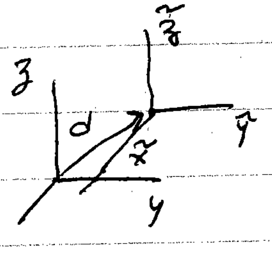
$$\vec{E} = \frac{1}{r^3}\left[\,3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}\,\right]$$ expresses $\vec{E}$ of dipole in coord free form

<u>Origin of coordinates</u>

The definition of the multipole moments <u>depends</u> on the choice of origin of the coordinates.



Suppose transform to $\tilde{\vec{r}} = \vec{r} - \vec{d}$

In the $\tilde{\vec{r}}$ coord system

$$\tilde{q} = \int d^3\tilde{r}\; \rho(\tilde{r}) = \int d^3r\; \rho(r) = q$$

monopole <u>does</u> <u>not</u> depend on choice of origin.

$$\tilde{\vec{p}} = \int d^3\tilde{r}\; \rho(\tilde{r})\,\tilde{\vec{r}} = \int d^3r\; \rho\,(\vec{r} - \vec{d})$$

$$= \int d^3r\, \rho\, \vec{r} - \vec{d}\int d^3r\, \rho$$

$$\tilde{\vec{p}} = \vec{p} - \vec{d}q$$ $\tilde{\vec{p}} = \vec{p}$ only if $q = 0$!

if $q \neq 0$, then $\tilde{\vec{p}} \neq \vec{p}$

$\Rightarrow$ ~~One coord~~ If $q \neq 0$, one could always choose an origin of coords for which $\vec{p} = 0$!

For HW you will show that $\tilde{Q} = Q$ only if both $q = 0$ and $\vec{p} = 0$

Quadupole moment in new coordinates

$$\overleftrightarrow{\tilde{Q}} = \int d^3\tilde{r}\, \rho \left[3\tilde{\vec{r}}\,\tilde{\vec{r}} - (\tilde{\vec{r}})^2 \overleftrightarrow{I} \right]$$

where $\tilde{\vec{r}} = \vec{r} - \vec{d}$

substitute in above

$$\overleftrightarrow{\tilde{Q}} = \int d^3r\, \rho \left[3(\vec{r}-\vec{d})(\vec{r}-\vec{d}) - (\vec{r}-\vec{d})^2 \overleftrightarrow{I} \right]$$

$$= \int d^3r\, \rho \left[3\vec{r}\,\vec{r} - 3\vec{r}\,\vec{d} - 3\vec{d}\,\vec{r} + 3\,\vec{d}\,\vec{d} - (r^2 + d^2 - 2\vec{r}\cdot\vec{d}) \overleftrightarrow{I} \right]$$

$$= \int d^3r\, \rho \left[3\vec{r}\,\vec{r} - r^2 \overleftrightarrow{I} \right] - 3\left[\int d^3r\, \rho\, \vec{r}\right]\vec{d} - 3\vec{d}\left[\int d^3r\, \rho\, \vec{r}\right]$$

$$+ 3\vec{d}\,\vec{d}\left[\int d^3r\, \rho\right] - d^2 \overleftrightarrow{I}\left[\int d^3r\, \rho\right]$$

$$+ 2\left[\int d^3r\, \rho\, \vec{r}\right]\cdot\vec{d}\, \overleftrightarrow{I}$$

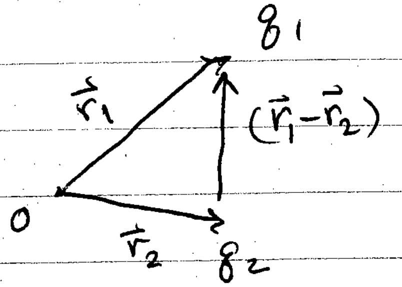
$$\overleftrightarrow{\tilde{Q}} = \overleftrightarrow{Q} - 3\vec{p}\,\vec{d} - 3\vec{d}\,\vec{p} + 3\vec{d}\,\vec{d}\,q - \left(d^2 q - 2\vec{p}\cdot\vec{d}\right)\overleftrightarrow{I}$$

we see that $\overleftrightarrow{Q}$ is independent of choice of origin only when both q and $\vec{p}$ vanish. When this happens the quadrupole term is the <u>leading</u> term in the multipole expansion.

In general, the leading term in multipole expansion will be indep of origin of coordinates.

Example two charges q_1 at $\vec{r}_1$ and q_2 at $\vec{r}_2$

$$q_1 + q_2 = q \neq 0$$



monopole $q_1 + q_2 = q$

dipole $\vec{p} = q_1 \vec{r}_1 + q_2 \vec{r}_2$

quadrupole $\overleftrightarrow{Q} = (3\vec{r}_1\vec{r}_1 - r_1^2 \overleftrightarrow{I})q_1 + (3\vec{r}_2\vec{r}_2 - r_2^2 \overleftrightarrow{I})q_2$

We can make the dipole moment vanish by shifting to a new coord system $\vec{r}\,' = \vec{r} - \vec{d}$ where $\vec{d} = \dfrac{\vec{p}}{q}$

$$\vec{r}\,' = \vec{r} - \frac{q_1\vec{r}_1 + q_2\vec{r}_2}{q_1 + q_2} = \frac{q_1(\vec{r} - \vec{r}_1) + q_2(\vec{r} - \vec{r}_2)}{q_1 + q_2}$$

positions of q_1, q_2 in new coords are

$$\vec{r}_1\,' = \frac{q_2}{q_1 + q_2}(\vec{r}_1 - \vec{r}_2)$$

$$\vec{r}_2\,' = \frac{-q_1}{q_1 + q_2}(\vec{r}_1 - \vec{r}_2)$$

lies along vector from $\vec{r}_2$ to $\vec{r}_1$

origin of new coord system is at

$$\vec{r}\,' = 0 \Rightarrow \vec{r} = \frac{q_1\vec{r}_1 + q_2\vec{r}_2}{q_1 + q_2}$$ "center of charge"

for many charges q_i at positions $\vec{r}_i$, the origin that makes dipole moment vanish is at

$$\vec{r} = \frac{\sum_i q_i \vec{r}_i}{\sum q_i}$$

In this coord system

$$\vec{p}\,' = q_1 \vec{r}_1\,' + q_2 \vec{r}_2\,' = \frac{q_1 q_2}{q_1+q_2}(\vec{r}_1 - \vec{r}_2) - \frac{q_2 q_1}{q_1+q_2}(\vec{r}_1 - \vec{r}_2)$$

$$= 0 \quad \text{as it must be!}$$

<u>Quadrupole moment</u> in the coord system in which $\vec{p}\,' = 0$ the quadrupole tensor is

$$\overleftrightarrow{Q}\,' = \left[3\vec{r}_1\,'\vec{r}_1\,' - (r_1\,')^2 \overleftrightarrow{I}\right] q_1 + \left[3\vec{r}_2\,'\vec{r}_2\,' - (r_2\,')^2 \overleftrightarrow{I}\right] q_2$$

let us choose ~~coord~~ spherical coordinates with origin at O' and $\hat{z}$ axis aligned along $\vec{r}_1 - \vec{r}_2$, so that

$$\vec{r}_1 - \vec{r}_2 = s\,\hat{z} \quad \text{where } s = |\vec{r}_1 - \vec{r}_2| \text{ is separation between the charges}$$

Then
$$\vec{r}_1\,' = \frac{q_2}{q_1+q_2} s\,\hat{z}$$
$$\vec{r}_2\,' = \frac{-q_1}{q_1+q_2} s\,\hat{z}$$

$$\overleftrightarrow{Q}\,' = \left(\frac{q_2}{q_1+q_2}\right)^2 q_1 \left[3 s^2 \hat{z}\hat{z} - s^2 \overleftrightarrow{I}\right] + \left(\frac{-q_1}{q_1+q_2}\right)^2 q_2 \left[3 s^2 \hat{z}\hat{z} - s^2 \overleftrightarrow{I}\right]$$

$$\overleftrightarrow{Q}' = \frac{q_2^2 q_1 + q_1^2 q_2}{(q_1+q_2)^2} s^2 \left[3\hat{z}\hat{z} - \overleftrightarrow{I} \right]$$

$$= \frac{q_1 q_2}{q_1+q_2} s^2 \left[3\hat{z}\hat{z} - \overleftrightarrow{I} \right]$$

$$Q'_{ij} = \frac{q_1 q_2}{q_1+q_2} s^2 \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

in xyz coord system

as $\hat{z}\hat{z} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$\overleftrightarrow{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

the contribution of quadrupole to the potential is

$$\Phi_{quad} = \frac{1}{2} \frac{\hat{r} \cdot \overleftrightarrow{Q} \cdot \hat{r}}{r^3} \qquad \hat{r} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$$

in xyz coords

with origin at O' this becomes

$$\Phi_{quad} = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1+q_2} (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$$

do matrix multiplications

$$\Phi_{quad} = \frac{s^2}{2r^3} \frac{q_1 q_2}{q_1+q_2} (2\cos^2\theta - \sin^2\theta)$$

independent of φ as it must be due to azimuthal symmetry

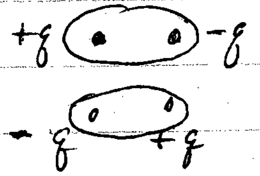
Example

sample charge config's

$\circ\ q$ $\Rightarrow$ monopole is leading term

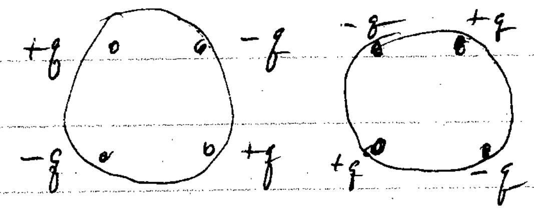
$\overset{\circ}{+q}\ \ \overset{\circ}{-q}$ $\Rightarrow$ monopole $= 0$ $\Rightarrow$ dipole is leading term

$\vec{p}$ is indep of origin



$\Rightarrow$ monopole $= 0$ $\Rightarrow$ total dipole is sum of dipoles of individual neutral pairs

$\leftarrow + \rightarrow = 0$ leading term is quadrapole



when monopole $= 0$ and dipole $= 0$, quadrapole is indep of origin.

$\rightarrow$ total quadrapole is sum of quadrapoles of individual clusters with $q = 0$ and $\vec{p} = 0$

$Q = Q_1 + Q_2$

with $Q_2 = -Q_1$

$\Rightarrow Q = 0$ leading term is <u>octopole</u>

Eigenfunction expansion for Green Functions

Suppose $\mathbb{D}$ is some linear differential operator, for example ∇^2.

Solutions to the equation

$$\mathbb{D}\,\psi(\vec{r}) = -4\pi f(\vec{r})$$

can be solved if one knows the Green function, which is the solution to the problem with a point source

$$\mathbb{D}\,G(\vec{r},\vec{r}\,') = -4\pi\,\delta(\vec{r}-\vec{r}\,')$$

$\uparrow$ operates on $\vec{r}$

Then

$$\psi(\vec{r}) = \int d^3r'\, G(\vec{r},\vec{r}\,')\, f(\vec{r}\,') \qquad \text{is solution}$$

If we need to solve for ψ subject to certain boundary conditions, then we can always add to the Green function a $\phi(\vec{r})$ such that $\mathbb{D}\phi(\vec{r}) = 0$ in the desired region and then choose ϕ accordingly as we did for Dirichlet or Neumann b.c. for ∇^2.

One way to find $G(\vec{r},\vec{r}\,')$ is to find the eigenvalues and eigenfunctions of $\mathbb{D}$.

$$\underbrace{\mathbb{D}\,\psi_n(\vec{r})}_{\text{eigenfunction}} = \underbrace{\lambda_n}_{\text{eigenvalue}}\,\psi_n(r)$$

Depending on the problem, the spectrum of eigenvalues might be discrete or might be continuous.

Note: when we solved Laplace's equation by separation of variables method, what we wound up doing was solving the eigenvalue problem for the (in spherical case) radial, θ, and φ pieces of the differential operator.

In many cases (you would have to prove this for the particular operator $\mathbb{D}$) the eigenfunctions $\psi_n(\vec{r})$ form an orthogonal and complete set of basis functions over the region of interest (ie in the volume in which we are seeking a solution)

orthogonal $\Rightarrow$ $\boxed{\int_V d^3r \; \psi_m^*(\vec{r})\,\psi_n(\vec{r}) = \delta_{m,n}}$

complete $\Rightarrow$ $f(\vec{r}) = \sum_n a_n \psi_n(\vec{r})$.

any function f can be expanded in a linear combination of the ψ_n.

The expansion coefficients a_n are obtained by

$$\int_V d^3r \; f(\vec{r})\,\psi_m^*(\vec{r}) = \sum_n a_n \int_V d^3r \; \psi_m^*(\vec{r})\,\psi_n(\vec{r}) = \sum_n a_n \delta_{m,n}$$

So $\boxed{a_m = \int_V d^3r \; f(\vec{r})\,\psi_m^*(\vec{r})}$ "Fourier" coefficient for basis ψ_n

In particular, the function $\delta(\vec{r}-\vec{r}\,')$ can be expanded as

$$\delta(\vec{r}-\vec{r}\,') = \sum_n a_n \psi_n(\vec{r})$$

where

$$a_n = \int_V d^3r \; \delta(\vec{r}-\vec{r}\,')\, \psi_n^*(\vec{r}) = \psi_n^*(\vec{r}\,') \qquad \text{assuming } \vec{r}\,' \in V$$

So we have $$\boxed{\delta(\vec{r}-\vec{r}\,') = \sum_n \psi_n^*(\vec{r}\,')\psi_n(\vec{r})}$$

Now we can solve for the Green function!

Expand $G(\vec{r},\vec{r}\,')$ as, $\underbrace{\text{a series in } \psi_n(\vec{r})}_{\text{a function of } \vec{r}, \text{ in}}$

$$G(\vec{r},\vec{r}\,') = \sum_n a_n \psi_n(\vec{r})$$

Now use

$$\mathbb{D}\, G(\vec{r},\vec{r}\,') = -4\pi\, \delta(\vec{r}-\vec{r}\,')$$

since $\mathbb{D}$ is linear

$$\hookrightarrow \sum_n a_n \mathbb{D}\psi_n(\vec{r}) = \sum_n a_n \lambda_n \psi_n(\vec{r}) = -4\pi \sum_n \psi_n^*(\vec{r}\,')\psi_n(\vec{r})$$

$$\Rightarrow \sum_n \left[a_n \lambda_n + 4\pi\, \psi_n^*(\vec{r}\,') \right] \psi_n(\vec{r}) = 0$$

If a series in a set of basis functions vanishes then each coefficient in the series must vanish

$$\Rightarrow \quad a_n = \frac{-4\pi\, \psi_n^*(\vec{r}\,')}{\lambda_n}$$

$$\boxed{G(\vec{r},\vec{r}\,') = -4\pi \sum_n \left[\frac{\psi_n^*(\vec{r}\,')\psi_n(\vec{r})}{\lambda_n} \right]}$$

Example: ∇^2 in rectangular coordinate, V = all space

$$\nabla^2 \psi(\vec{r}) = \lambda \psi(\vec{r})$$

call the eigenvalues $\lambda = -k^2$

eigen functions are then $\psi \sim e^{i\vec{k}\cdot\vec{r}}$

check $\vec{\nabla}\psi = i\vec{k}\, e^{i\vec{k}\cdot\vec{r}}$

$$\nabla^2\psi = \vec{\nabla}\cdot(\vec{\nabla}\psi) = (i\vec{k})\cdot(i\vec{k})\, e^{i\vec{k}\cdot\vec{r}} = -k^2\psi$$

normalize ψ for orthogonality condition $\boxed{\psi_k(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}}$

$$\int d^3r\, \psi^*_{k'}(\vec{r})\, \psi_k(\vec{r}) = \int d^3r \frac{1}{(2\pi)} e^{-i\vec{k}'\cdot\vec{r}} e^{i\vec{k}\cdot\vec{r}}$$

$$= \int d^3r \frac{e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}}{(2\pi)^3} = \delta(\vec{k}-\vec{k}')$$

$$\Rightarrow G(\vec{r},\vec{r}') = -4\pi \int \frac{d^2k}{(2\pi)^3} \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{(-k^2)} = \int \frac{d^3k}{(2\pi)^3} \left(\frac{4\pi}{k^2}\right) e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}$$

Now we already know that the Green function for this problem is

$$G(\vec{r},\vec{r}') = \frac{1}{|\vec{r}-\vec{r}'|}$$

So from this we see that the Fourier transf of

$\frac{1}{|\vec{r}-\vec{r}'|}$ is $\frac{4\pi}{k^2}$

Example Green's function for Dirichlet problem inside rectangular box $x \in [0, a]$, $y \in [0, b]$, $z \in [0, c]$

We are looking for eigenfunction of

$$\nabla^2 \psi = \lambda \psi$$

with $\psi = 0$ on boundaries of the rectangular box.

Solutions are.

$$\psi_{lmn} = \sqrt{\frac{8}{abc}} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{n\pi z}{c}\right)$$

with eigenvalue $\lambda_{lmn} = -\pi^2\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)$, $lmn = 1, \ldots$

check normalization for yourselves!

$$G(\vec{r}, \vec{r}') = -4\pi \sum_{lmn=1}^{\infty} \frac{8}{abc} \frac{\sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \times \sin\left(\frac{n\pi z}{c}\right) \sin\left(\frac{n\pi z'}{c}\right)}{-\pi^2\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)}$$

$$G(\vec{r}, \vec{r}') = \frac{32}{\pi abc} \sum_{lmn=1}^{\infty} \frac{\sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right) \sin\left(\frac{n\pi z}{c}\right) \sin\left(\frac{n\pi z'}{c}\right)}{\left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2}\right)}$$

Note that in this case, $G(\vec{r}, \vec{r}')$ is NOT a function of $\vec{r} - \vec{r}'$. The boundary breaks the translational invariance.