PHY 712 Electrodynamics
10-10:50 AM MWF Online

Class notes for Lecture 8:

Finish reading Chap. 3 and start Chap. 4

Multipole moment expansion of electrostatic potential –

A. Spherical coordinates

B. Cartesian coordinates

Course schedule for Spring 2021

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Wed: 01/27/2021	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/29/2021
2	Fri: 01/29/2021	Chap. 1	Electrostatic energy calculations	#2	02/01/2021
3	Mon: 02/01/2021	Chap. 1 & 2	Electrostatic potentials and fields	#3	02/03/2021
4	Wed: 02/03/2021	Chap. 1 - 3	Poisson's equation in 2 and 3 dimensions	#4	02/05/2021
5	Fri: 02/05/2021	Chap. 1 - 3	Brief introduction to numerical methods	#5	02/08/2021
6	Mon: 02/08/2021	Chap. 2 & 3	Image charge constructions	#6	02/10/2021
7	Wed: 02/10/2021	Chap. 2 & 3	Cylindrical and spherical geometries		
8	Fri: 02/12/2021	Chap. 3 & 4	Spherical geometry and multipole moments	#7	02/15/2021
9	Mon: 02/15/2021	Chap. 4	Dipoles and Dielectrics		
10	Wed: 02/17/2021	Chap. 4	Polarization and Dielectrics		
11	Fri: 02/19/2021	Chap. 5	Magnetostatics		
12	Mon: 02/22/2021	Chap. 5	Magnetic dipoles and hyperfine interaction		
13	Wed: 02/24/2021	Chap. 5	Magnetic dipoles and dipolar fields		

PHY 712 -- Assignment #7

February 12, 2021

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

1. Consider the charge density of an electron bound to a proton in 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.

Your questions –

From Gao -- We bring up multipole moments for changing expression of Phi. What other purposes does it have?

From Tim -- So you say the equation on slide 7 is important. Is the method to describe your charge density (normally in factors of sines and cosines) into spherical harmonics such as Y_lm so that we can use the equation on slide 7?

From Nick -- On a different note from yesterday's lecture. When we are discussing the cylindrical shell, we say it only works for m=0 and I get cosine integral argument, but we have a factor of 1/m, so how can m=0?

Brief comment about cylindrical geometry case --

$$G(r,r',\varphi,\varphi') = -\ln\left(r_>^{\;2}\right) + 2\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{r_<}{r_>}\right)^m \cos\left(m\left(\varphi-\varphi'\right)\right)$$

$$\Phi(r,\varphi) = \frac{1}{4\pi\epsilon_0}\int_0^{2\pi} d\varphi' \int_0^{\infty} r'dr' G(r,r',\varphi,\varphi')\rho(r',\varphi')$$

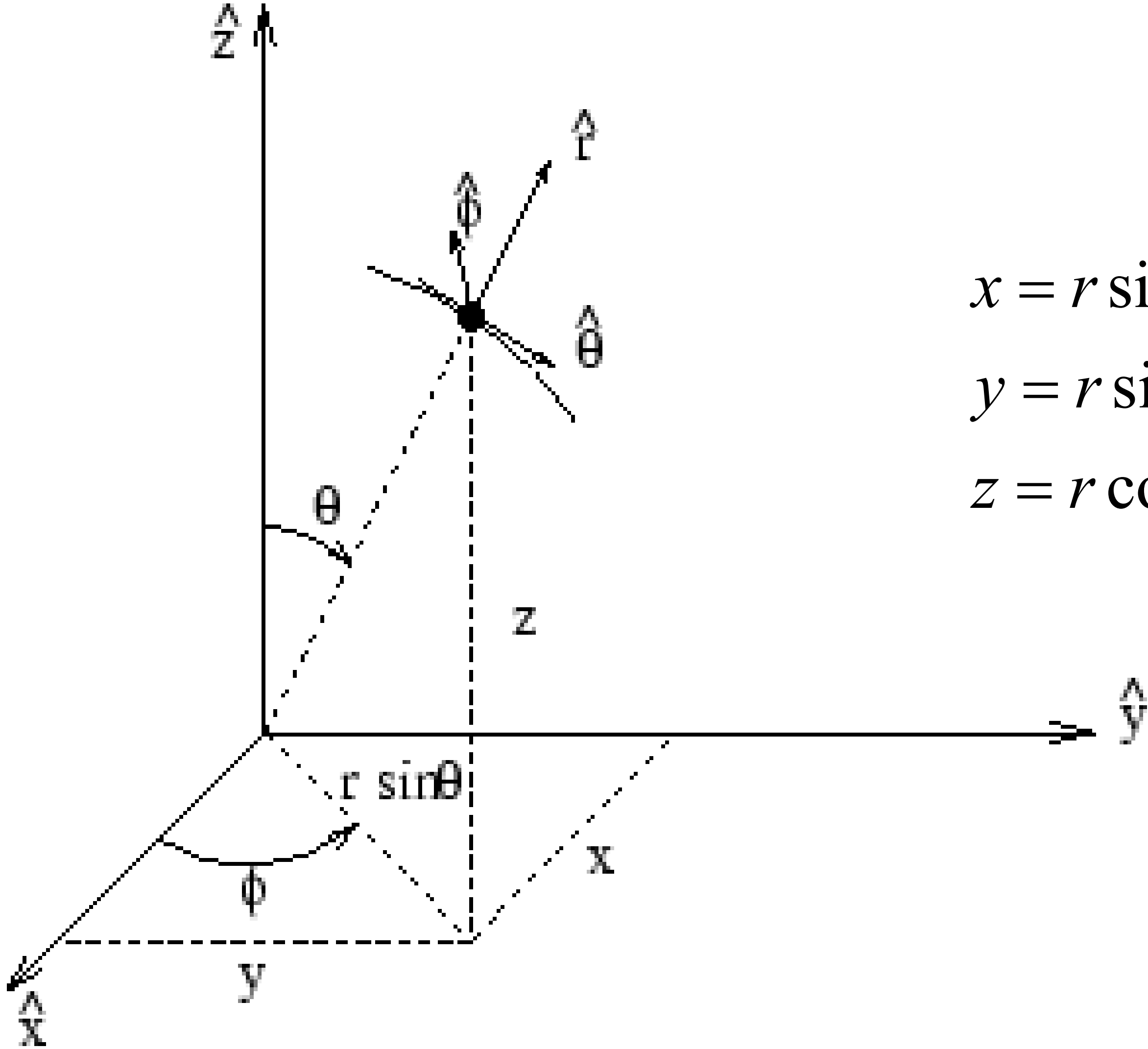
Suppose that $\rho(r',\varphi') = f(r')$ that is independent of φ'

$$\int_0^{2\pi} d\varphi' \cos(m(\varphi-\varphi')) = 0 \text{ for any integer } m > 0$$

$\Rightarrow$ In our example, only the $m = 0$ part contributes.

$$\Phi(r,\varphi) = \frac{-2\pi}{4\pi\epsilon_0}\int_0^{\infty} r'dr' \ln(r_>) f(r')$$

Poisson and Laplace equation in spherical polar coordinates



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

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta$$

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

Poisson and Laplace equation in spherical polar coordinates -- continued

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

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

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

Spherical harmonic functions:

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

Properties of spherical harmonic functions

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

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

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:

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

Legendre and Associated Legendre functions

Legendre differential equation :

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

Associated Legendre differential equation :

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

For $m \geq 0$

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

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

Legendre polynomials --

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

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

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

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

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

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

Some spherical harmonic functions:

$$Y_{00}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{4\pi}}$$

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

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

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

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

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

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

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

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

Even more useful identity:

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

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

$$\Phi(\mathbf{r})=\frac{1}{4\pi\varepsilon_0}\int d^3r'\,\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$=\frac{1}{4\pi\varepsilon_0}\int d^3r'\,\rho(\mathbf{r}')\left(\sum_{lm}\frac{4\pi}{2l+1}\frac{r_<^{\,l}}{r_>^{\,l+1}}Y_{lm}(\theta,\varphi)Y_{lm}^{\,*}(\theta',\varphi')\right)$$

General form of electrostatic potential with boundary value

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

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$= \frac{1}{4\pi\varepsilon_0}\int d^3r' \rho(\mathbf{r}')\left(\sum_{lm}\frac{4\pi}{2l+1}\frac{r_<^{\,l}}{r_>^{\,l+1}} Y_{lm}(\theta,\varphi) Y_{lm}^*(\theta',\varphi')\right)$$

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

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

$$F_{lm}(r) = \frac{1}{\varepsilon_0}\frac{1}{2l+1}\left(\frac{1}{r^{l+1}}\int_0^r r'^{2+l}\, dr' \rho_{lm}(r') + r^l \int_r^\infty r'^{1-l}\, dr' \rho_{lm}(r')\right)$$

In summary:

$$\Phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\sum_{lm}\frac{1}{2l+1} Y_{lm}(\theta,\varphi)\left(\frac{1}{r^{l+1}}\int_0^r r'^{2+l}\, dr' \rho_{lm}(r') + r^l \int_r^\infty r'^{1-l}\, dr' \rho_{lm}(r')\right)$$

Example:

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

$$\Phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\sum_{lm}\frac{1}{2l+1}Y_{lm}(\theta,\varphi)\left(\frac{1}{r^{l+1}}\int_0^r r'^{2+l}\,dr'\,\rho_{lm}(r') + r^l\int_r^\infty r'^{1-l}\,dr'\rho_{lm}(r')\right)$$

For $r \le a$

$$\Phi(\mathbf{r}) = \frac{q}{Va\varepsilon_0}\left(\frac{1}{6}\sqrt{\frac{8\pi}{3}}\left(Y_{1-1}(\theta,\varphi) - Y_{11}(\theta,\varphi)\right)\right)\left(\frac{1}{r^2}\int_0^r r'^4\,dr' + r\int_r^a r'\,dr'\right)$$

For $r > a$

$$\Phi(\mathbf{r}) = \frac{q}{Va\varepsilon_0}\left(\frac{1}{6}\sqrt{\frac{8\pi}{3}}\left(Y_{1-1}(\theta,\varphi) - Y_{11}(\theta,\varphi)\right)\right)\left(\frac{1}{r^2}\int_0^a r'^4\,dr'\right)$$

Example -- continued:

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

For $r \le a$

$$\Phi(\mathbf{r}) = \frac{q}{Va\varepsilon_0}\left(\frac{1}{6}\sqrt{\frac{8\pi}{3}}\left(Y_{1-1}(\theta,\varphi) - Y_{11}(\theta,\varphi)\right)\right)\left(\frac{1}{r^2}\int_0^r r'^4\, dr' + r\int_r^a r'\,dr'\right)$$

$$= \frac{q}{6Va\varepsilon_0}\sin\theta\cos\varphi\left(r\left(a^2 - \tfrac{3}{5}r^2\right)\right)$$

For $r > a$

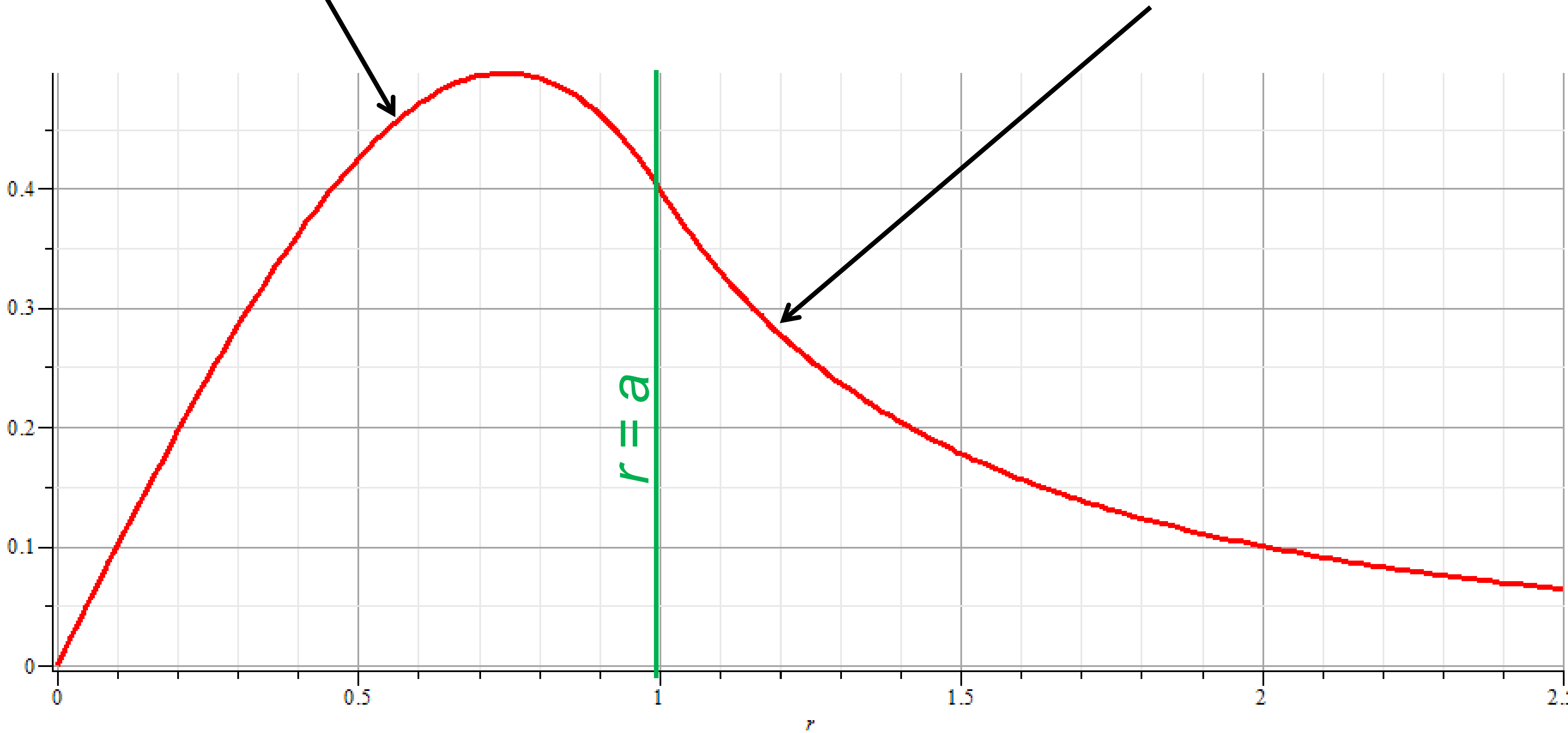
$$\Phi(\mathbf{r}) = \frac{q}{Va\varepsilon_0}\left(\frac{1}{6}\sqrt{\frac{8\pi}{3}}\left(Y_{1-1}(\theta,\varphi) - Y_{11}(\theta,\varphi)\right)\right)\left(\frac{1}{r^2}\int_0^a r'^4\, dr'\right)$$

$$= \frac{q}{6Va\varepsilon_0}\sin\theta\cos\varphi\left(\frac{\tfrac{2}{5}a^5}{r^2}\right)$$

Example -- continued:

For $r \le a$: $\Phi(\mathbf{r}) = \frac{q}{6Va\varepsilon_0} \sin\theta\cos\varphi\left(r\left(a^2 - \frac{3}{5}r^2\right)\right)$

For $r > a$: $\Phi(\mathbf{r}) = \frac{q}{6V\varepsilon_0} \sin\theta\cos\varphi\left(\frac{\frac{2}{5}a^5}{r^2}\right) = \frac{qa^5}{15V\varepsilon_0} \; \frac{x}{r^3}$



Notion of multipole moment:

In the spherical harmonic representation --

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

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

In the Cartesian representation --

define the monopole moment q:

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

define the dipole moment $\mathbf{p}$:

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

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

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

Significance of multipole moments

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

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$= \frac{1}{4\pi\varepsilon_0}\int d^3r' \rho(\mathbf{r}')\left(\sum_{lm}\frac{4\pi}{2l+1}\frac{r_<^{\,l}}{r_>^{\,l+1}}Y_{lm}(\theta,\varphi)Y_{lm}^*(\theta',\varphi')\right)$$

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

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\sum_{lm}\frac{4\pi}{2l+1}\frac{Y_{lm}(\theta,\varphi)}{r^{l+1}}\underbrace{\left(\int_0^\infty d^3r'\, r'^l\, Y_{lm}^*(\theta',\varphi')\rho(\mathbf{r}')\right)}_{q_{lm}}$$

$$= \frac{1}{4\pi\varepsilon_0}\sum_{lm}\frac{4\pi\, q_{lm}}{2l+1}\frac{Y_{lm}(\theta,\varphi)}{r^{l+1}}$$

Multipole moments continued:

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

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

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\sum_{lm}\frac{4\pi\ q_{lm}}{2l+1}\frac{Y_{lm}(\theta,\varphi)}{r^{l+1}}$$

Relationship between spherical harmonic and Cartesian forms of multipole moments:

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

$$q_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\left(p_x \mp ip_y\right)$$

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

$$q_{2\pm2} = \sqrt{\frac{15}{288\pi}}\left(Q_{xx} \mp 2iQ_{xy} - Q_{yy}\right)$$

$$q_{2\pm1} = \mp\sqrt{\frac{15}{72\pi}}\left(Q_{xz} \mp iQ_{yz}\right)$$

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

Consider previous example:

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

We previously showed that for $r > a$

$$\Phi(\mathbf{r}) = \frac{q}{Va\varepsilon_0}\left(\frac{1}{6}\sqrt{\frac{8\pi}{3}}\left(Y_{1-1}(\theta,\varphi) - Y_{11}(\theta,\varphi)\right)\right)\left(\frac{1}{r^2}\int_0^a r'^4\, dr'\right)$$

$$= \frac{q}{Va\varepsilon_0}\left(\frac{1}{6}\sqrt{\frac{8\pi}{3}}\left(Y_{1-1}(\theta,\varphi) - Y_{11}(\theta,\varphi)\right)\right)\frac{a^5}{5r^2} = \frac{q}{6V\varepsilon_0}\sin\theta\cos\varphi\left(\frac{2a^5}{5r^2}\right)$$

Note that: $q_{1\pm1} = \mp\dfrac{q}{Va}\dfrac{1}{2}\sqrt{\dfrac{8\pi}{3}}\dfrac{a^5}{5}$

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

General form of electrostatic potential in terms of multipole moments:

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

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\sum_{lm}\frac{4\pi}{2l+1}\frac{Y_{lm}(\theta,\varphi)}{r^{l+1}}\left(\int d^3r'\, r'^l\, Y_{lm}^*(\theta',\varphi')\rho(\mathbf{r}')\right)$$

$$= \frac{1}{4\pi\varepsilon_0}\sum_{lm}\frac{4\pi\, q_{lm}}{2l+1}\frac{Y_{lm}(\theta,\varphi)}{r^{l+1}}$$

In terms of Cartesian expansion:

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\left(\frac{q}{r}+\frac{\mathbf{p}\cdot\mathbf{r}}{r^3}+\frac{1}{2}\sum_{i,j}Q_{ij}\frac{r_i r_j}{r^5}\cdots\right)$$

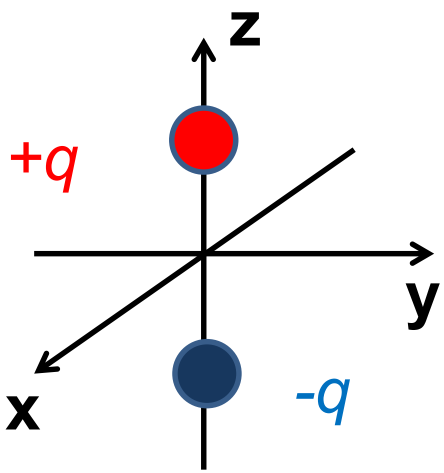
Example of multipole expansion in evaluating energy of a very localized charge density $\rho(\mathbf{r})$ in a electrostatic field $\Phi(\mathbf{r})$ (such as an nucleus in the field produced by electrons in an atom).

$$W = \int d^3r \, \rho(\mathbf{r})\Phi(\mathbf{r})$$

$$\approx \int d^3r \, \rho(\mathbf{r})\left(\Phi(0) + \mathbf{r}\cdot\nabla\Phi(\mathbf{r})\Big|_{r=0} + \frac{1}{2}(\mathbf{r}\cdot\nabla)^2\Phi(\mathbf{r})\Big|_{r=0} + \cdots \right)$$

$$= q\Phi(0) - \mathbf{p}\cdot\mathbf{E}(0) + \frac{1}{6}\sum_{i,j} Q_{ij}\,\frac{\partial^2\Phi(0)}{\partial r_i \partial r_j} + \cdots$$

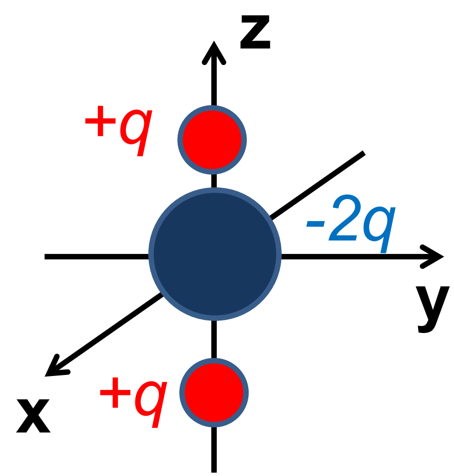
Simple examples of multipole distributions



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

$$p_z = 2qd$$

$$p_x = p_y = 0$$



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

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

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

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

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

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

$$\Phi_{lm} = \frac{1}{4\pi\varepsilon_0}\frac{4\pi}{2l+1}\left(\frac{1}{r^{l+1}}\int_0^r r'^{2+l}\,dr'\,\rho_{lm}(r') + r^l\int_r^\infty r'^{1-l}\,dr'\rho_{lm}(r')\right)$$

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

Another example of multipole distribution -- continued

$$\Phi_{00}(r) = \frac{1}{4\pi\varepsilon_0}\sqrt{4\pi}\,\frac{q}{r}\left(1 - e^{-r/a}\left(1 + \frac{3r}{4a} + \frac{r^2}{4a^2} + \frac{r^3}{24a^3}\right)\right)$$

$$\Phi_{20}(r) = -\frac{6}{4\pi\varepsilon_0}\sqrt{\frac{4\pi}{5}}\,\frac{qa^2}{r^3}\left(1 - e^{-r/a}\left(1 + \frac{r}{a} + \frac{r^2}{2a^2} + \frac{r^3}{6a^3} + \frac{r^4}{24a^3} + \frac{r^5}{144a^5}\right)\right)$$

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

$$\Phi(\mathbf{r}) \to \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{r} - \frac{6a^2}{r^3}P_2(\cos\theta)\right) \qquad Y_{l0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)$$

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

$$\Phi(\mathbf{r}) \to \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{4a} - \frac{r^2}{120a^3}P_2(\cos\theta)\right)$$

Another example of multipole distribution -- continued

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

$$\Phi(\mathbf{r}) \to \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{4a} - \frac{r^2}{120a^3}P_2(\cos\theta)\right)$$

Implications for electric quadrupole interaction:

$$W = \frac{1}{6}\sum_{i,j} Q_{ij}\frac{\partial^2\Phi(0)}{\partial r_i \partial r_j} + \cdots$$

$$P_2(\cos\theta) = \tfrac{3}{2}\cos^2\theta - \tfrac{1}{2} = \tfrac{1}{2r^2}\left(3z^2 - r^2\right)$$
$$= \tfrac{1}{2r^2}\left(2z^2 - x^2 - y^2\right)$$

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

$$\Phi(\mathbf{r}) \to \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{4a} - \frac{2z^2 - x^2 - y^2}{240a^3}\right)$$

$$\frac{\partial^2\Phi(0)}{\partial x^2} = \frac{\partial^2\Phi(0)}{\partial y^2} = -\frac{1}{2}\frac{\partial^2\Phi(0)}{\partial z^2} = \frac{q}{4\pi\varepsilon_0}\frac{1}{120a^3}$$

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

$$W \approx -\frac{q^2}{4\pi\varepsilon_0} \frac{Q}{240 a^3}$$