Lec. 12  Multipole Moments Cont.

Midterm Oct 28, No class Oct 14. 10/7/10

Configuration is

\[ \uparrow s \]

\[ \uparrow p \]

\[ \uparrow n \]

Last time

EDM greatly constrained by \( \Omega \) \( T \) symmetries.

Quadrupole moment not constrained

\[ q_{lm} = S \delta x^i \rho (x^i) \left( r^l y^m \right) \]

This leads to a positive electric quadrupole moment where deuteron charge distribution is elongated along spin axis (cigar shaped) and (flat and pancake shaped).

\[ Q_{33} = \sum_{ij} 5 \delta x^i \rho (x^i) \left( 3 x_i x_j - r^l y^m \right) \]

\[ Q_{20} = \sum_{ij} \frac{1}{2} \delta x^i \rho (x^i) \]

May have heavy nuclei such as 238U

Indeed

Prolate shape

\[ \Rightarrow \]
Indeed, Uranium fissions along axis.

Expand $\Phi$ in Taylor series using simple rectangular coordinates.

$\Phi = \frac{\Phi_0}{4\pi\varepsilon_0} \sum_{l,m} \left( \frac{2l+1}{2l+1} \right) y_l^m e^{im\phi} / r^{l+1}$

$\Phi(x) = \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{r} + \sum_{i,j} \frac{P_{ij}}{r^3} + \frac{1}{2} \sum_{i,j} \frac{Q_{ij}}{r^5} \right] x_i x_j + \ldots$

Note expression in Cartesian coordinates becomes very tedious for higher order.

Electric field for a given multipole

$E = \nabla \Phi + \partial \Phi + \phi \hat{E}_\phi$

$E_r = \frac{l+1}{2l+1} \frac{q_l m_n}{\varepsilon_0} \frac{Y_l^m(\phi, \theta)}{r^{l+2}}$

$E(\theta) = \frac{1}{\varepsilon_0} \frac{q_l m_n}{2l+1} \frac{Y_l^m(\phi, \theta)}{r^l}$

$E = -\nabla \Phi$

$E_\phi = -\frac{q_l m_n}{\varepsilon_0} \frac{1}{r^{l+2}} \frac{\partial}{\partial \theta} Y_l^m$
\[ E_\phi = \frac{q \rho_m}{\left( 2 \pi l \right) \epsilon_0 r^{l+2}} \frac{im}{\sin \theta} \ell m \]

For a dipole along Z axis:

\[ q_{11} = q_{1-1} = 0 \]

\[ q_{00} = \sqrt{\frac{3}{4\pi}} | \vec{p} | \]

\[ E_r = \frac{2p \cos \theta}{4\pi \epsilon_0 r^3}, \quad E_\theta = \frac{p \sin \theta}{4\pi \epsilon_0 r^3}, \quad E_\phi = 0 \]

Can express these in vector form:

\[ \vec{E}(\vec{r}) = 3 \frac{\vec{n} \left( \vec{p} \cdot \vec{n} \right) - \vec{p}}{4\pi \epsilon_0 \left( \vec{r} - \vec{r}_0 \right)^3} \]

Dipole located at \( \vec{r}_0 \)

Note, cartesian tensors of order \( l \) have

\[ (l+1)(l+2) \]

components. Spherical multipole moments of order \( l \) are \( 2l+1 \) numbers.

The extra components of the cartesian tensors are spherical multipoles.

Irreducible.
Note multipole moments in general depend on choice of origin. Consider a point charge located at \( x_0 = r_0 \angle \theta_0, \phi_0 \)

\[
q_{lm} = e \frac{r^l}{l!} y^l(\theta_0, \phi_0)
\]

The \( l=0 \) moment \( q_{00} = e / \sqrt{4\pi} \) is independent of \( x_0 \), but all higher moments depend on \( x_0 \).

Consider two charges \( +e, -e \) at \( x_0 \) and \( x_1 \)

\[
q_{lm} = e \left[ \frac{R}{l!} y^l(\theta_0, \phi_0) - \frac{r}{l!} y^l(\theta_1, \phi_1) \right]
\]

\[
q_{00} = 0
\]

\[
q_{10} = \sqrt{\frac{3}{4\pi}} e (2_0 - 2_1)
\]

\[
q_{11} = -\sqrt{\frac{3}{8\pi}} e \left[ (x_0 - x - i(y_0 - y_i)) \right]
\]

Dipole moment independent of choice of origin. However, all higher moments depend on choice of origin.

The values of \( q_{lm} \) for the lowest nonvanishing multipole moment of any charge distribution are independent of choice of origin, but all higher multipoles do depend on the location of the origin.
Consider the integral of $E^2$ from a charge distribution.

Calculate the volume integral of $E^2$:

$$
\int V E(x) \, d^3x = - \int \nabla \varphi \, d^3x
$$

for $r < R$.

$$
= - \int R^2 \, dS \cdot \varphi(x) \hat{n}
$$

where $\hat{n}$ is the outwardly directed normal.

$$
n = \frac{x}{R}
$$

$$
= - \frac{R^2}{4 \pi \varepsilon_0} \int d^3x' \rho(x') \int dS \cdot \frac{\hat{n}}{|x^2 - x^2'|}
$$
\[ \sum_{l=1}^{n} C_l \cos \phi + \sum_{s=1}^{n} \sin \phi \sin \theta + \sum_{t=1}^{n} \cos \theta \]

Linear combinations of \( Y_{lm} \) involving only

\[ \sum_{r=1}^{n} \frac{1}{\sin \phi} \frac{\cos \phi}{\cos \theta} = \sum_{r=1}^{n} \frac{1}{\sin \phi} \frac{\cos \phi}{\cos \theta} \]

\[ \cos \phi = \cos \phi' \cos \phi'' + \sin \phi \sin \phi' \cos (\phi - \phi'') \]

Note

\[ \sum_{r=1}^{n} \frac{1}{\sin \phi} \frac{\cos \phi}{\cos \theta} = \sum_{l=1}^{n} \frac{1}{\cos \phi} \cos \phi' \cos \phi'' + \sin \phi' \sin \phi'' \cos (\phi - \phi'') \]

Only \( l = 1 \) term survives \( \sum_{l=1}^{n} \) integral

\[ p_l (\cos \phi'') = \cos \phi'' \]

\[ \sum_{l=1}^{n} \frac{1}{\cos \phi} \frac{\cos \phi}{\cos \theta} \]
\[ S \Delta \Omega \ n \ \cos \gamma \]

\[ = \int_{\pi}^{\pi} d\phi \int_{0}^{1} \sin \phi \ \cos \phi + \int_{0}^{\pi} \sin \phi \ \sin \phi + k \ \cos \phi \int \cos \phi \ \cos \phi' \]

\[ + \sin \phi \ \sin \phi' \ \cos (\phi - \phi') \]

\[ = k \int_{0}^{\pi} x^2 \ dx \ \frac{2\pi}{3} \ \cos \phi' \]

\[ + \int_{0}^{\pi} (1 - x^2) \ dx \ \frac{2\pi}{3} \ \left( \int_{0}^{\pi} \left( \cos \phi + \int_{0}^{\pi} \sin \phi \right) \ \sin \phi' \ \cos (\phi - \phi') \right) \]

\[ = 4\pi \ \frac{4\pi}{3} \ \cos \phi' \]

\[ = 4\pi \ \frac{4\pi}{3} \ \left[ k \ \cos \phi' + \sin \phi' \left( \cos \phi' + \int_{0}^{\pi} \cos \phi' \right) \right] \]

\[ = 4\pi \ \frac{4\pi}{3} \ \cos \phi' \]

\[ S \Delta \Omega \ n \ \cos \gamma = 4\pi \ \frac{4\pi}{3} \ \cos \phi' \]

\[ S \Delta \Omega \ n \ \frac{n}{1 - r_x - r_x'} = \frac{4\pi}{3} \ \frac{4\pi}{3} \ \cos \phi' \]

\[ S \Delta \Omega \ \int_{r_x}^{r_x'} \frac{n}{r_x^2} = \frac{4\pi}{3} \ \frac{4\pi}{3} \ \cos \phi' \]

\[ S \in \ \Delta \Omega \ \int_{r_x}^{r_x'} \frac{n}{r_x^2} = \frac{4\pi}{3} \ \frac{4\pi}{3} \ \cos \phi' \]

If sphere encloses charge \( r' < R \)
\[ sE^2x = -\frac{1}{3\varepsilon_0} \bar{p} \]

\[ \bar{p} = \text{electric dipole moment of charge distribution} \]

Alternatively, if no charge enclosed

\[ r < R \]
\[ r > R \]

\[ sE^2x = \begin{cases} \frac{-R^2}{3\varepsilon_0} & \text{for } r < R \\ -\frac{4\pi\rho^3}{3} & \text{for } r > R \end{cases} \]

\[ E(0) = \frac{\bar{p}}{4\pi\varepsilon_0} \]

The average value of the electric field over any spherical region that does not contain charge is just the E field at the center of the sphere.
Look at E field from dipole configuration

In expression

$$E = \frac{3 \, n \left( \frac{q}{r} \right) - \frac{q}{r}}{4 \pi \varepsilon_0 \left| x - x_0 \right|^3}$$

The very strong flux from the + charge to the - charge is neglected.

Dipole is limit \( q \to \infty \)

So product \( q \cdot a \) is fixed.

Very strong \( |E| \approx \frac{q}{a^3} \)

E field between charges
\[ |E| \propto \frac{|p|}{a^3} \]

In limit \( a \to 0 \)

The E field becomes very large but it is confined to a very small volume of space between the two charges.

Write

\[
E(x) = \frac{1}{4\pi \varepsilon_0} \left\{ \frac{3}{5} \frac{n(\mathbf{p} \cdot \mathbf{n}) - \mathbf{p}}{|x - x_0|^3} - \frac{4\pi}{3} \mathbf{p} \delta(x - x_0) \right\}
\]

\[
\sum R^2 \times E(R) = -\frac{|p|}{3\varepsilon_0}
\]

First term has angular integral that gives zero.

Note we only desire the dipole pt. and E field assuming \( r > r' \) outside of charge dist.
Energy of a charge distribution in an external field:

\[ W = \int \rho(x) \varphi(x) \, d^3x \]

Taylor expand \( \varphi \):

\[ \varphi(x) = \varphi(0) + x \cdot \nabla \varphi(0) + \frac{1}{2} x \cdot \nabla \frac{\partial \varphi(0)}{\partial x} \cdot x + \cdots \]

\[ E = -\nabla \varphi \]

\[ \varphi(x) = \varphi(0) - x \cdot E(0) - \frac{1}{6} \sum_{ij} x_i x_j \frac{\partial^3 \varphi(0)}{\partial x_i \partial x_j \partial x_k} + \cdots \]

\[ \nabla \cdot E = 0 \quad \text{for external field} \]

Add \( \frac{1}{6} \sum x^2 \nabla \cdot E(0) \) to above:

\[ \varphi(x) = \varphi(0) - x \cdot E(0) - \frac{1}{6} \sum_{ij} (3x_i x_j - \delta_{ij} x^2) \frac{\partial^3 \varphi(0)}{\partial x_i \partial x_j \partial x_k} + \cdots \]

\[ W = q \varphi(0) - p \cdot E(0) - \frac{1}{6} \sum_{ij} q_{ij} \frac{\partial^3 E(0)}{\partial x_i \partial x_j \partial x_k} + \cdots \]

Quadrupole moment of a nucleus:

In an atom or condensed matter, electrons produce \( E \) at nucleus. \( \partial E / \partial x \) is only zero if there is some symmetry.

Can measure the quadrupole moment of the nucleus by looking at energy differences of states with different nuclear angular momenta.
Nuclear quad. moment.

\[ Q_{J\alpha} = \frac{1}{2} \int (3z^2 - r^2) \rho_{J\alpha} (r) \, r^2 \, dz \]

\[ Q = \int Q_{J\alpha} \, J\alpha \]

has dimensions of length^2.

\[ \rho_{J\alpha} = \text{charge density of nucleus in state } J\alpha \]

Shapes of nuclei:

\[ ^{16}\text{O}, \quad ^{40}\text{Ca}, \quad ^{208}\text{Pb} \]

\[ 2Z - N = 8, \quad 2Z - N = 20, \quad 2Z - N = 126 \]

are closed shell nuclei (both neutrons and protons) (analog of noble gases) (doubly magic)

Closed shell nuclei are spherical.

Tensor force between n and proton in spin one favors favors

\[ \uparrow \downarrow \quad \text{over} \quad \uparrow \uparrow \]

\[ \uparrow \downarrow \quad \text{over} \quad \uparrow \uparrow \]

\[ \text{configurations} \quad \Rightarrow \quad \text{so deuteron has} \]

\[ \text{positive } Q \quad \text{and is relatively} \]

\[ \text{bound, since system is weakly} \]
Also has a big positive Q

\[ \Rightarrow \]

\text{Fissions of Q along axis}

Interaction dipole energy between two dipoles can be found by one dipole

\[ W_{12} = \frac{p_1 \cdot p_2 - 3 n \cdot p_1 n \cdot p_2}{4\pi \varepsilon_0 \left| x_1 - x_2 \right|^3} \]

\[ \Rightarrow \]

\[ f_{12} \rightarrow \]

Attractive \text{ repulsive}