- **Nuclear magnetic resonance, first demonstrated in 1946, takes advantage of the fact that certain atomic nuclei possess magnetic dipole moments -- that is, these nuclei act like tiny bar magnets, each with a north magnetic pole at one end and a south magnetic pole at the other.**

- **The laws of quantum mechanics dictate that when such nuclei are subjected to an externally applied magnetic field, they must align themselves along it.**
    - **But the magnetic moments of these nuclei, usually depicted as arrows, are allowed only two possible orientations: in the same direction as the applied magnetic field or opposite to it.**

- **Although alignment with the applied field is favored (this being the lower-energy condition), the energy difference between the two orientations is such that thermal agitation is usually sufficient to ensure that only slightly more than half the nuclei are in the lower-energy state.**

- **The key is that the nuclei can occupy two distinct states separated by a well-defined increment in energy.**

- **A ground-state electron shifts to an excited state when the atom receives a dollop of electromagnetic radiation of just the right energy to put it there –**
    - **That is, when it absorbs a photon of just the right frequency.**

- **Nuclear Quadrupole Resonance is very similar to Nuclear Magnetic Resonance (NMR) except that the nuclear energy level splittings are due to electric field gradients internal to the sample, rather than an externally applied magnetic field.**

- **It does not rely on nuclei aligning themselves in an externally applied magnetic field.**

- **Instead, NQR exploits the fact that some nuclei possess an electric quadrupole moment, which can be thought of as arising from two back-to-back electric dipoles**
    - **Positive and negative charges separated by a short distance.**

- **Since unlike NMR, NQR is done in an environment without a static (or DC) magnetic field, it is sometimes called "zero-field NMR".**

- **Why do some atomic nuclei have an electric quadrupole moment?**
    - **Physicists would say because they have a spin quantum number greater than 1/2.**

NQR works pretty much the same way, but there are some striking differences.

- **First of all, NQR works by applying an external electrical field, rather than a magnetic field.**
- **Electric fields are easier to generate, and a device to produce an electric field of a given strength is considerably more portable than its magnetic equivalent.**
- **The drawback is that NQR only works when the substance contains an appreciable quadrupole moment.**
- **The quantum physical basis for the arisal of quadrupole moments in some substances is due to their nuclei having a spin number greater than 1/2.**
- **When this is the case, the charge density is no longer spherically symmetrical.**
    - **In stead, the charge density is described by the so-called quadrupole tensor Q.**
- **Some 74% of NMR active nuclei have a spin greater than 1/2, and as a consequence possesses a quadrupole moment.**
    - **Most studied examples include Deuterium, Nitrogen 14, Chlorine 37, Copper 63, Zinc 67, or Iodine 127.**
- **The quadrupole moment interacts with any electric field gradient.**
    - **In particular, it interacts with the local electric field generated by the molecular structure of the compound containing the quadrupole moment -from which it gets its compound-specific NQR spectrum-**

It interacts with any externally applied field. By applying an external RF field, we can align the spins and see them relax when we terminate the field.

- **When a nucleus possessing such an electric quadrupole moment is subjected to an electric field that varies from place to place, interesting things happen.**

- **The internal electric field gradients are a characteristic of the material, and hence each material will have characteristic resonance frequencies. This makes NQR an obvious candidate method for the detection of different chemical species.**

- **The intrinsic electric quadrupole moment of the nucleus and the electric-field gradient imposed from outside together create distinct energy states.**

- **This result is analogous to the multiple energy states in NMR, where the critical ingredients were the intrinsic magnetic dipole moment of the nucleus and a magnetic field imposed from the outside.**

- **The key difference between NMR and NQR is the definition of "outside."**

- **In NMR, the outside magnetic field arises because the experimenter has invested considerable effort in setting it up, perhaps using a superconducting electromagnet.**

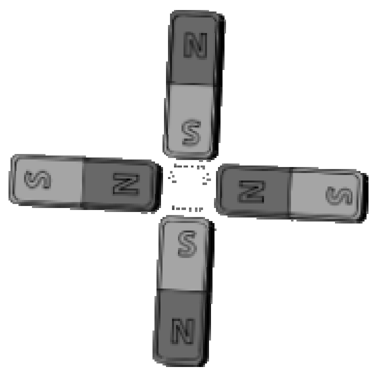
- **In NQR, the required electric field (or, more precisely, the required electric-field gradient) comes free:**
  - **It reflects the local arrangement of electrons around the nucleus under study.**
  - **That arrangement, in turn, depends not only on the nature of the atom but also on its chemical environment.**

  This feature accounts for one of the chief benefits of NQR -- the method is exquisitely sensitive to chemistry.

- **Nuclear quadrupole resonance (NQR) has much in common with nuclear magnetic resonance (NMR), the fundamental physical process that makes magnetic resonance imaging possible.**

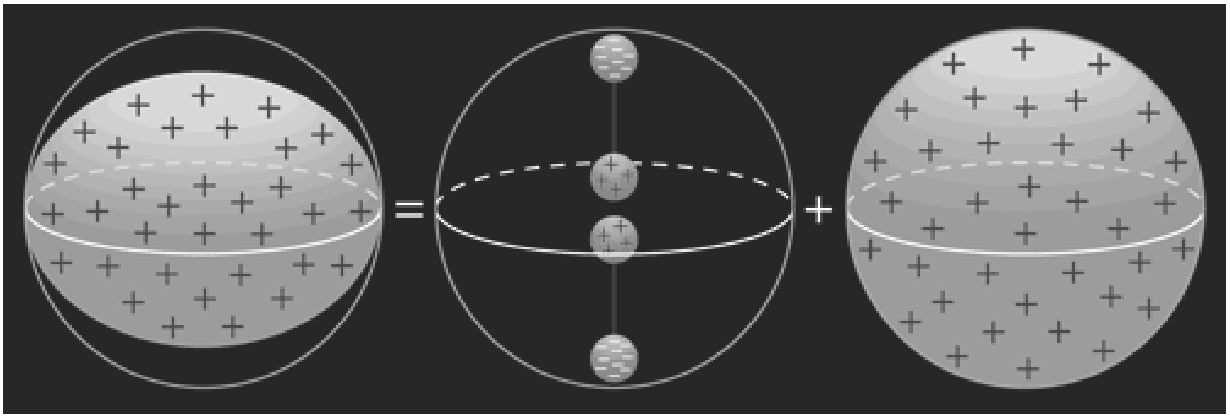
- **It is a well-known spectroscopic technique that is used to detect and identify molecular structures by the characteristic NQR of atomic species contained within.**

- **It is related to nuclear magnetic resonance (NMR) which is used to detect atoms whose nuclei have a nuclear quadrupole moment, such as ^{14}N, ^{35}Cl and ^{63}Cu.**



- **A quadrupole is one of a sequence of configurations of electric charge or gravitational mass that can exist in ideal form, but it is usually just part of a multipole expansion of a more complex structure reflecting various orders of complexity.**

Common NQR isotopes				
Isotopes	Abundances/%	I	eQ/ b	QCCo/ MHza
^{10}B	19.6	3	8.5 x 10-2	
^{11}B	80.4	3/2	4.1 x 10-2	
^{14}N	99.6	1	1 x 10-2	ca 10
^{35}Cl	75.5	3/2	-1 x 10-1	110
^{37}Cl	24.5	3/2	-7.9 x 10-2	86.7
^{55}Mn	100	5/2	4 x 10-1	
^{59}Co	100	7/2	3.8 x 10-1	
^{63}Cu	69.1	3/2	-2.1 x 10-1	
^{65}Cu	30.1	3/2	-2.0 x 10-1	
^{75}As	100	3/2	2.9 x 10-1	ca 150
^{79}Br	50.5	3/2	3.7 x 10-1	770
^{81}Br	49.5	3/2	3.1 x 10-1	645
^{121}Sb	57.3	5/2	-2.8 x 10-1	ca 780
^{123}Sb	42.7	7/2	-3.6 x 10-1	ca 1000
^{127}I	100	5/2	-7.9 x 10-1	ca 2293



- **Nuclear quadrupole resonance requires that the nuclei under scrutiny display electric quadrupole moments.**
- **Such quadrupole moments arise when the distribution of positive electric charge in the nucleus is not perfectly spherical.**
    - **For example, a slightly oblate (pumpkin-like) distribution of positive charge (*left*) can be thought of as the sum of a quadrupolar distribution (*center*) and a spherical distribution (*right*).**

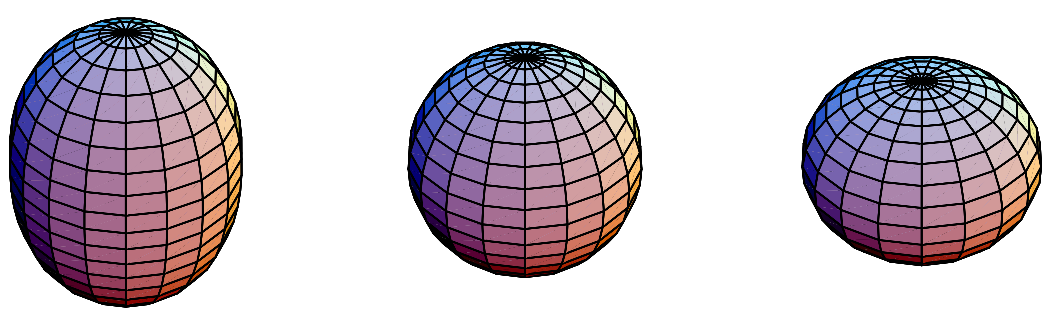
- A more intuitive explanation is because the positive electric charge these nuclei carry is not distributed with perfect spherical symmetry.

- Consider for a moment a spherical nucleus with its positive charge distributed uniformly throughout.

- Now squeeze that nucleus in your mind's eye so that what was originally shaped like a basketball is flattened into a pumpkin.

- A pumpkin of positive charge can be thought of, to a rough approximation, as being the sum of a sphere of positive charge and two oppositely directed electric dipoles, one at the top and one at the bottom.

- That is, the only requirement for an electric quadrupole moment is that the nucleus be squashed (or stretched) along one axis.

- 

The nuclei having integral and half integral nuclear spins i.e. I = 1, 3/2, 2, 5/2, 3, 7/2 etc are known as quadrupole nuclei.

- **These nuclei possess nuclear electric quadrupole moments Q or (eQ) which interact with the electric field gradient created at the nuclei by the asymmetric distribution of charge arising from the extra nuclear electrons or the nonbonding electrons of which the nuclei forms a part.**
- **The product of the quadrupole moment Q (or eQ) and the electric field gradient q (or eq) is known as the Nuclear Quadrupole coupling constant (Cq)**

$$Cq = \frac{e^2Qq}{h}$$

Electric quadrupole moment (EQM)

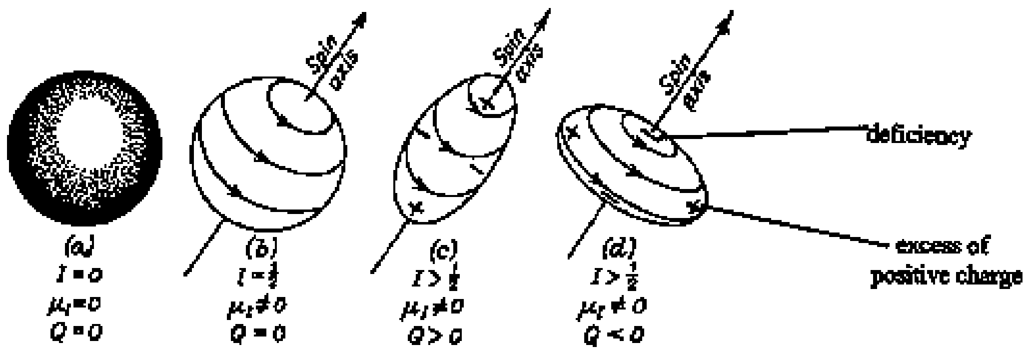
$$eQ = \int \rho r^2 (3\cos^2\alpha - 1)\, d\tau$$

where

e - proton charge C
Q - in cm^2
ρ - nuclear charge density
r - distance from center of gravity of positive charge to volume element dx dy dz = $d\tau$
α - angle between r and spin axis

eQ = electric quadrupole moment, EQM

- **If I > ½, Nucleus has EQM. EQM measures deviation of nuclear charge distribution from spherical symmetry.**



Elongated flattened

- **Charge distribution for nucleus, (a) which does not spin (i.e. I=0), (b) which has I= ½, and (c) and (d) where I > ½**

- **Spinning nuclear charge has electric field, extends outside nucleus.**
- **Interacts with non-spherical (asymmetric) charge distribution caused by :**

nonbonding electrons (lone pairs, p, d)

$>$

bonding electrons

$>$

Low symmetry environment,
charges on neighbouring ions

- **So nucleus orients in certain quantized directions with respect to this field, with different energy.**

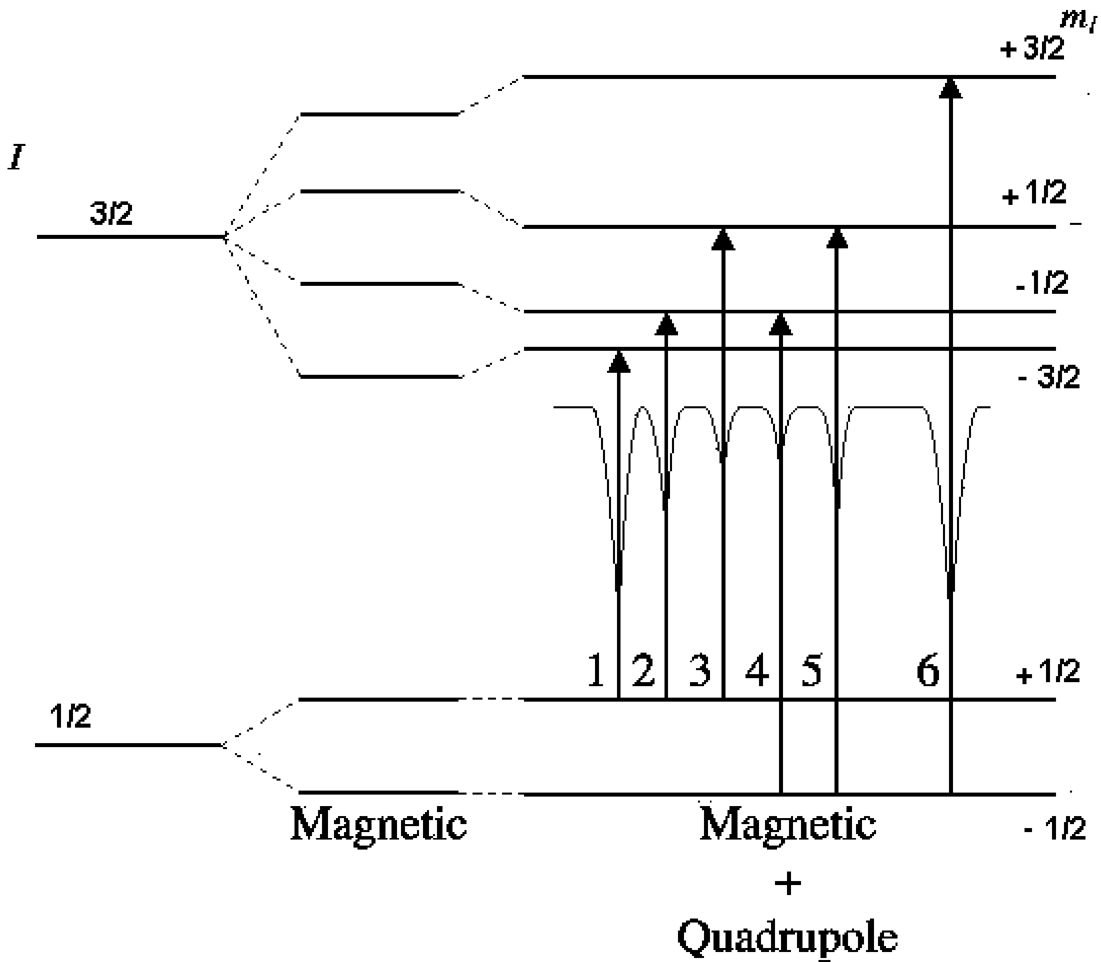
- **NQR spectra have been observed in the approximate range 1–1000 MHz.**

- **Most of the NQR work has been on molecular crystals.**
  - **For such crystals the coupling constants found do not differ very much from those measured for the isolated molecules in microwave spectroscopy.**

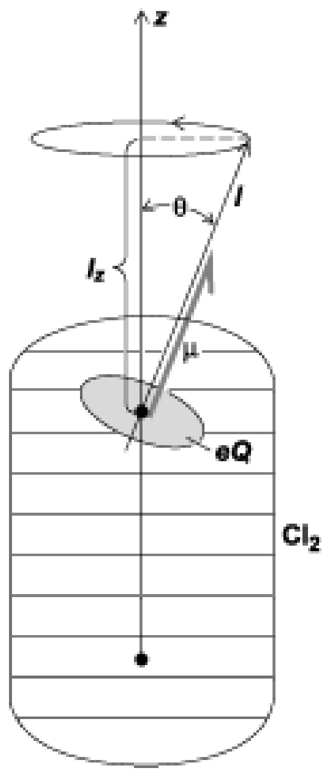
- **The most precise nuclear information which may be extracted from NQR data are quadrupole moment ratios of isotopes of the same element.**

- **If values for the axial gradient of the molecular electric field can be estimated from atomic fine structure data, then fair values of the quadrupole moment may be obtained.**

- **However, it has also proved very productive to use the quadrupole nucleus as a probe of bond character and orientation and crystalline electric fields and lattice sites, and extensive data have been accumulated in this area.**



The effect of a first order quadrupole perturbation on a magnetic hyperfine spectrum for a 3/2 → 1/2 transition. Lines 2,3,4,5 are shifted relative to line 1,6.



Interaction of ^{35}Cl nucleus with the electric field of a Cl_2 molecule.

Applications

- **NQR has been used principally for investigating the electronic structure of molecules**

- **Information regarding hybridization and the ionic character of the bond can be determined by comparing the quadrupole coupling constant in atomic and molecular state in the same nuclei**

- **Study of the structure of charge transfer complexes**

- **Detection of crystal imperfections**
  - **Small imperfections destroy symmetry of internal electric field, lead to splitting or broadening of NQR lines.**

- **Confirmation of nuclear spin Q. N. of an isotope from observed NQR lines.**

- **It can be used to detect certain chemical elements which have a magnetic dipole moment.**
  - **Amongst these is nitrogen-14 (^{14}N) which is a major constituent of explosives used in landmines, such as RDX and TNT. NQR has been described as "an electromagnetic resonance screening technique with the specificity of chemical spectroscopy" as it not only detects but can be used to identify the exact chemical compound used.**