Chapter 4 – Multipole expansions + dielectrics

Next we consider:

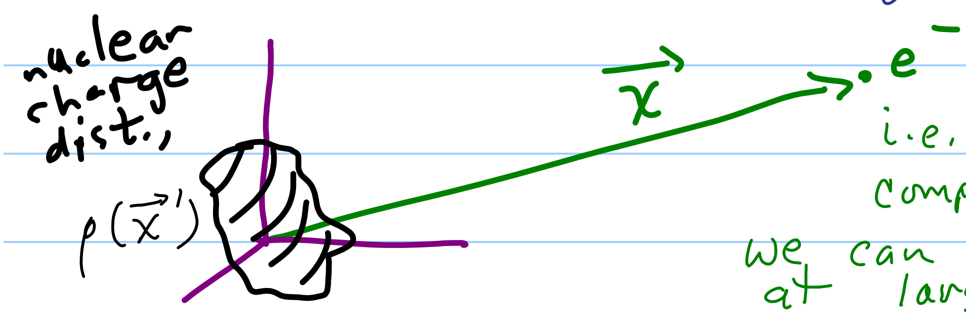
(i) Multipole expansion of $\Phi(\vec{x})$ produced by a localized $\rho(\vec{x})$

(ii) Electric fields and energy in macroscopic media, including charge rearrangement in response to an external field.

i.e. induced dipoles modify the electric field, as in $\vec{E} = \vec{E}_{ext} + \vec{E}_{induced}$

<u>Multipole expansion</u> First, our goal is to find properties like $\Phi(\vec{x})$, $\vec{E}(\vec{x})$, etc., produced by a localized $\rho(\vec{x}\,')$, e.g. when a nucleus produces a potential and then an e^- moves through it.

<u>Concept</u> Let's try to characterize effects of the charge distribution through a few parameters, = charge, electric dipole moment, electric quadrupole moment, etc.



i.e. the full $\rho(\vec{x}\,')$ could be complicated and detailed, but we can summarize its effects at large $|\vec{x}|$ more simply, For now, develop the theory for only localized charges in free space, i.e. with no boundaries:

$$\Rightarrow \quad \Phi(\vec{x}) = \frac{1}{4\pi\epsilon_0}\int d^3x' \, \frac{\rho(\vec{x}\,')}{|\vec{x}-\vec{x}\,'|}$$

or if we plug in our spherical harmonic expansion, for $r > r'$, this gives

$$\Phi(\vec{x}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{4\pi}{2l+1}\frac{1}{4\pi\epsilon_0}\left[\int d^3x' \, r'^l \, Y^*_{lm}(\hat{x}')\rho(\vec{x}\,')\right] \times \frac{1}{r^{l+1}} Y_{lm}(\hat{x})$$

or $\Phi(\vec{x}) = \frac{1}{\epsilon_0}\sum_{lm} \frac{q_{lm}}{2l+1} \frac{Y_{lm}(\hat{x})}{r^{l+1}}$

where the $q_{lm} \equiv \int d^3x' \, r'^l \, Y^*_{lm}(\hat{x}')\rho(\vec{x}\,')$ are called the multipole moments of $\rho(\vec{x}\,')$

Some basic properties

(1) Note that $q_{l,-m} = (-1)^m q^*_{lm}$, simply from the Y_{lm} properties

(2) $q_{0,0} = \frac{1}{\sqrt{4\pi}}\int \rho(\vec{x}\,')\,d^3x' = \frac{q}{\sqrt{4\pi}}$ ← electric monopole moment

where q = total charge

(3) ELECTRIC DIPOLE, $\ell=1$

$$q_{11} = -\int d^3x'\, r' \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta'\, e^{-i\phi'} \rho(\vec{x}\,')$$

It is instructive to rewrite this in terms of the "SPHERICAL UNIT VECTORS", defined as $\hat{\epsilon}_{\pm 1} = \dfrac{\mp \hat{x} - i\hat{y}}{\sqrt{2}}$, $\hat{\epsilon}_0 = \hat{z}$

which shows that the $\ell=1$ spherical harmonics are in fact just:

$$Y_{1,\mu}(\theta',\phi') = \left(\frac{3}{4\pi}\right)^{1/2} \frac{\vec{x}\,'}{r} \cdot \hat{\epsilon}_\mu$$

Quick check

does $Y_{1,1}(\theta',\phi') \stackrel{?}{=} \left(\frac{3}{4\pi}\right)^{1/2} \left(\frac{x}{r}\hat{x} + \frac{y}{r}\hat{y} + \frac{z}{r}\hat{z}\right) \cdot \left(\frac{-\hat{x} - i\hat{y}}{\sqrt{2}}\right)$

$$= -\left(\frac{3}{8\pi}\right)^{1/2} (\sin\theta\cos\phi + i\sin\theta\sin\phi)$$

$$= -\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{i\phi} \quad \checkmark \text{ it checks!}$$

Note also that the spherical unit vectors obey:

$$\hat{\epsilon}_\mu^* \cdot \hat{\epsilon}_\nu = \delta_{\mu\nu}$$

Addendum ANY vector in 3D can be written in terms of its spherical (tensor) components as follows:

$$\vec{P} = \sum_{\mu=-1}^{1} \hat{\epsilon}_\mu \left(\hat{\epsilon}_\mu^* \cdot \vec{P}\right)$$

which is formally analogous to the Hilbert Space expansion in quantum mechanics,

$$|\psi\rangle = \sum_\mu |\mu\rangle \left(\langle\mu|\psi\rangle\right)$$

Using this notation, we have

$$q_{11} = \left(\frac{3}{4\pi}\right)^{1/2} \hat{\epsilon}_{+1}^{*} \cdot \int d^3x' \,\vec{x}'\rho(\vec{x}')$$

$$= \sqrt{\frac{3}{4\pi}}\ \hat{\epsilon}_{+1}^{*} \cdot \vec{p}$$

where $\vec{p} \equiv \int d^3x' \,\vec{x}'\rho(\vec{x}')$ is the usual ELECTRIC DIPOLE MOMENT of ρ

e.g. $q_{11} = -\frac{1}{\sqrt{2}}(p_x - ip_y)\left(\frac{3}{4\pi}\right)^{1/2}$

$$q_{10} = \left(\frac{3}{4\pi}\right)^{1/2} \hat{\epsilon}_{0}^{*} \cdot \vec{p} = \left(\frac{3}{4\pi}\right)^{1/2} p_z$$

$$q_{1,-1} = \left(\frac{3}{4\pi}\right)^{1/2} \hat{\epsilon}_{-1}^{*} \cdot \vec{p} = \left(\frac{3}{4\pi}\right)^{1/2} \frac{p_x + ip_y}{\sqrt{2}}$$

(4) Electric quadrupole moment ($l=2$)

$$q_{22} = \int d^3x' \, r'^2 \, Y_{22}^{*}(\hat{x}')\rho(\vec{x}')$$

and $Y_{22}^{*} = \frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2} \sin^2\theta' \, e^{-2i\phi'}$,

which we can also rewrite in terms of Cartesian components as

$$\frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2}\left(\frac{x' - iy'}{r}\right)^2$$

or $q_{22} = \frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2} \int (x' - iy')^2 \rho(\vec{x}') \, d^3x'$

It is conventional to write this in terms of a Cartesian quadrupole moment tensor, Q, i.e.

$$q_{22} = \frac{1}{12}\left(\frac{15}{2\pi}\right)^{1/2}\left(Q_{11} - 2iQ_{12} - Q_{22}\right)$$

and similarly $q_{21} = -\left(\frac{15}{8\pi}\right)^{1/2}\int z'(x-iy')\rho(\vec{x}')\,d^3x'$

$$\equiv -\frac{1}{3}\left(\frac{15}{8\pi}\right)^{1/2}\left(Q_{13} - iQ_{23}\right)$$

and

$$q_{20} = \frac{1}{2}\left(\frac{5}{4\pi}\right)^{1/2}\int\left(3z'^2 - r'^2\right)\rho(\vec{x}')\,d^3x'$$

$$\equiv \frac{1}{2}\left(\frac{5}{4\pi}\right)^{1/2} Q_{33}$$

makes Q_{ij} traceless

where

$$Q_{ij} \equiv \int\left(3x_i x_j - r'^2\delta_{ij}\right)\rho(\vec{x}')\,d^3x'$$

called the electric quadrupole moment tensor

Then the external electric potential beyond the range of ρ can be expanded as

$$\Phi(\vec{x}) = \frac{1}{4\pi\epsilon_0}\left\{\frac{q}{r} + \frac{\vec{p}\cdot\vec{x}}{r^3} + \frac{1}{2}\sum_{ij}\frac{\overbrace{x_i Q_{ij} x_j}^{\equiv\,\vec{x}\cdot Q\,\vec{x}}}{r^5} + \ldots\right.$$

Next, let's work out the electric field of a single l,m multipole, using $\vec{E} = -\nabla\Phi$:

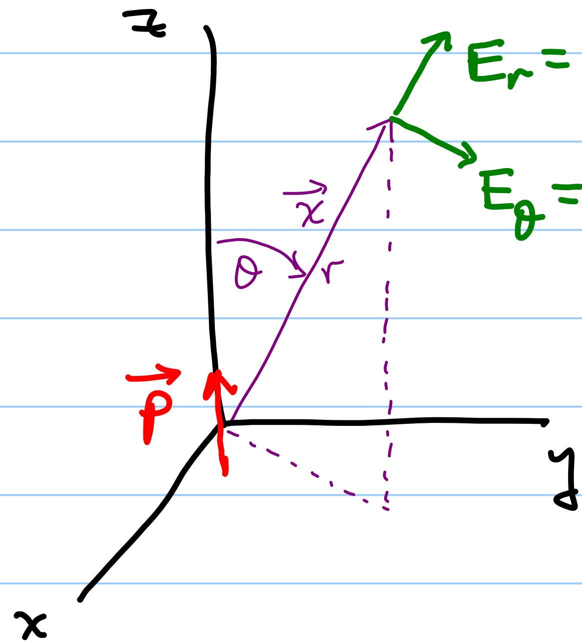
Here, use $\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial\theta} + \frac{\hat{\phi}}{r\sin\theta}\frac{\partial}{\partial\phi}$

$$\Rightarrow \boxed{E_r = \frac{q_{lm}}{\epsilon_0}\frac{l+1}{2l+1}\frac{Y_{lm}(\hat{x})}{r^{l+2}}} \quad \boxed{E_\theta = \frac{-q_{lm}}{\epsilon_0(2l+1)}\frac{1}{r^{l+2}}\frac{\partial}{\partial\theta}Y_{lm}(\hat{x})}$$

$$\boxed{E_\phi = \frac{-q_{lm}}{\epsilon_0(2l+1)}\frac{im}{r^{l+2}\sin\theta}Y_{lm}(\hat{x})}$$

Specialize now to the case of an <u>electric dipole</u> and align it with the z-axis: $\vec{p} = p\hat{z}$

$\Rightarrow \ell = 1, m = 0$ only



$$E_r = \frac{2p\cos\theta}{4\pi\epsilon_0 r^3}$$

$$E_\theta = \frac{p\sin\theta}{4\pi\epsilon_0 r^3} \qquad E_\phi = 0$$

We can recast these expressions into a more general form, involving $\vec{x}$ and $\vec{p}$ only.

First observe that $\vec{p} = \hat{r}(\vec{p}\cdot\hat{r}) + \hat{\theta}(\vec{p}\cdot\hat{\theta})$

hence $$\hat{\theta} = \frac{\vec{p} - \hat{r}(\vec{p}\cdot\hat{r})}{\vec{p}\cdot\hat{\theta}}$$

whereby
$$\vec{E} = \frac{1}{4\pi\epsilon_0 r^3}\left\{2p\cos\theta\,\hat{r} + p\sin\theta\left(\frac{\vec{p} - \hat{r}(\vec{p}\cdot\hat{r})}{\vec{p}\cdot\hat{\theta}}\right)\right\}$$

and by inspection,
$$\vec{p}\cdot\hat{\theta} = p\cos\left(\tfrac{\pi}{2}+\theta\right) = -p\sin\theta, \quad \vec{p}\cdot\hat{r} = p\cos\theta$$
which simplifies $\vec{E}$ to the form:

$$\boxed{\vec{E} = \frac{1}{4\pi\epsilon_0 r^3}\left[3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}\right]}$$

Or if $\vec{p}$ is located at $\vec{x}_0$, this reads,

This form is no longer restricted to a dipole oriented along $\hat{z}$!

$$\vec{E}(\vec{x}) = \frac{1}{4\pi\epsilon_0|\vec{x}-\vec{x}_0|^5}\left\{3\left[\vec{p}\cdot(\vec{x}-\vec{x}_0)\right](\vec{x}-\vec{x}_0) - \vec{p}\,|\vec{x}-\vec{x}_0|^2\right\}$$

It is worth noting that this expression gives 0 when $\vec{E}$ is integrated over a sphere centered on $\vec{p}$:

i.e. $$\int_{r<R} \frac{3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}}{r^3}\, d^3r = 0$$

This is because the components of $\vec{E}$ are proportional to $Y_{2m}(\theta,\phi)$ and of course $\int Y_{lm}\, d\Omega = 0$ <u>unless</u> $l = m = 0$

$\Rightarrow$ To see this explicitly, we use a few identities to work out the Cartesian components of $\vec{E}$.

First, observe that
$$\hat{r} = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta$$

and
$$\hat{\phi} = \frac{\partial\hat{r}}{\partial\phi} \Big/ \left|\frac{\partial\hat{r}}{\partial\phi}\right|$$
$$= -\hat{x}\sin\phi + \hat{y}\cos\phi$$

and $$\hat{\theta} = \hat{\phi}\times\hat{r} = \hat{x}\cos\theta\cos\phi + \hat{y}\cos\theta\sin\phi - \hat{z}\sin\theta$$

So for a dipole aligned with $\hat{z}$, i.e. $\vec{p} = p\hat{z}$

$$\Rightarrow 4\pi\epsilon_0 r^3\vec{E} = 2p\cos\theta\,\hat{r} + p\sin\theta\,\hat{\theta}$$
$$= 2p\cos\theta(\hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta)$$
$$+ p\sin\theta(\hat{x}\cos\theta\cos\phi + \hat{y}\cos\theta\sin\phi - \hat{z}\sin\theta)$$

or comparing to the $l=2$ spherical harmonics gives

$$\boxed{\vec{E} = \frac{p}{4\pi\epsilon_0 r^3}\left(\frac{8\pi}{15}\right)^{1/2}\left\{\hat{x}\,\frac{3}{2}\left(-Y_{2,1}+Y_{2,-1}\right)+\hat{y}\,\frac{3}{2i}\left(-Y_{21}-Y_{2,-1}\right) + \hat{z}\sqrt{2}\;Y_{2,0}\right\}}$$

Comments

(1) In general (see problem 4.4a), all multipoles of rank l HIGHER than the lowest nonzero one (l_{min}) depend on the coordinate origin.

illustration: a charge q at the origin has only one nonvanishing moment, namely

$$q_{0,0} = \frac{q}{\sqrt{4\pi}} = \text{the monopole moment}$$

However a charge q placed at $\vec{x}_0$ has the same monopole moment q_{00}, but also the other $q_{lm} = q\, r_0^{\,l}\, Y^*_{lm}(\theta_0, \phi_0) \neq 0$ for all l, m, in general.

(2) We have not yet investigated carefully the behavior near $r=0$, i.e. at the singularity. In fact a careful analysis shows that there is an additional δ-contribution, giving

an analogous term is important in atomic hyperfine structure, for magnetic moments

$$\vec{E}(\vec{x}) = \frac{1}{4\pi\epsilon_0}\left[\frac{3\hat{n}(\vec{p}\cdot\hat{n})-\vec{p}}{|\vec{x}-\vec{x}_0|^3} - \frac{4\pi}{3}\vec{p}\,\delta(\vec{x}-\vec{x}_0)\right]$$

Here of course $\hat{n} = \frac{\vec{x} - \vec{x}_0}{|\vec{x} - \vec{x}_0|}$

Proof Consider the volume integral of $\vec{E}(\vec{x})$ over a tiny spherical volume, $r<R$

$$\Rightarrow \int_{r<R} \vec{E}(\vec{x})\, d^3r = -\int_{r<R} \nabla \Phi(\vec{x})\, d^3x = -\underbrace{\int R^2 d\Omega\, \Phi(\vec{x})\, \hat{n}}_{\text{surface integral of radius } R}$$

this identity can be proved by applying the divergence theorem to $\vec{b}\, \Phi(\vec{x})$ where $\vec{b}$ = any constant vector

i.e. consider

$$\int_V \nabla \cdot (\vec{b}\, \Phi(\vec{x}))\, d^3x = \vec{b} \cdot \int \vec{\nabla} \Phi\, d^3x = \oint_S \vec{b} \cdot \hat{n}\, \Phi(\vec{x})\, d^3x$$

So since $\vec{b} \cdot \int \vec{\nabla}\Phi\, d^3x = \vec{b} \cdot \oint_S \hat{n}\, \Phi(\vec{x})\, da$ holds for arbitrary constant $\vec{b}$

$$\Rightarrow \boxed{\int \nabla \Phi(\vec{x})\, d^3x = \oint_S \Phi(\vec{x})\, \hat{n}\, da}$$

And returning to our above derivation, we have

$$\int_{r<R} \vec{E}(\vec{x})\, d^3x = \frac{-R^2}{4\pi\epsilon_0} \int d^3x' \rho(\vec{x}') \int_{r=R} \frac{d\Omega\, \hat{n}}{|\vec{x} - \vec{x}'|}$$

(i.e. $|\vec{x}| = R$ on surface)

and $\hat{n} = \hat{x} \sin\theta \cos\phi + \hat{y} \sin\theta \sin\phi + \hat{z} \cos\theta$

then recall $\hat{n} = \left(\frac{4\pi}{3}\right)^{1/2} \sum_\mu Y^*_{1\mu}(\hat{x})\, \hat{\epsilon}_\mu$

$$\Rightarrow \int \frac{\hat{n}\, d\Omega}{|\vec{x}-\vec{x}'|} = \int d\Omega \sum_{lm} \frac{4\pi}{2l+1}\left(\frac{4\pi}{3}\right)^{1/2} \sum_{\mu} Y^*_{1\mu}(\hat{x})\,\hat{\epsilon}_\mu \frac{r_<^l}{r_>^{l+1}} Y^*_{lm}(\hat{x}')\, Y_{lm}(\hat{x})$$

$\delta_{l,1}\,\delta_{m,\mu}$

$$= \underbrace{\frac{4\pi}{3}\left(\frac{4\pi}{3}\right)^{1/2} \sum_{\mu} Y^*_{1\mu}(\hat{x}')\,\hat{\epsilon}_\mu}_{\text{"}\hat{n}'\text{"}} \frac{r_<}{r_>^2}$$

and so we see that

$$\int_{r<R} \vec{E}(\vec{x})\, d^3r = \left(-\frac{4}{3}\pi R^2\right)\frac{1}{4\pi\epsilon_0}\int \frac{r_<}{r_>^2}\,\rho(\vec{x}')\,\hat{n}'\, d^3x'$$

Thus if <u>all</u> $\rho(\vec{x}')$ is INSIDE the sphere, then $r_< = r'$, $r_> = R$, whereby

$$\int \vec{E}(\vec{x})\, d^3x = -\frac{\left(\frac{4}{3}\pi R^2\right)}{4\pi\epsilon_0 R^2}\underbrace{\left(\int \rho(\vec{x}')\,\vec{x}'\, d^3x'\right)}_{\text{"}\vec{p}\text{"}}$$

$$= -\frac{1}{4\pi\epsilon_0}\frac{4\pi}{3}\vec{p},$$ this is <u>independent</u> of the sphere radius R provided R is outside of the charges ρ

In conclusion, for a dipole $\vec{p}$ at $\vec{x}'=0$,

$$\boxed{\vec{E}_{dipole}(\vec{x}) = \frac{3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}}{4\pi\epsilon_0 r^3} - \frac{\vec{p}}{3\epsilon_0}\,\delta(\vec{x})}$$