Lec. 12 Multipole Moments Cont.

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

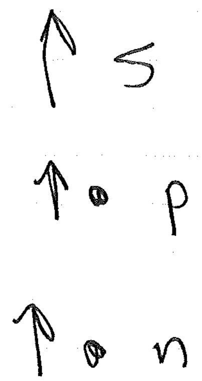
Last time

EDM greatly constrained by P, T symmetries.

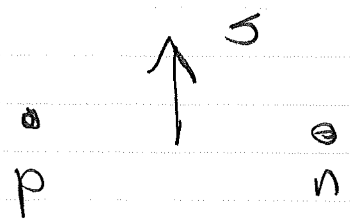
Quadrupole moment not constrained

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

Configuration is



with lower energy than



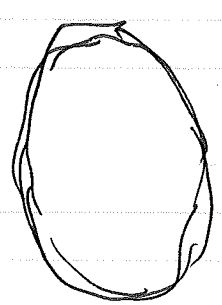
This leads to a positive electric qudrupole moment where deuteron charge distribution is ~~cigar~~ cigar shaped (elongated along spin axis) and not pancake shaped (flattened along spin).

$$Q_{33} = \langle 3z^2 - r^2 \rangle > 0$$

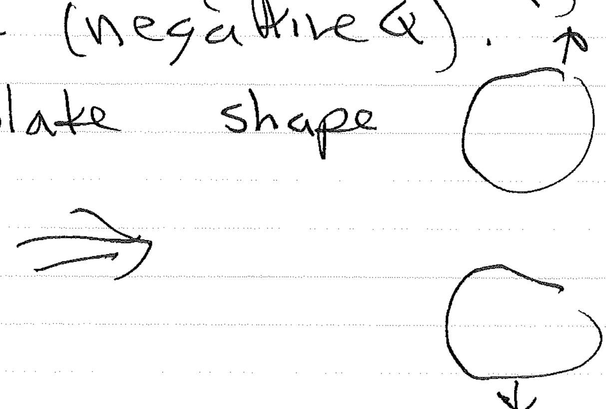
$$Q_{ij} = \int d^3x' \rho(x') (3x_i'x_j' - r'^2 \delta_{ij})$$

$$q_{20} = \frac{1}{2}\sqrt{\frac{5}{4\pi}} Q_{33}$$

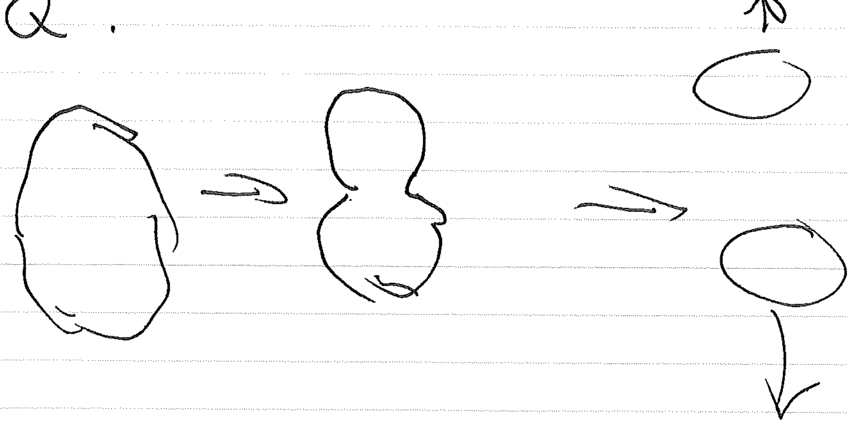
Many heavy nuclei such as ^{238}U also have nonzero Q. Indeed Uranium is prolate (positive Q) and not oblate (negative Q).



Prolate shape



Indeed Uranium fissions along axis of Q.



Expand Φ in rectangular coordinates use simple Taylor series

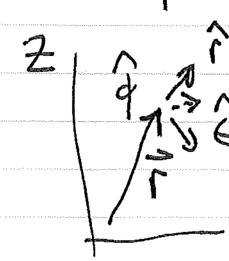
$$\Phi = \frac{1}{4\pi\epsilon_0} \sum_{lm} \left(\frac{4\pi}{2l+1}\right) q_{lm} \, Y_{lm}(\theta\phi) / r^{l+1}$$

$$\Phi(\vec{x}) = \frac{1}{4\pi\epsilon_0}\left[\frac{q}{r} + \frac{\vec{p}\cdot\vec{x}}{r^3} + \frac{1}{2}\sum_{ij} Q_{ij}\frac{x_i x_j}{r^5} + \cdots\right]$$

Note expression in Cartesian ~~coot~~ coordinates becomes very tedius for higher order terms.

Electric field for a given multipole

$$\vec{E} = \hat{r}\,E_r + \hat{\theta}\,E_\theta + \hat{\phi}\,E_\phi$$



$$E_r = \left(\frac{l+1}{2l+1}\right)\frac{1}{\epsilon_0} q_{lm} \frac{Y_{lm}(\theta\phi)}{r^{l+2}}$$

$$\Phi(\vec{x}) = \frac{1}{\epsilon_0}\sum_{lm}\frac{q_{lm}}{2l+1}\, Y_{lm}(\theta,\phi)$$

$$E = -\vec{\nabla}\Phi$$

$$E_\theta = -\frac{q_{lm}}{(2l+1)\epsilon_0}\frac{1}{r^{l+2}}\frac{d}{d\theta}Y_{lm}$$

$$E_\phi = \frac{q_{lm}}{(2l+1)\epsilon_0 r^{l+2}} \frac{im}{\sin\theta} Y_{lm}$$

For a dipole along z axis

$$q_{11} = q_{1-1} = 0$$

$$q_{10} = \sqrt{\frac{3}{4\pi}} |\vec{p}|$$

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

Can express these in vector form

$$\vec{E}(\vec{x}) = \frac{3\vec{n}(\vec{p}\cdot\vec{n}) - \vec{p}}{4\pi\epsilon_0 |\vec{x} - \vec{x}_0|^3}$$

dipole located at x_0

Note, cartesian tensors of order l have

$$\frac{(l+1)(l+2)}{2}$$

components. Spherical multipole moments of order l are $2l+1$ numbers.

The extra components of the cartesian tensors are related to lower order multipoles. Spherical multipoles are <u>irreducible</u>

Note multipole moments in general depend on choice of origin.

Consider a point charge located at $\vec{x}_0 = r_0, \theta_0, \phi_0$

$$q_{lm} = e\, r_0^l\, Y^*_{lm}(\theta_0 \phi_0)$$

The $l=0$ moment $q_{00} = e/\sqrt{4\pi}$ is independent of $\vec{x}_0$, but all higher moments depend on $\vec{x}_0$

Consider two charges $+e, -e$ at $\vec{x}_0$ and $\vec{x}_1$

$$q_{lm} = e\left[r_0^l\, Y^*_{lm}(\theta_0 \phi_0) - r_1^l\, Y^*_{lm}(\theta_1 \phi_1)\right]$$

$$q_{00} = 0$$

$$q_{10} = \sqrt{\frac{3}{4\pi}}\, e\,(z_0 - z_1)$$

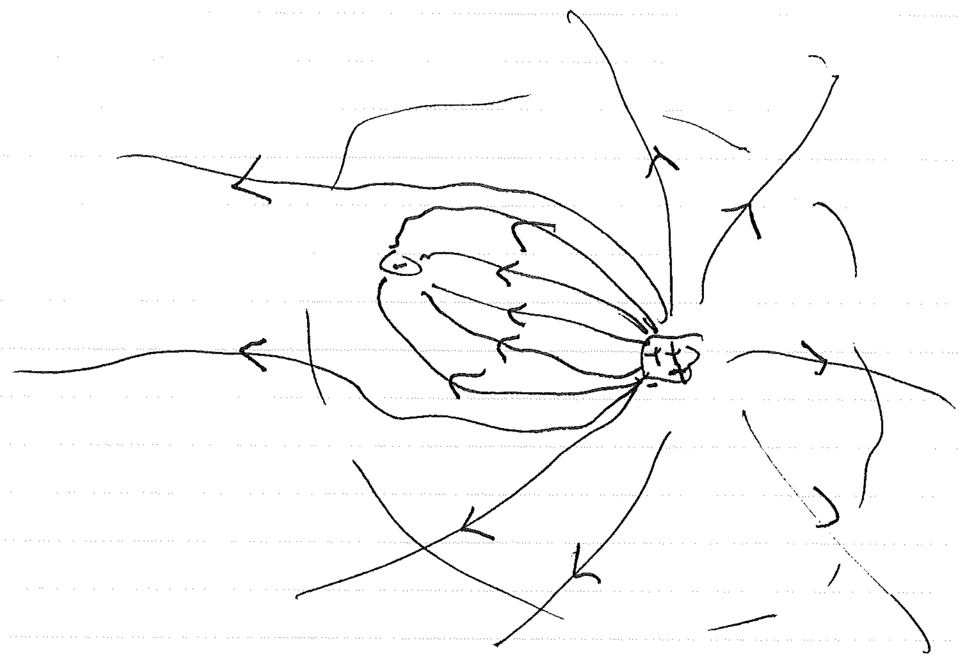
$$q_{11} = -\sqrt{\frac{3}{8\pi}}\, e\left[x_0 - x_1 - i\,(y_0 - y_1)\right]$$

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!

Konstantin Novoselov 36 + Andre Geim 51
Graphene

Consider integral of $\vec{E}$ from a charge dist.



Calculate volume integral of $\vec{E}$

$$\int_{r<R} \vec{E}(x)\, d^3x = -\int_{r<R} \nabla \Phi \, d^3x$$

$$= -\int_{\text{sphere}} R^2 \, d\Omega \; \Phi(\vec{x})\, \vec{n}$$

$n = \dfrac{\vec{x}}{R}$ outwardly directed normal

$$= -\frac{R^2}{4\pi\epsilon_0} \int d^3x' \, \rho(\vec{x}') \int_{r=R} d\Omega \, \frac{\vec{n}}{|\vec{x}-\vec{x}'|}$$

$$\vec{n} = \hat{i} \sin\theta \cos\phi + \hat{j} \sin\theta \sin\phi + \hat{k} \cos\theta$$

linear combinations of Y_{lm} involving only $l=1$

$$\int_{r=R} d\Omega \, \frac{n}{|\vec{x}-\vec{x}'|} = \frac{r_<}{r_>^2} \int d\Omega \, n \cos\gamma$$

$$\cos\gamma = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi-\phi')$$

Note $$\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\gamma) \qquad 3.38$$

$$= \sum_{lm} \frac{r_<^l}{r_>^{l+1}} \frac{4\pi}{(2l+1)} Y_{lm}^* Y_{lm}$$

only $l=1$ term survives $\int d\Omega$ integral

$$P_1(\cos\gamma) = \cos\gamma$$

$$\int d\Omega \, \vec{n} \cos\gamma = \int_0^{\pi} \sin\theta' d\theta' \int_0^{2\pi} d\phi' \, \vec{n} \{ \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi-\phi') \}$$

$$= 2\pi \int_{-1}^{1} d\cos\theta' \, \vec{n} \cos\theta \cos\theta'$$

$$= \cdot \quad \frac{x^2}{2}$$

$$\int d\Omega \; n \cos\gamma$$

$$= \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi \left[\hat{i} \sin\theta \cos\phi + \hat{j} \sin\theta \sin\phi + \hat{k} \cos\theta\right] \left[\cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi - \phi')\right]$$

$$= \hat{k} \int_{-1}^{1} x^2 \, dx \; 2\pi \cos\theta'$$

$$+ \int_{-1}^{1} (1 - x^2) \, dx \quad \int_0^{2\pi} d\phi \left(\hat{i} \cos\phi + \hat{j} \sin\phi\right) \sin\theta' \cos(\phi - \phi')$$

$$\left(2 - \frac{2}{3}\right) \sin\theta' \, \pi \left(\hat{j} \sin\phi' + \hat{i} \cos\phi'\right)$$

$$= \hat{k} \, \frac{4\pi}{3} \cos\theta'$$

$$= \frac{4\pi}{3} \left[\hat{k} \cos\theta' + \sin\theta' \left(\hat{j} \sin\phi' + \hat{i} \cos\phi'\right)\right]$$

$$= \frac{4\pi}{3} \, n'$$

$$\int d\Omega \; n \cos\gamma = \frac{4\pi}{3} \, n'$$

$$\int_{r=R} d\Omega \; \frac{n}{|x - x'|} = \frac{r_<}{r_>^2} \, \frac{4\pi}{3} \, n'$$

$$\int_{r<R} E \, d^3x = - \frac{R^2}{4\pi\epsilon_0} \int d^3x' \, \rho(x') \, \frac{r_<}{r_>^2} \, \frac{4\pi}{3} \, n'$$

If sphere encloses charge $r' < R$

$$= -\frac{1}{3\epsilon_0} \int d^3x' \, \rho(x') \, r' \hat{n}'$$

$$\int_{r<R} \vec{E} \, d^3x = -\frac{1}{3\epsilon_0} \vec{p}$$

$\vec{p}$ = electric dipole moment of charge distribution.

alternatively if no charge enclosed

$r_< = R$

$r_> = r'$

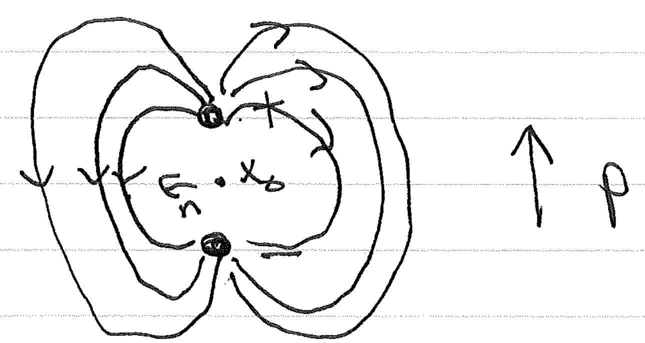
$$\int_{r<R} E \, d^3x = -\frac{R^3}{3\epsilon_0} \int d^3x' \, \frac{\rho(x') \, n'}{r'^2}$$

$$= -\frac{4\pi R^3}{3} \vec{E}(0) = V \vec{E}(0)$$

$$\vec{E}(x) = \frac{1}{4\pi\epsilon_0} \int d^3x' \, \frac{\rho(x')}{|x' - x|^2} n_{x'-x}$$

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



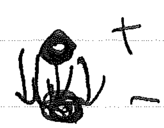
In expression

$$E = \frac{3\, n(\vec{p}\cdot\vec{n}) - \vec{p}}{4\pi\epsilon_0 |\vec{X} - \vec{X}_0^*|^3}$$

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

Dipole is limit $q \to \infty$, $a \to 0$

so product $q \cdot a$ is fixed.



Very strong E field between charges

$$|E| \sim \frac{q}{a^2} \sim \frac{qa}{a^3}$$

$$|E| \sim \frac{p}{a^3}$$

In limit ~~a^3~~ $a \to 0$
The E field becomes very large but it is confined to a very small volume of space between the two charges.

Write

$$E(\vec{x}) = \frac{1}{4\pi\epsilon_0}\left\{ \frac{3\,n\,(p\cdot n) - p}{|x - x_0|^3} - \frac{4\pi}{3}\vec{p}\,\delta(x - x_0) \right\}$$

$$\int_{r<R} d^3x \; E(\vec{x}) = -\frac{\vec{p}}{3\epsilon_0}$$

First term has angular integral that gives zero.

Note we only derived the dipole pot. and E field assuming $r > r'$ outside of charge dist.

Energy of a charge distribution in an external field.

$$W = \int \rho(x)\, \Phi(x)\, d^3x$$

Taylor expand Φ

$$\Phi(x) = \Phi(0) + x \cdot \nabla \Phi(0) + \frac{1}{2} \sum_i \sum_j x_i x_j \frac{\partial^2 \Phi(0)}{\partial x_i x_j} + \ldots$$

$$E = -\nabla \Phi$$

$$\Phi(x) = \Phi(0) - \vec{x} \cdot E(0) - \frac{1}{2} \sum_{ij} x_i x_j \partial E_j$$

$\nabla \cdot E = 0$ for external field

add $\frac{1}{6} r^2 \nabla \cdot E(0)$ to above

$$\Phi(x) = \Phi(0) - \vec{x} \cdot \vec{E}(0) - \frac{1}{\cancel{2}6} \sum_{ij} \left(3 x_i x_j - \delta_{ij} r^2\right) \frac{\partial E_j}{\partial x_i} + \ldots$$

$$W = q\Phi(0) - \vec{p} \cdot \vec{E}(0) - \frac{1}{6} \sum_{ij} Q_{ij} \frac{\partial E_j(0)}{\partial x_i} + \ldots$$

~~Quadrupole moment of a nuclea~~

In an atom or condensed matter electrons produce $\vec{E}$ at nucleus. $\frac{\partial \vec{E}}{\partial x}$ 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.

$$Q_{JM\alpha} = \frac{1}{e}\int (3z^2 - r^2)\, \rho_{JM\alpha}(\vec{x})\, d^3x$$

$$Q \equiv Q_{JJ\alpha}$$

has dimensions of length^2

$\rho_{JM\alpha}$ = charge density of nucleus in state $JM\alpha$

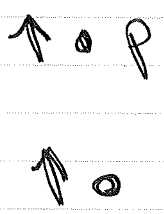
Shapes of nuclei

^{16}O, ^{40}Ca, ^{208}Pb
$Z=N=8$, $Z=N=20$, $Z=82$, $N=126$

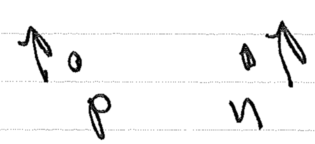
are closed shell nuclei (both neutrons and protons, analog of Noble gases)
Doubly magic

Closed shell nuclei are spherical.
$Q \cong 0$

Tensor force between n and proton in spin one deuteron favors



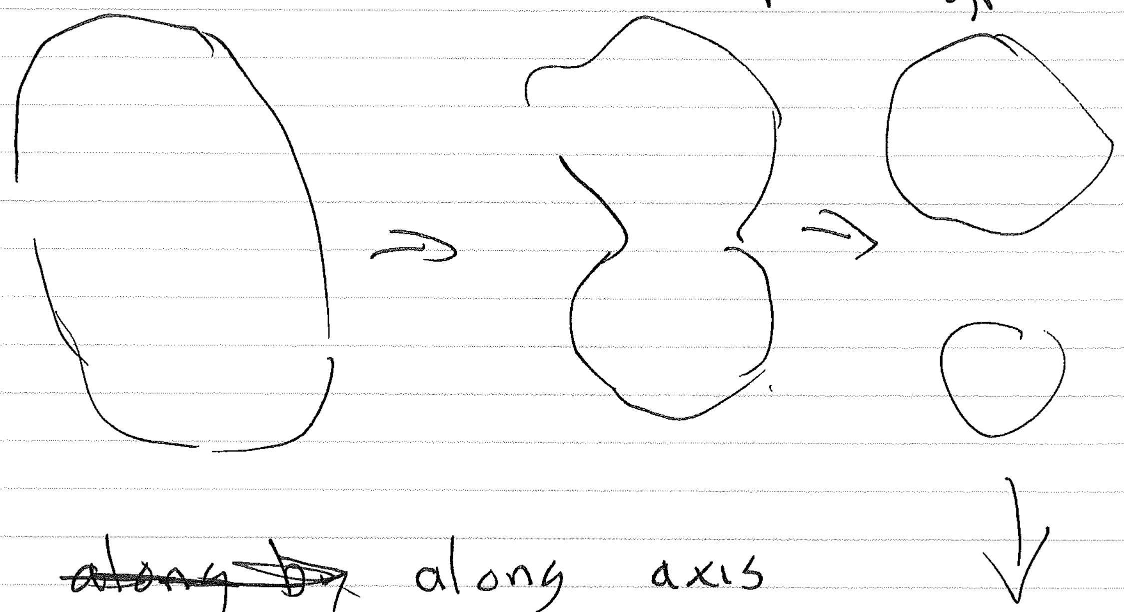
over



configurations so deuteron has a positive Q and is relatively large since system is weakly bound.

^{238}U

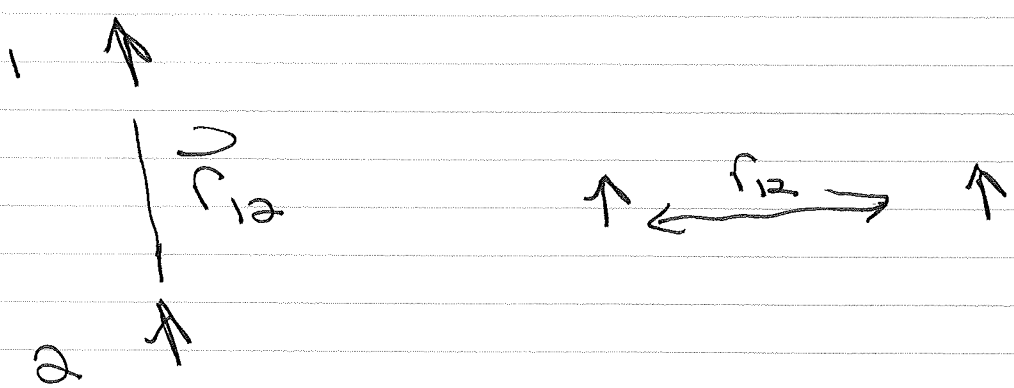
~~is~~ also has a big positive Q



Fissions ~~along by~~ along axis of Q

Interaction energy between two dipoles can be found by using E field of one dipole

$$W_{12} = \frac{p_1 \cdot p_2 - 3\, n \cdot p_1 \; n \cdot p_2}{4\pi\epsilon_0 \, |x_1 - x_2|^3}$$



attractive repulsive