PHY 712 Electrodynamics
11-11:50 AM MWF Olin 107

Plan for Lecture 8:

Start reading Chapter 4

Multipole moment expansion of electrostatic potential –

A. Spherical coordinates

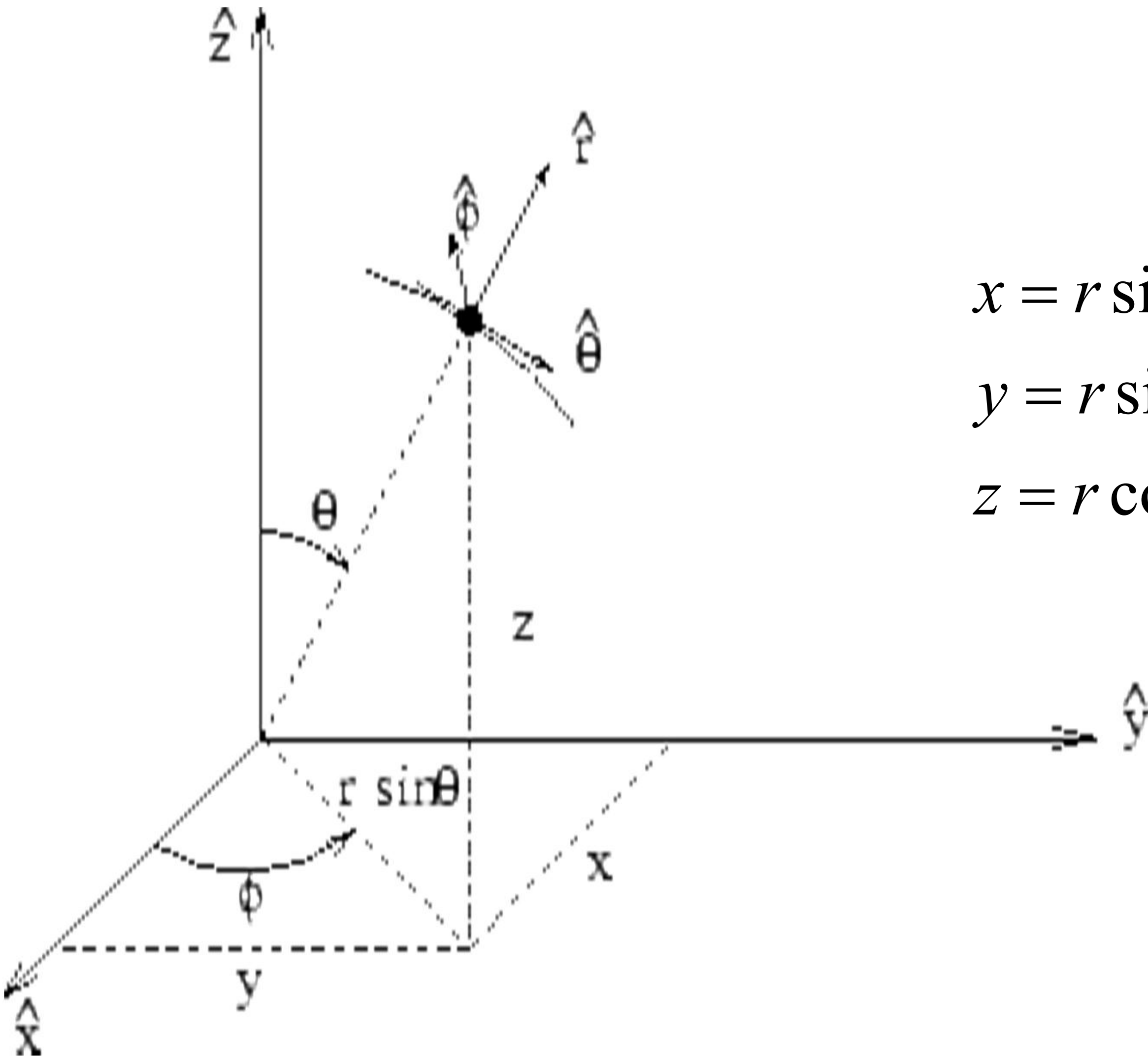
B. Cartesian coordinates

Course schedule for 2013

(Preliminary schedule -- subject to frequent adjustment.)

Date	JDJ Reading	Topic	Assign.
01-16(Wed)	Chap. 1	Introduction, units and Poisson equation.	#1
01-18(Fri)	Chap. 1	Electronstatic energy calculations	#2
01-21(Mon)	*No class*	*MKL Holiday*	
01-23(Wed)	Chap. 1	Poisson Equation and Green's Functions	#3
01-25(Fri)	Chap. 1 & 2	Green's Theorem and Functions	#4
01-28(Mon)	Chap. 1 & 2	Brief introduction to numerical methods	#5
01-30(Wed)	Chap. 2	Method of images	#6
02-01(Fri)	Chap. 3	Cylindrical and spherical geometries	#7
02-04(Mon)	Chap. 4	Multipole moments	#8

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 $\Phi(r,\theta,\phi)$:

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

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

Spherical harmonic functions:

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

Properties of spherical harmonic functions

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

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

Completeness :

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

Relationship to Legendre polynomials :

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

Relationship to Associated Legendre polynomials :

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

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 $m \geq 0$

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

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

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 $r \to \infty$:

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

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

Some spherical harmonic functions:

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

$$Y_{1(\pm1)}(\hat{\mathbf{r}}) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

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

$$Y_{2(\pm2)}(\hat{\mathbf{r}}) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$$

$$Y_{2(\pm1)}(\hat{\mathbf{r}}) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$$

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

Example:

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

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

Example:

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

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

For $r \leq a$

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

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 $r \le a$

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

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

For $r > a$

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

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

Example -- continued:

For $r \leq a$

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

For $r > a$

$$\Phi(\mathbf{r}) = \frac{q}{6V\varepsilon_0} \sin\theta \cos\phi \left(\frac{\tfrac{2}{5} a^5}{r^2} \right)$$

Notion of multipole moment:

In the spherical harmonic representation --

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

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

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 $\rho(\mathbf{r})$:

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

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

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 $r > a$

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

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

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

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

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:

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

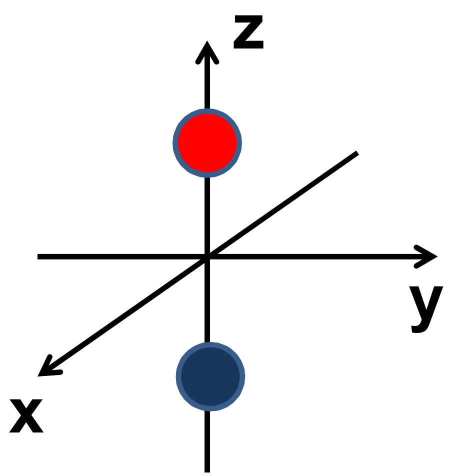
Example of multipole expansion in evaluating energy of a very localized charge density $\rho(\mathbf{r})$ in a electrostatic field $\Phi(\mathbf{r})$ (such as an nucleus in the field due to the electrons in an atom).

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

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

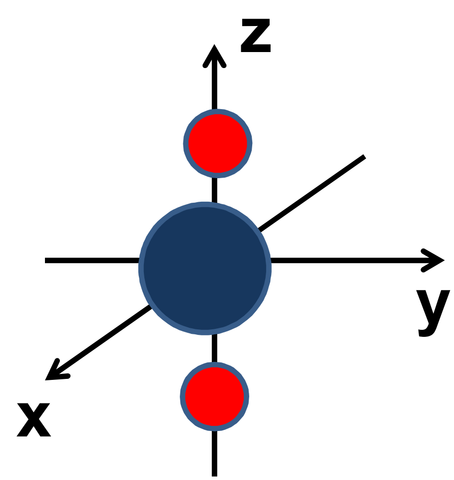
$$= q\Phi(0) - \mathbf{p} \cdot \mathbf{E}(0) + \frac{1}{6} \sum_{i,j} Q_{ij} \frac{\partial^2 \Phi(0)}{\partial r_i \partial r_j} + \cdots$$

Simple examples of multipole distributions



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

$$p_z = 2qd$$



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

$$Q_{zz} = 4qd^2 = -\tfrac{1}{2}Q_{xx} = -\tfrac{1}{2}Q_{yy}$$