

PHY 712 Electrodynamics
10-10:50 AM MWF Olin 103

Class notes for Lecture 9:

Finish reading Chap. 3 and start Chap. 4

**Multipole moment expansion of
electrostatic potential –**

A. Spherical coordinates

B. Cartesian coordinates

Course schedule for Spring 2023

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/9/2023	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/13/2023
2	Wed: 01/11/2023	Chap. 1	Electrostatic energy calculations	#2	01/18/2023
3	Fri: 01/13/2023	Chap. 1	Electrostatic energy calculations thanks to Ewald	#3	01/18/2023
	Mon: 01/16/2023		MLK Holiday -- no class		
4	Wed: 01/18/2023	Chap. 1 & 2	Electrostatic potentials and fields	#4	01/20/2023
5	Fri: 01/20/2023	Chap. 1 - 3	Poisson's equation in 2 and 3 dimensions	#5	01/23/2023
6	Mon: 01/23/2023	Chap. 1 - 3	Brief introduction to numerical methods	#6	01/25/2023
7	Wed: 01/25/2023	Chap. 2 & 3	Image charge constructions	#7	01/30/2023
8	Fri: 01/27/2023	Chap. 2 & 3	Cylindrical and spherical geometries		
9	Mon: 01/30/2023	Chap. 3 & 4	Spherical geometry and multipole moments	#8	02/01/2023
10	Wed: 02/01/2023	Chap. 4	Dipoles and Dielectrics		

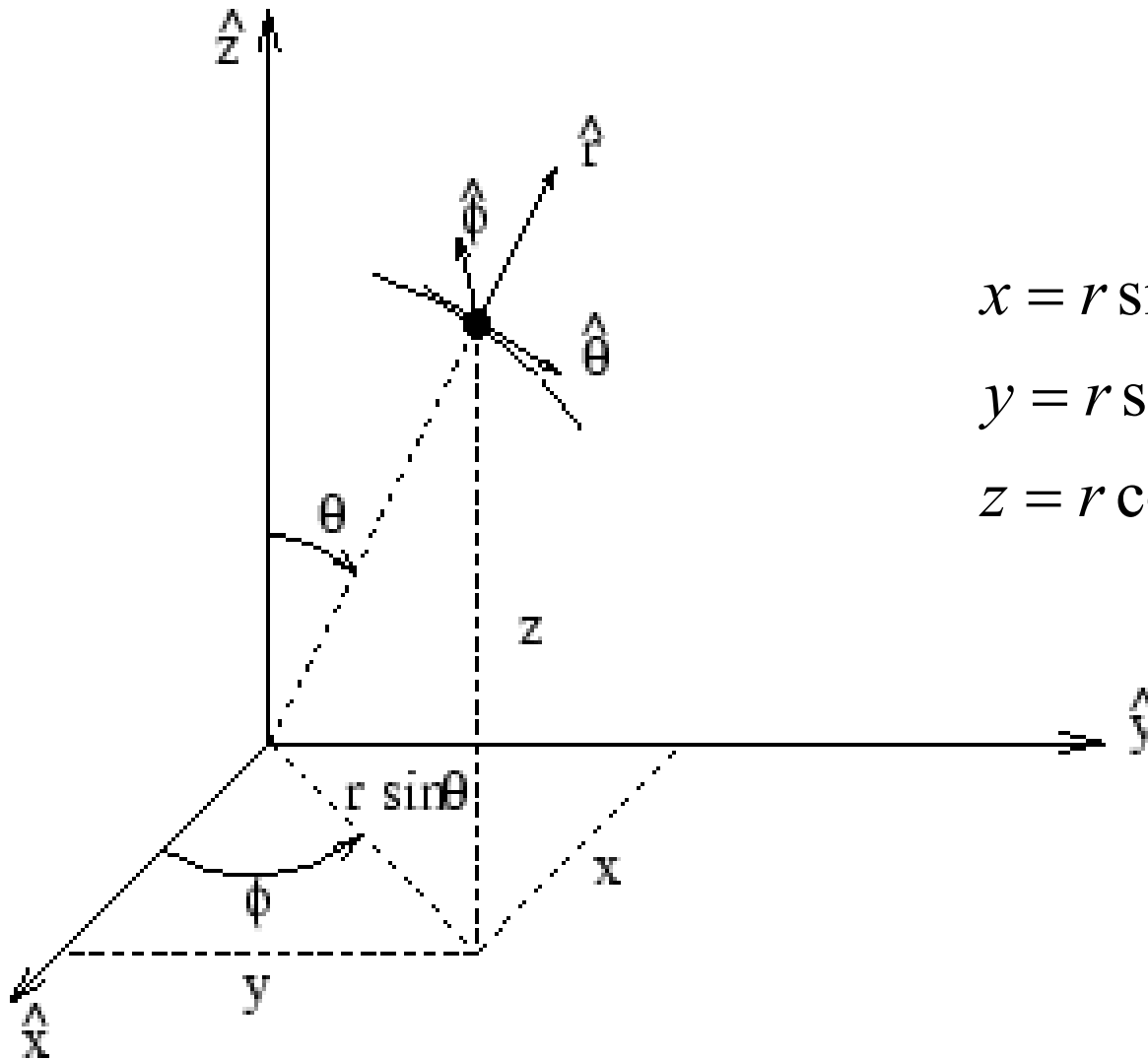
PHY 712 -- Assignment #8

January 30, 2023

Complete reading Chapter 3 and start Chapter 4 in **Jackson** .

1. Consider the charge density of an electron bound to a proton in the ground state of a hydrogen atom -- $\rho(r) = (1/\pi a_0^3) e^{-2r/a_0}$, where a_0 denotes the Bohr radius. Find the electrostatic potential $\Phi(r)$ associated with $\rho(r)$. Compare your result to HW#1.

Poisson and Laplace equation in spherical polar coordinates



$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

<http://www.uic.edu/classes/eecs/eecs520/textbook/node32.html>

Poisson and Laplace equation in spherical polar coordinates -- continued

Laplace equation for electrostatic potential $\Phi(r, \theta, \varphi)$:

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

$$\Phi(r, \theta, \varphi) = \sum_{lm} R_{lm}(r) Y_{lm}(\theta, \varphi)$$

Spherical harmonic functions:

$$\left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right) Y_{lm}(\theta, \varphi) = -l(l+1) Y_{lm}(\theta, \varphi)$$

Properties of spherical harmonic functions

$$Y_{lm}(\theta, \varphi) = (-1)^m Y_{l(-m)}^*(\theta, \varphi) \quad (\text{standard Condon-Shortley convention})$$

$$\int d\Omega Y_{lm}(\theta, \varphi) Y_{l'm'}^*(\theta, \varphi) \equiv \int \sin\theta d\theta d\varphi Y_{lm}(\theta, \varphi) Y_{l'm'}^*(\theta, \varphi) = \delta_{ll'} \delta_{mm'}$$

Completeness:

$$\sum_{lm} Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi') = \delta(\hat{\mathbf{r}} - \hat{\mathbf{r}}') \equiv \delta(\cos\theta - \cos\theta') \delta(\varphi - \varphi')$$

Relationship to Legendre polynomials:

$$Y_{l0}(\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

Relationship to Associated Legendre polynomials:

$$Y_{lm}(\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi}$$

Legendre and Associated Legendre functions

Legendre differential equation :

$$\left(\frac{d}{dx} \left((1-x^2) \frac{d}{dx} \right) + l(l+1) \right) P_l(x) = 0$$

Associated Legendre differential equation :

$$\left(\frac{d}{dx} \left((1-x^2) \frac{d}{dx} \right) + l(l+1) - \frac{m^2}{1-x^2} \right) P_l^m(x) = 0$$

For $m \geq 0$

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \left(\frac{d^m}{dx^m} P_l(x) \right)$$

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x)$$

This is the Condon and Shortley convention and the most common.

Legendre polynomials --

$$m = 0: \quad P_0(x) = 1$$

$$m = 1: \quad P_1(x) = x$$

$$m = 2: \quad P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$m = 3: \quad P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

$$m = 4: \quad P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

$$\int_{-1}^1 dx P_n(x) P_m(x) = \frac{2}{2m+1} \delta_{n,m}$$

Some spherical harmonic functions:

$$Y_{00}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{4\pi}} \quad \int d\Omega Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi) = \delta_{ll'} \delta_{mm'}$$

$$Y_{1(\pm 1)}(\hat{\mathbf{r}}) = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$$

$$Y_{10}(\hat{\mathbf{r}}) = \sqrt{\frac{3}{4\pi}} \cos \theta$$

$$Y_{2(\pm 2)}(\hat{\mathbf{r}}) = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}$$

$$Y_{2(\pm 1)}(\hat{\mathbf{r}}) = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi}$$

$$Y_{20}(\hat{\mathbf{r}}) = \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$$

Useful expansion:

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{l=0}^{\infty} \frac{r_{<}^l}{r_{>}^{l+1}} P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}')$$

Another useful expansion:

$$P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{r}}')$$

Check: $\hat{\mathbf{r}} = \sin(\theta) \cos(\varphi) \hat{\mathbf{x}} + \sin(\theta) \sin(\varphi) \hat{\mathbf{y}} + \cos(\theta) \hat{\mathbf{z}}$

$$P_0(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = 1$$

$$P_1(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = \hat{\mathbf{r}} \cdot \hat{\mathbf{r}}' = \sin(\theta) \sin(\theta') \cos(\varphi - \varphi') + \cos(\theta) \cos(\theta')$$

Note that for $\hat{\mathbf{r}} = \hat{\mathbf{r}}'$, $P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = 1$

$$\Rightarrow \frac{4\pi}{2l+1} \sum_{m=-l}^l |Y_{lm}(\hat{\mathbf{r}})|^2 = 1$$

Some details --

Useful expansion:

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{l=0}^{\infty} \frac{r_{<}^l}{r_{>}^{l+1}} P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}')$$

Elements of "proof":

$$\begin{aligned} \frac{1}{|\mathbf{r} - \mathbf{r}'|} &= \frac{1}{r_{>} \left(1 + \left(\frac{r_{<}}{r_{>}} \right)^2 - 2 \left(\frac{r_{<}}{r_{>}} \right) \hat{\mathbf{r}} \cdot \hat{\mathbf{r}}' \right)^{1/2}} = \\ &= \frac{1}{r_{>}} \left(1 + \left(\frac{r_{<}}{r_{>}} \right) \hat{\mathbf{r}} \cdot \hat{\mathbf{r}}' + \left(\frac{r_{<}}{r_{>}} \right)^2 \left(\frac{3}{2} (\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}')^2 - \frac{1}{2} \right) + \dots \right) \\ &= \frac{1}{r_{>}} \left(\sum_{l=0}^{\infty} \left(\frac{r_{<}}{r_{>}} \right)^l P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') \right) \end{aligned}$$

Even more useful identity:

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{lm} \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi')$$

Which follows from the identity: $P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{r}}')$

Example for isolated charge density $\rho(\mathbf{r})$ with electrostatic potential vanishing for $r \rightarrow \infty$:

$$\begin{aligned} \Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ &= \frac{1}{4\pi\epsilon_0} \int d^3r' \rho(\mathbf{r}') \left(\sum_{lm} \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi') \right) \end{aligned}$$

General form of electrostatic potential with boundary value

$r \rightarrow \infty$, for isolated charge density $\rho(\mathbf{r})$:

$$\begin{aligned}\Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ &= \frac{1}{4\pi\epsilon_0} \int d^3r' \rho(\mathbf{r}') \left(\sum_{lm} \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi') \right)\end{aligned}$$

Suppose that $\rho(\mathbf{r}) = \sum_{lm} \rho_{lm}(r) Y_{lm}(\theta, \varphi)$

$$\Rightarrow \Phi(\mathbf{r}) = \sum_{lm} F_{lm}(r) Y_{lm}(\theta, \varphi) \quad \text{where}$$

$$F_{lm}(r) = \frac{1}{\epsilon_0} \frac{1}{2l+1} \left(\frac{1}{r^{l+1}} \int_0^r r'^{2+l} dr' \rho_{lm}(r') + r^l \int_r^\infty r'^{1-l} dr' \rho_{lm}(r') \right)$$

In summary:

$$\Phi(\mathbf{r}) = \frac{1}{\epsilon_0} \sum_{lm} \frac{1}{2l+1} Y_{lm}(\theta, \varphi) \left(\frac{1}{r^{l+1}} \int_0^r r'^{2+l} dr' \rho_{lm}(r') + r^l \int_r^\infty r'^{1-l} dr' \rho_{lm}(r') \right)$$

Example --

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int d^3r' \rho(\mathbf{r}') \left(\sum_{lm} \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi') \right)$$

Suppose: $\rho(\mathbf{r}') = \frac{Q}{a^3 \pi^{3/2}} e^{-r'^2/a^2}$

$$\int d\Omega' Y_{lm}^*(\theta', \varphi') = \sqrt{4\pi} \delta_{l0} \delta_{m0}$$

$$\Phi(\mathbf{r}) = \frac{4\pi}{4\pi\epsilon_0} \int_0^\infty r'^2 dr' \frac{r_{<}^0}{r_{>}^1} \frac{Q}{a^3 \pi^{3/2}} e^{-r'^2/a^2} = \frac{Q}{a^3 \pi^{3/2} \epsilon_0} \left(\frac{1}{r} \int_0^r r'^2 dr' e^{-r'^2/a^2} + \int_r^\infty r' dr' e^{-r'^2/a^2} \right)$$

Note that: $\text{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du$ and $\int_A^B r' dr' e^{-r'^2/a^2} = \frac{a^2}{2} \left(e^{-A^2/a^2} - e^{-B^2/a^2} \right)$

Integrating by parts and simplifying --

$$\Phi(\mathbf{r}) = \frac{Q}{a^3 \pi^{3/2} \epsilon_0} \frac{a^3}{2r} \int_0^{r/a} e^{-u^2} du = \frac{Q}{4\pi\epsilon_0} \frac{\text{erf}(r/a)}{r}$$

Another example:

$$\text{Suppose } \rho(\mathbf{r}) = \begin{cases} \frac{qr \sin \theta \cos \varphi}{Va} = \frac{qr}{Va} \left(\frac{1}{2} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) & r \leq a \\ 0 & r > a \end{cases}$$

$$\Phi(\mathbf{r}) = \frac{1}{\epsilon_0} \sum_{lm} \frac{1}{2l+1} Y_{lm}(\theta, \varphi) \left(\frac{1}{r^{l+1}} \int_0^r r'^{2+l} dr' \rho_{lm}(r') + r^l \int_r^\infty r'^{1-l} dr' \rho_{lm}(r') \right)$$

For $r \leq a$

$$\Phi(\mathbf{r}) = \frac{q}{Va\epsilon_0} \left(\frac{1}{6} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) \left(\frac{1}{r^2} \int_0^r r'^4 dr' + r \int_r^a r' dr' \right)$$

For $r > a$

$$\Phi(\mathbf{r}) = \frac{q}{Va\epsilon_0} \left(\frac{1}{6} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) \left(\frac{1}{r^2} \int_0^a r'^4 dr' \right)$$

Example -- continued:

$$\text{Suppose } \rho(\mathbf{r}) = \begin{cases} \frac{qx}{Va} = \frac{qr}{Va} \left(\frac{1}{2} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) & r \leq a \\ 0 & r > a \end{cases}$$

For $r \leq a$

$$\begin{aligned} \Phi(\mathbf{r}) &= \frac{q}{Va\epsilon_0} \left(\frac{1}{6} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) \left(\frac{1}{r^2} \int_0^r r'^4 dr' + r \int_r^a r' dr' \right) \\ &= \frac{q}{6Va\epsilon_0} \sin \theta \cos \varphi \left(r \left(a^2 - \frac{3}{5} r^2 \right) \right) \end{aligned}$$

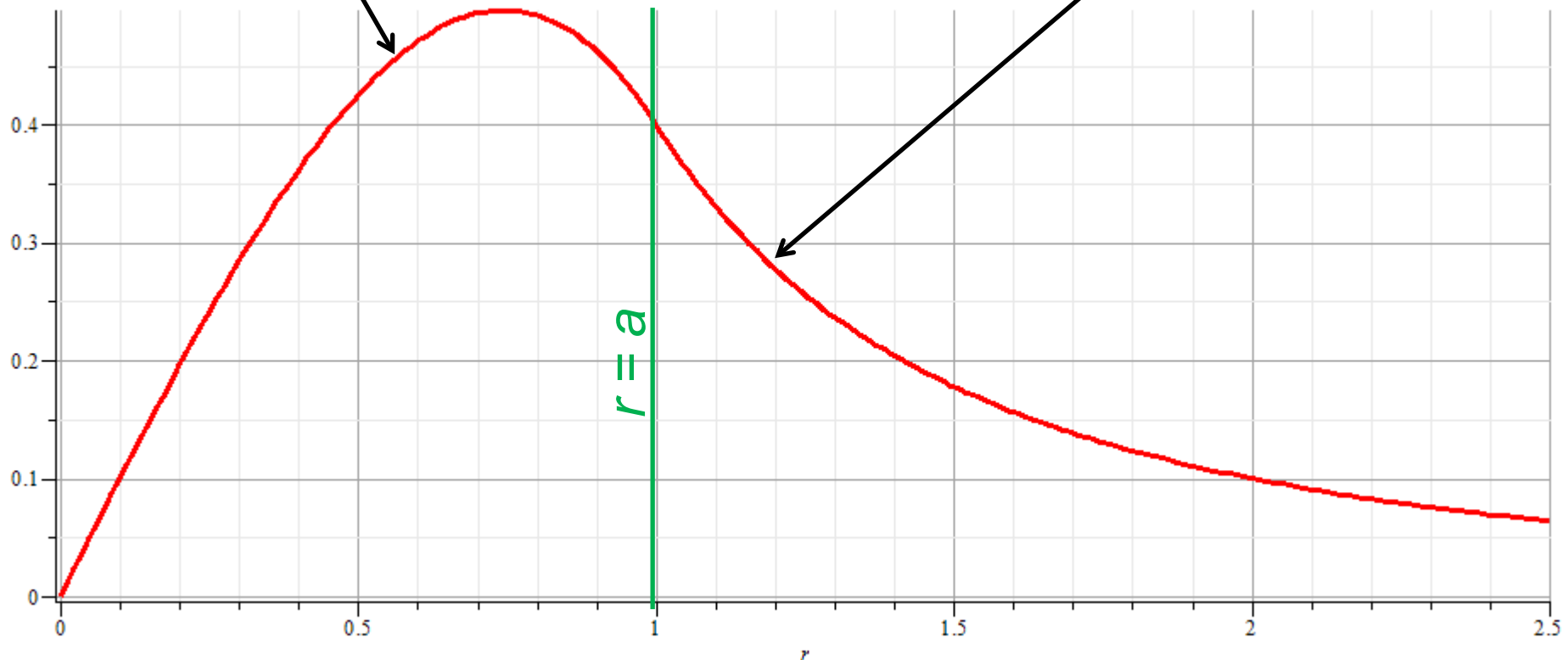
For $r > a$

$$\begin{aligned} \Phi(\mathbf{r}) &= \frac{q}{Va\epsilon_0} \left(\frac{1}{6} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) \left(\frac{1}{r^2} \int_0^a r'^4 dr' \right) \\ &= \frac{q}{6Va\epsilon_0} \sin \theta \cos \varphi \left(\frac{\frac{2}{5} a^5}{r^2} \right) \end{aligned}$$

Example -- continued:

For $r \leq a$: $\Phi(\mathbf{r}) = \frac{q}{6Va\epsilon_0} \sin \theta \cos \varphi \left(r \left(a^2 - \frac{3}{5} r^2 \right) \right)$

For $r > a$: $\Phi(\mathbf{r}) = \frac{q}{6Va\epsilon_0} \sin \theta \cos \varphi \left(\frac{\frac{2}{5} a^5}{r^2} \right) = \frac{qa^4}{15V\epsilon_0} \frac{x}{r^3}$



Notion of multipole moment:

In the spherical harmonic representation --

define the moment q_{lm} of the (confined) charge distribution $\rho(\mathbf{r})$:

$$q_{lm} \equiv \int d^3 r' r'^l Y_{lm}^*(\theta', \varphi') \rho(\mathbf{r}')$$

In the Cartesian representation --

define the monopole moment q :

$$q \equiv \int d^3 r' \rho(\mathbf{r}')$$

define the dipole moment \mathbf{p} :

$$\mathbf{p} \equiv \int d^3 r' \mathbf{r}' \rho(\mathbf{r}')$$

define the quadrupole moment components Q_{ij} ($i, j \rightarrow x, y, z$):

$$Q_{ij} \equiv \int d^3 r' \left(3r'_i r'_j - r'^2 \delta_{ij} \right) \rho(\mathbf{r}')$$

Significance of multipole moments

Recall general form of electrostatic potential with boundary value $r \rightarrow \infty$, for isolated charge density $\rho(\mathbf{r})$:

$$\begin{aligned}\Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ &= \frac{1}{4\pi\epsilon_0} \int d^3r' \rho(\mathbf{r}') \left(\sum_{lm} \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\theta, \varphi) Y_{lm}^*(\theta', \varphi') \right)\end{aligned}$$

For r outside the extent of $\rho(\mathbf{r})$:

$$\begin{aligned}\Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \sum_{lm} \frac{4\pi}{2l+1} \frac{Y_{lm}(\theta, \varphi)}{r^{l+1}} \underbrace{\left(\int_0^\infty d^3r' r'^l Y_{lm}^*(\theta', \varphi') \rho(\mathbf{r}') \right)}_{q_{lm}} \\ &= \frac{1}{4\pi\epsilon_0} \sum_{lm} \frac{4\pi q_{lm}}{2l+1} \frac{Y_{lm}(\theta, \varphi)}{r^{l+1}}\end{aligned}$$

Multipole moments continued:

For r outside the extent of $\rho(\mathbf{r})$:

$$q_{lm} = \int_0^\infty d^3r' r'^l Y_{lm}^*(\theta', \varphi') \rho(\mathbf{r}')$$

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{lm} \frac{4\pi q_{lm}}{2l+1} \frac{Y_{lm}(\theta, \varphi)}{r^{l+1}}$$

Relationship between spherical harmonic and Cartesian forms of multipole moments:

$$q_{00} = \sqrt{\frac{1}{4\pi}} q$$

$$q_{2\pm 2} = \sqrt{\frac{15}{288\pi}} (Q_{xx} \mp 2iQ_{xy} - Q_{yy})$$

$$q_{1\pm 1} = \mp \sqrt{\frac{3}{8\pi}} (p_x \mp ip_y)$$

$$q_{2\pm 1} = \mp \sqrt{\frac{15}{72\pi}} (Q_{xz} \mp iQ_{yz})$$

$$q_{10} = \sqrt{\frac{3}{4\pi}} p_z$$

$$q_{20} = \sqrt{\frac{5}{16\pi}} Q_{zz}$$

Consider previous example:

$$\rho(\mathbf{r}) = \begin{cases} \frac{qx}{Va} = \frac{qr}{Va} \left(\frac{1}{2} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) & r \leq a \\ 0 & r > a \end{cases}$$

We previously showed that for $r > a$

$$\begin{aligned} \Phi(\mathbf{r}) &= \frac{q}{Va\epsilon_0} \left(\frac{1}{6} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) \left(\frac{1}{r^2} \int_0^a r'^4 dr' \right) \\ &= \frac{q}{Va\epsilon_0} \left(\frac{1}{6} \sqrt{\frac{8\pi}{3}} (Y_{1-1}(\theta, \varphi) - Y_{11}(\theta, \varphi)) \right) \frac{a^5}{5r^2} = \frac{q}{6V\epsilon_0} \sin\theta \cos\varphi \left(\frac{2a^5}{5r^2} \right) \end{aligned}$$

Note that: $q_{1\pm 1} = \mp \frac{q}{Va} \frac{1}{2} \sqrt{\frac{8\pi}{3}} \frac{a^5}{5}$

$$p_x = \frac{1}{2} \sqrt{\frac{8\pi}{3}} (-q_{11} + q_{1-1}) = \frac{4\pi}{3} \frac{q}{Va} \frac{a^5}{5}$$

General form of electrostatic potential in terms of multipole moments:

For r outside the extent of $\rho(\mathbf{r})$:

$$\begin{aligned}\Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \sum_{lm} \frac{4\pi}{2l+1} \frac{Y_{lm}(\theta, \varphi)}{r^{l+1}} \left(\int d^3r' r'^l Y_{lm}^*(\theta', \varphi') \rho(\mathbf{r}') \right) \\ &= \frac{1}{4\pi\epsilon_0} \sum_{lm} \frac{4\pi q_{lm}}{2l+1} \frac{Y_{lm}(\theta, \varphi)}{r^{l+1}}\end{aligned}$$

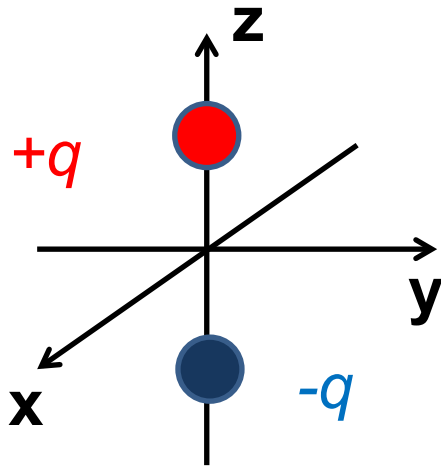
In terms of Cartesian expansion :

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \left(\frac{q}{r} + \frac{\mathbf{p} \cdot \mathbf{r}}{r^3} + \frac{1}{2} \sum_{i,j} Q_{ij} \frac{r_i r_j}{r^5} \dots \right)$$

Example of multipole expansion in evaluating energy of a very localized charge density $\rho(\mathbf{r})$ in a electrostatic field $\Phi(\mathbf{r})$ (such as an nucleus in the field produced by electrons in an atom).

$$\begin{aligned} W &= \int d^3r \rho(\mathbf{r})\Phi(\mathbf{r}) \\ &\approx \int d^3r \rho(\mathbf{r}) \left(\Phi(0) + \mathbf{r} \cdot \nabla \Phi(\mathbf{r}) \Big|_{r=0} + \frac{1}{2} (\mathbf{r} \cdot \nabla)^2 \Phi(\mathbf{r}) \Big|_{r=0} + \dots \right) \\ &= q\Phi(0) - \mathbf{p} \cdot \mathbf{E}(0) + \frac{1}{6} \sum_{i,j} Q_{ij} \frac{\partial^2 \Phi(0)}{\partial r_i \partial r_j} + \dots \end{aligned}$$

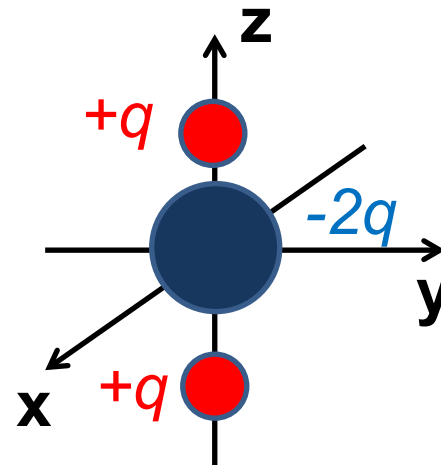
Simple examples of multipole distributions



$$\rho(\mathbf{r}) = q(\delta^3(\mathbf{r} - d\hat{\mathbf{z}}) - \delta^3(\mathbf{r} + d\hat{\mathbf{z}}))$$

$$p_z = 2qd$$

$$p_x = p_y = 0$$



$$\rho(\mathbf{r}) = q(\delta^3(\mathbf{r} - d\hat{\mathbf{z}}) + \delta^3(\mathbf{r} + d\hat{\mathbf{z}}) - 2\delta^3(\mathbf{r}))$$

$$Q_{zz} = 4qd^2 = -2Q_{xx} = -2Q_{yy}$$

Another example of multipole distribution

$$\rho(\mathbf{r}) = \frac{q}{64\pi a^3} \left(\frac{r}{a}\right)^2 e^{-r/a} \sin^2 \theta$$

Note that: $\sqrt{\frac{4\pi}{5}} Y_{20}(\theta, \phi) = \frac{3}{2} \cos^2 \theta - \frac{1}{2} = 1 - \frac{3}{2} \sin^2 \theta$

$$\sin^2 \theta = \frac{2}{3} - \frac{2}{3} \sqrt{\frac{4\pi}{5}} Y_{20}(\theta, \phi) = \frac{2}{3} \sqrt{\frac{4\pi}{1}} Y_{00}(\theta, \phi) - \frac{2}{3} \sqrt{\frac{4\pi}{5}} Y_{20}(\theta, \phi)$$

$$\Rightarrow \rho(\mathbf{r}) = \rho_{00}(r) Y_{00}(\theta, \phi) + \rho_{20}(r) Y_{20}(\theta, \phi)$$

$$\Phi(\mathbf{r}) = \Phi_{00}(r) Y_{00}(\theta, \phi) + \Phi_{20}(r) Y_{20}(\theta, \phi)$$

$$\Phi_{lm} = \frac{1}{4\pi\epsilon_0} \frac{4\pi}{2l+1} \left(\frac{1}{r^{l+1}} \int_0^r r'^{2+l} dr' \rho_{lm}(r') + r^l \int_r^\infty r'^{1-l} dr' \rho_{lm}(r') \right)$$

$$\rho_{00}(r) = \frac{2}{3} \sqrt{4\pi} \frac{q}{64\pi a^3} \left(\frac{r}{a}\right)^2 e^{-r/a} \quad \rho_{20}(r) = -\frac{2}{3} \sqrt{\frac{4\pi}{5}} \frac{q}{64\pi a^3} \left(\frac{r}{a}\right)^2 e^{-r/a}$$

Another example of multipole distribution -- continued

$$\Phi_{00}(r) = \frac{1}{4\pi\epsilon_0} \sqrt{4\pi} \frac{q}{r} \left(1 - e^{-r/a} \left(1 + \frac{3r}{4a} + \frac{r^2}{4a^2} + \frac{r^3}{24a^3} \right) \right)$$

$$\Phi_{20}(r) = -\frac{6}{4\pi\epsilon_0} \sqrt{\frac{4\pi}{5}} \frac{qa^2}{r^3} \left(1 - e^{-r/a} \left(1 + \frac{r}{a} + \frac{r^2}{2a^2} + \frac{r^3}{6a^3} + \frac{r^4}{24a^3} + \frac{r^5}{144a^5} \right) \right)$$

For $r \rightarrow \infty$; in terms for Legendre polynomials:

$$\Phi(\mathbf{r}) \rightarrow \frac{q}{4\pi\epsilon_0} \left(\frac{1}{r} - \frac{6a^2}{r^3} P_2(\cos\theta) \right) \quad Y_{l0}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

For $r \rightarrow 0$; in terms for Legendre polynomials :

$$\Phi(\mathbf{r}) \rightarrow \frac{q}{4\pi\epsilon_0} \left(\frac{1}{4a} - \frac{r^2}{120a^3} P_2(\cos\theta) \right)$$

Another example of multipole distribution -- continued

For $r \rightarrow 0$; in terms for Legendre polynomials :

$$\Phi(\mathbf{r}) \rightarrow \frac{q}{4\pi\epsilon_0} \left(\frac{1}{4a} - \frac{r^2}{120a^3} P_2(\cos\theta) \right)$$

Implications for electric quadrupole interaction :

$$W = \frac{1}{6} \sum_{i,j} Q_{ij} \frac{\partial^2 \Phi(0)}{\partial r_i \partial r_j} + \dots \quad P_2(\cos\theta) = \frac{3}{2} \cos^2 \theta - \frac{1}{2} = \frac{1}{2r^2} (3z^2 - r^2) \\ = \frac{1}{2r^2} (2z^2 - x^2 - y^2)$$

For $r \rightarrow 0$; in terms of Cartesian coordinates

$$\Phi(\mathbf{r}) \rightarrow \frac{q}{4\pi\epsilon_0} \left(\frac{1}{4a} - \frac{2z^2 - x^2 - y^2}{240a^3} \right)$$

$$\frac{\partial^2 \Phi(0)}{\partial x^2} = \frac{\partial^2 \Phi(0)}{\partial y^2} = -\frac{1}{2} \frac{\partial^2 \Phi(0)}{\partial z^2} = \frac{q}{4\pi\epsilon_0} \frac{1}{120a^3}$$

Another example of multipole distribution -- continued

Electric quadrupole interaction:

$$W = \frac{1}{6} \sum_{i,j} Q_{ij} \frac{\partial^2 \Phi(0)}{\partial r_i \partial r_j} = \frac{1}{6} \left(Q_{xx} \frac{\partial^2 \Phi(0)}{\partial x^2} + Q_{yy} \frac{\partial^2 \Phi(0)}{\partial y^2} + Q_{zz} \frac{\partial^2 \Phi(0)}{\partial z^2} \right)$$

For symmetric nuclei, $Q_{zz} \equiv Qq = -\frac{1}{2} Q_{xx} = -\frac{1}{2} Q_{yy}$

$$W \approx \frac{q^2}{4\pi\epsilon_0} \frac{Q}{240a^3}$$