

PHY 712 Electrodynamics
10-10:50 AM MWF Olin 107

Plan for Lecture 8:

Start reading Chapter 4

Multipole moment expansion of electrostatic potential –

A. Spherical coordinates

B. Cartesian coordinates

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Course schedule for Spring 2014

Preliminary schedule -- subject to frequent adjustment. Please note that makeup lectures (indicated in red) are scheduled for Tuesdays or Thursdays at 11 AM - 12:15 PM in Olin 107.

Lecture date	JDJ Reading	Topic	Assign.	Due date
1 Wed 01/15/2014	Chap. 1	Introduction, units and Poisson equation	#1	01/31/2014
2 Thu 01/16/2014	Chap. 1	Electrostatic energy calculations	#2	01/31/2014
3 Fri 01/17/2014	Chap. 1	Poisson equation and Green's theorem	#3	01/31/2014
Mon 01/20/2014		MILK Holiday - no class		
4 Wed 01/22/2014	Chap. 1	Green's functions for cartesian coordinates	#4	01/31/2014
5 Thu 01/23/2014	Chap. 1	Brief introduction to numerical methods	#5	01/31/2014
6 Fri 01/24/2014	Chap. 2	Method of images	#6	01/31/2014
Mon 01/27/2014		NAWH out of town - no class		
Wed 01/29/2014		NAWH out of town - no class		
7 Fri 01/31/2014	Chap. 3	Cylindrical and spherical geometries	#7	02/05/2014
8 Mon 02/03/2014	Chap. 4	Multipole analysis of charge distributions	#8	02/05/2014
9 Wed 02/05/2014	Chap. 4	Dipoles and dielectrics	#9	02/07/2014

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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>

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Poisson and Laplace equation in spherical polar coordinates -- continued

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

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

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

Spherical harmonic functions :

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

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Properties of spherical harmonic functions

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

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

Completeness :

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

Relationship to Legendre polynomials :

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

Relationship to Associated Legendre polynomials :

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

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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 $m \geq 0$

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

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

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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 $r \rightarrow \infty$:

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

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Some spherical harmonic functions:

$$\begin{aligned} Y_{00}(\hat{\mathbf{r}}) &= \frac{1}{\sqrt{4\pi}} \\ Y_{1(\pm 1)}(\hat{\mathbf{r}}) &= \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi} \\ Y_{10}(\hat{\mathbf{r}}) &= \sqrt{\frac{3}{4\pi}} \cos \theta \\ Y_{2(\pm 2)}(\hat{\mathbf{r}}) &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi} \\ Y_{2(\pm 1)}(\hat{\mathbf{r}}) &= \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi} \\ Y_{20}(\hat{\mathbf{r}}) &= \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right) \end{aligned}$$

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Example:

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

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

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Example:

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

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

For $r \leq a$

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

For $r > a$

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

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Example -- continued:

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

For $r \leq a$

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

$$= \frac{q}{6Va\epsilon_0} \sin \theta \cos \phi \left(r \left(a^2 - \frac{2}{3} r^2 \right) \right)$$

For $r > a$

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

$$= \frac{q}{6Va\epsilon_0} \sin \theta \cos \phi \left(\frac{\frac{2}{5} a^5}{r^2} \right)$$

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Example -- continued:

For $r \leq a$

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

For $r > a$

$$\Phi(\mathbf{r}) = \frac{q}{6Va\epsilon_0} \sin \theta \cos \phi \left(\frac{\frac{2}{5} a^5}{r^2} \right)$$

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

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

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Significance of multipole moments

Recall general form of electrostatic potential with boundary value

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

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

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

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

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Relationship between spherical harmonic and Cartesian forms of multipole moments:

$$\begin{aligned} q_{00} &= \sqrt{\frac{1}{4\pi}} q & q_{2\pm 2} &= \sqrt{\frac{15}{288\pi}} (Q_{xx} \mp 2iQ_{xy} - Q_{yy}) \\ q_{1\pm 1} &= \mp \sqrt{\frac{3}{8\pi}} (p_x \mp ip_y) & q_{2\pm 1} &= \mp \sqrt{\frac{15}{72\pi}} (Q_{xz} \mp iQ_{yz}) \\ q_{10} &= \sqrt{\frac{3}{4\pi}} p_z & q_{20} &= \sqrt{\frac{5}{16\pi}} Q_{zz} \end{aligned}$$

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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 $r > a$

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

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

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

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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:

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

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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).

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

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Simple examples of multipole distributions

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

$\rho(\mathbf{r}) = q(\delta^3(\mathbf{r} - d\hat{z}) + \delta^3(\mathbf{r} + d\hat{z}) - 2\delta^3(\mathbf{r}))$
 $Q_{zz} = 4qd^2 = -\frac{1}{2}Q_{xx} = -\frac{1}{2}Q_{yy}$

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

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

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

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

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

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Another example of multipole distribution -- continued

$\Phi_{00}(r) = \frac{1}{4\pi\epsilon_0} \sqrt{\frac{4\pi}{5}} \frac{q}{r} \left(1 - e^{-r/a} \left(1 + \frac{3r}{4a} + \frac{r^2}{4a^2} + \frac{r^3}{24a^3} \right) \right)$

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

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

$\Phi(\mathbf{r}) \rightarrow \frac{q}{4\pi\epsilon_0} \left(\frac{1}{r} - \frac{6a^2}{r^3} P_2(\cos \theta) \right)$

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

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

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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 :

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

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

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

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

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

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

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