PHY 712 Electrodynamics
9-9:50 AM MWF Olin 103

Plan for Lecture 8:

Start reading Chapter 4

Multipole moment expansion of electrostatic potential –

A. Spherical coordinates

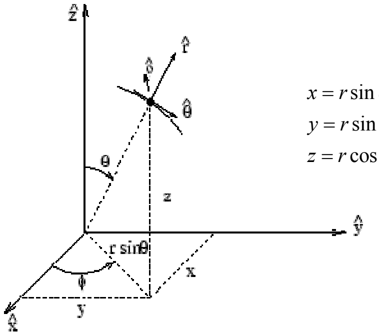
B. Cartesian coordinates

Course schedule for Spring 2015

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	Assign.	Due date
1	Mon: 01/12/2015	Chap. 1	Introduction, units and Poisson equation	#1	01/23/2015
2	Wed: 01/14/2015	Chap. 1	Electrostatic energy calculations	#2	01/23/2015
	Fri: 01/16/2015	No class	NAWH out of town		
	Mon: 01/19/2015	No class	MLK Holiday		
3	Wed: 01/21/2015	Chap. 1	Poisson equation and Green's theorem	#3	01/23/2015
4	Fri: 01/23/2015	Chap. 1 & 2	Green's functions in Cartesian coordinates	#4	01/26/2015
5	Mon: 01/26/2015	Chap. 1 & 2	Brief introduction to grid solution methods	#5	01/28/2015
6	Wed: 01/28/2015	Chap. 2	Method of images	#6	01/30/2015
7	Fri: 01/30/2015	Chap. 3	Cylindrical and spherical geometries	#7	02/02/2015
➡	Mon: 02/02/2015	Chap. 4	Multipole analysis	#8	02/04/2015
9	Wed: 02/04/2015	Chap. 4	Dipoles and dielectrics	#9	02/06/2015
10	Fri: 02/06/2015	Chap. 4	Dipoles and dielectrics	#10	02/09/2015

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

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

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

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:

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

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 $m\geq 0$

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

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

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:

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

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

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:

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

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 $r > a$

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

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

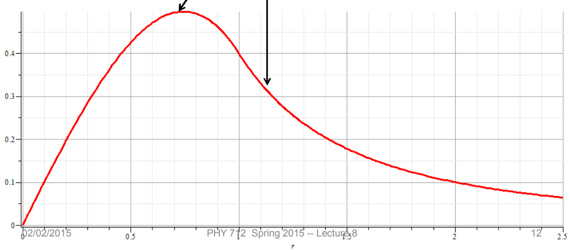
Example -- continued:

For $r \le a$

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

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} $(i,j \rightarrow x,y,z)$:

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

Significance of multipole moments

Recall general form of electrostatic potential with boundary value $r \rightarrow \infty$, 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:

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

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

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

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:

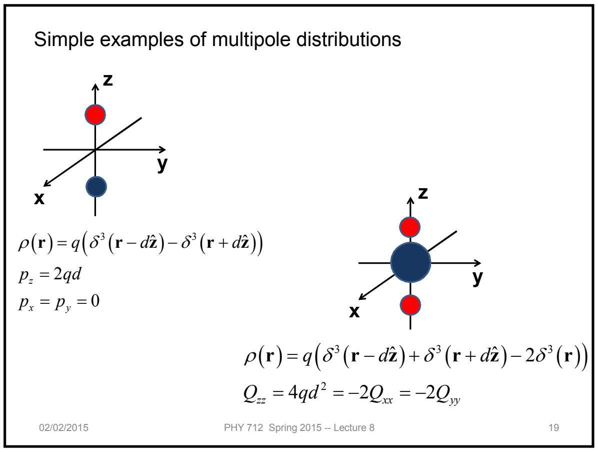
$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\left(\frac{q}{r} + \frac{\mathbf{p}\cdot\mathbf{r}}{r^3} + \frac{1}{2}\sum_{i,j} Q_{ij}\frac{r_i r_j}{r^5}\cdots\right)$$

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 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

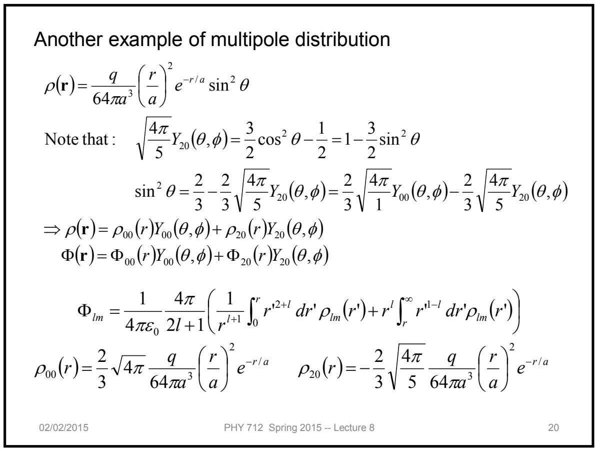
$$\rho(\mathbf{r}) = q\left(\delta^3(\mathbf{r} - d\hat{\mathbf{z}}) - \delta^3(\mathbf{r} + d\hat{\mathbf{z}})\right)$$

$$p_z = 2qd$$

$$p_x = p_y = 0$$

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

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



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

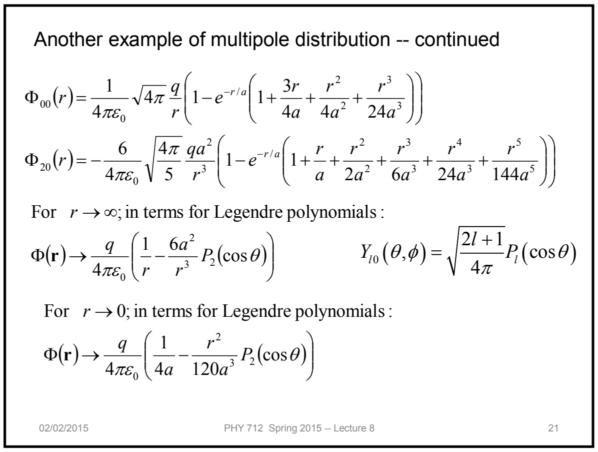
$$\sin^2\theta = \frac{2}{3} - \frac{2}{3}\sqrt{\frac{4\pi}{5}}Y_{20}(\theta,\phi) = \frac{2}{3}\sqrt{\frac{4\pi}{1}}Y_{00}(\theta,\phi) - \frac{2}{3}\sqrt{\frac{4\pi}{5}}Y_{20}(\theta,\phi)$$

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

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

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

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



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

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

Implications for electric quadrupole interaction:

$$W = \frac{1}{6}\sum_{i,j} Q_{ij}\frac{\partial^2\Phi(0)}{\partial r_i \partial r_j} + \cdots \qquad P_2(\cos\theta) = \tfrac{3}{2}\cos^2\theta - \tfrac{1}{2} = \tfrac{1}{2r^2}\left(3z^2 - r^2\right)$$

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

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

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

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

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

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