}{4\pi\epsilon_0}\frac{1}{6}\iiint \sum_{\alpha,\beta}(3x'_\alpha x'_\beta - \xi^2\delta_{\alpha\beta})\rho dV'\sum\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right)\delta_{\alpha\beta} = 0$

$\therefore \phi^{2^2} = \frac{1}{4\pi\epsilon_0}\frac{1}{6}\sum_{\alpha,\beta} Q_{\alpha,\beta}\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right)$ Where $Q_{\alpha,\beta} = \iiint(3x'_\alpha x'_\beta - \xi^2\delta_{\alpha\beta})\rho dV'$

The nine equation $Q_{\alpha,\beta}$ forms a 3×3 array, which is a tensor of rank 2. The α,β^th component of quadrupole tensor {Q} is given by,

$$\{Q\} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}$$

[Note that, it is clear that the tensor is symmetric i.e. $Q_{\alpha,\beta} = Q_{\beta,\alpha}$, then {Q}can contain at most six independent elements. There is an additional relation $\sum Q_{\alpha,\alpha} = 0$. Which reduces the no. of independent elements to 'five'.]

Show that $\sum Q_{\alpha,\alpha} = 0$.

$Q_{\alpha,\alpha} = \iiint(3x'_\alpha x'_\alpha - \xi^2\delta_{\alpha\alpha})\rho dV'$, then $\sum_\alpha Q_{\alpha,\alpha} = \iiint[3\sum_\alpha(x'_\alpha)^2 - \xi^2(\sum_\alpha \delta_{\alpha\alpha})]\rho dV'$,

Then $\sum Q_{\alpha,\alpha} = \iiint[3\xi^2 - \xi^2 3]\rho dV' = 0$ [As α-component of $\vec{\xi}$ is x'_α]

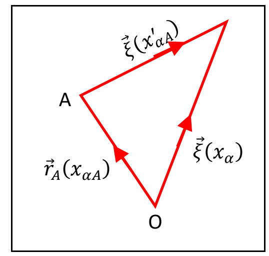
Show that $\phi^{2^2} = \frac{1}{4\pi\epsilon_0}\frac{1}{2R^5}\sum Q_{\alpha,\beta}x_\alpha x_\beta$.

$\phi^{2^2} = \frac{1}{4\pi\epsilon_0}\frac{1}{6}\sum \frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right) Q_{\alpha\beta}$ [Now $\frac{\partial}{\partial x_\beta}\left(\frac{1}{R}\right) = -\left(\frac{x_\beta}{R}\right)$ as $\vec{\nabla}\left(\frac{1}{R}\right) = -\frac{\vec{R}}{R^3}$, then, $\frac{\partial^2}{\partial x_\alpha \partial x_\beta}\left(\frac{1}{R}\right) = -\frac{\partial}{\partial x_\alpha}\left(\frac{x_\beta}{R^3}\right) = -\frac{1}{R^3}\delta_{\alpha\beta} + \frac{3x_\alpha x_\beta}{R^5}$]

$\phi^{2^2} = \frac{1}{4\pi\epsilon_0}\frac{1}{6}\sum Q_{\alpha\beta}\left[\frac{3x_\alpha x_\beta}{R^5} - \frac{\delta_{\alpha\beta}}{R^3}\right] = \frac{1}{4\pi\epsilon_0}\frac{1}{6}\left[\frac{\sum 3Q_{\alpha\beta}x_\alpha x_\beta}{R^5} - \frac{\sum Q_{\alpha\beta}\delta_{\alpha\beta}}{R^3}\right] = \frac{1}{4\pi\epsilon_0}\frac{1}{6}\left[\frac{3\sum Q_{\alpha\beta}x_\alpha x_\beta}{R^5} - \frac{\sum Q_{\alpha\alpha}}{R^3}\right] = \frac{1}{4\pi\epsilon_0}\frac{1}{2R^5}\sum Q_{\alpha,\beta}x_\alpha x_\beta$ [As $\sum Q_{\alpha\alpha} = 0$]

Note that: if the quadrupole tensor is referred to principle axis, then all the off diagonal element vanishes. As we have $\sum_\alpha Q_{\alpha\alpha} = 0$ i.e. together with vanishing of trace then number of independent elements becomes 'two'.
In many important situation the charge distribution possesses an axis of symmetry. If we can choose the x'_3-axis corresponding symmetric axis, then $Q_{11} = Q_{22}$. Hence there is only 'one' independent element of {Q} is $Q_{33} = -(Q_{11} + Q_{22}) = -2Q_{11} = -2Q_{22}$.
If x'_3-axis is symmetric axis of charge distribution in continuous, then the quadrupole moment is given by $Q = \iiint (3x'_3 - \xi^2)\rho dV'$.
Again note that if $Q_{33} = 0$ then charge distribution is spherical in shape (for +ve charges)
if $Q_{33} > 0$ then charge distribution is polate in shape (for +ve charge distribution)
if $Q_{33} < 0$ then charge distribution is oblate in shape (for +ve charge distribution)
Hence quadrupole moment of a nucleus may be a measurement of its deviation from spherical shape.
N.B. $Q_{11} = \sum\left(2{x'_k}^2 - {y'_k}^2 - {z'_k}^2\right)q_k$ $\quad Q_{22} = \sum\left(2{y'_k}^2 - {x'_k}^2 - {z'_k}^2\right)q_k$ $\quad Q_{33} = \sum\left(2{z'_k}^2 - {x'_k}^2 - {y'_k}^2\right)q_k$

$Q_{12} = \sum\left(3{x'_k}^2{y'_k}^2\right)q_k = Q_{21}$ $\quad Q_{13} = \sum\left(3{x'_k}^2{z'_k}^2\right)q_k = Q_{31}$ $\quad Q_{23} = \sum\left(3{y'_k}^2{z'_k}^2\right)q_k = Q_{32}$



Dependence of multiple moments on the choice of origin.

Suppose we consider a new coordinate system whose origin 'O'. 'A' is at a distance $\vec{r}_A$ w.r.t the origin 'O' of old coordinate system. As monopole moment $\iiint \rho dV' = qQ = total\ charge$. As total charge is independent of origin then monopole moment is independent of origin. Now dipole moment (new),
$P_A = \iiint x'_{\alpha A}\rho dV' = \iiint (x'_\alpha + x_{\alpha A})\rho dV'$ $\therefore P_A = \iiint x'_\alpha \rho dV' + x_{\alpha A}\iiint \rho dV'$ [As $x_{\alpha A} = constant$]
Then if total charge of the distribution $q = \iiint \rho dV' = 0$ then $P_A = P$ i.e. then dipole moment is independent of origin. Otherwise in general dipole moment depends upon origin.

Now for quadrupole moment $Q^A_{\alpha\beta} = \iiint\left(3x'_{\alpha A}x'_{\beta A} - \xi_A^2\delta_{\alpha\beta}\right)\rho dV' = \iiint\left\{3(x'_\alpha + x_{\alpha A})(x'_\beta + x_{\beta A}) - \left|\vec{\xi} - \vec{r}_A\right|^2\delta_{\alpha\beta}\right\}\rho dV'$

$= \iiint\left\{3x'_\alpha x'_\beta + 3x'_\alpha x_{\beta A} + 3x_{\alpha A}x'_\beta + 3x_{\alpha A}x_{\beta A} - \xi^2\delta_{\alpha\beta} - {r_A}^2\delta_{\alpha\beta} + 2\vec{\xi}\cdot\vec{r}_A\delta_{\alpha\beta}\right\}\rho dV'$

$= \iiint\left(3x'_\alpha x'_\beta - \xi^2\delta_{\alpha\beta}\right)\rho dV' + 3x_{\beta A}\iiint x'_\alpha\rho dV' + 3x_{\alpha A}\iiint x'_\beta\rho dV' + 3x_{\alpha A}x_{\beta A}\iiint \rho dV' - {r_A}^2\delta_{\alpha\beta}\iiint \rho dV' + 2\delta_{\alpha\beta}\vec{r}_A\cdot\iiint \vec{\xi}\rho dV'$

$\therefore Q^A_{\alpha\beta} = Q_{\alpha\beta} + 3x_{\beta A}P_\alpha + 3x_{\alpha A}P_\beta + 3x_{\alpha A}x_{\beta A}(q) - {r_A}^2\delta_{\alpha\beta}(q) + 2\delta_{\alpha\beta}\vec{r}_A\cdot\vec{P}$

Then if total charge and individual dipole moments are 'zero' then, $Q^A_{\alpha\beta} = Q_{\alpha\beta}$ i.e. then quadrupole moment is independent of origin. Otherwise in general quadrupole moment depends upon origin.

Note that: $\boldsymbol{\phi_P = \frac{1}{4\pi\epsilon_0}\iiint \frac{\rho dV'}{r(x_\alpha, x'_\alpha)}}$ **now** $\boldsymbol{\frac{1}{r} = \frac{1}{|\vec{R}-\vec{\xi}|} = \frac{1}{(R^2+\xi^2-2R\xi\cos\theta)^{\frac{1}{2}}} = \frac{1}{R}\frac{1}{\left(1+(\frac{\xi}{R})^2-2\frac{\xi}{R}\cos\theta\right)^{\frac{1}{2}}} = \frac{1}{R}\sum_{n=0}^{\infty}(\frac{\xi}{R})^n P_n\cos\theta}$

$\boldsymbol{\phi_P = \frac{1}{4\pi\epsilon_0}\sum_{n=0}^{\infty}\frac{1}{R^{n+1}}\iiint \xi^n P_n(\cos\theta)\rho dV' = \frac{1}{4\pi\epsilon_0}\frac{1}{R}\iiint \rho dV' + \frac{1}{4\pi\epsilon_0}\frac{1}{R^2}\iiint \xi(\cos\theta)\rho dV' + \frac{1}{4\pi\epsilon_0}\frac{1}{R^2}\iiint \xi^2\frac{1}{2}(3\cos^2\theta - 1)\rho dV' + \cdots}$

$\boldsymbol{\therefore\ \phi_P = \phi^{2^0} + \phi^{2^1} + \phi^{2^2} + \phi^{2^3} + \cdots}$

[Where $\boldsymbol{\iiint \rho dV'}$=monopole moment, $\boldsymbol{\iiint \xi(\cos\theta)\rho dV'}$=dipole moment, $\boldsymbol{\iiint \xi^2\frac{1}{2}(3\cos^2\theta - 1)\rho dV'}$=quadrupole]