M.Sc. II Sem

PHY-201 [Atomic and Molecular Physics]

Unit- III
Nuclear Magnetic Spectroscopy

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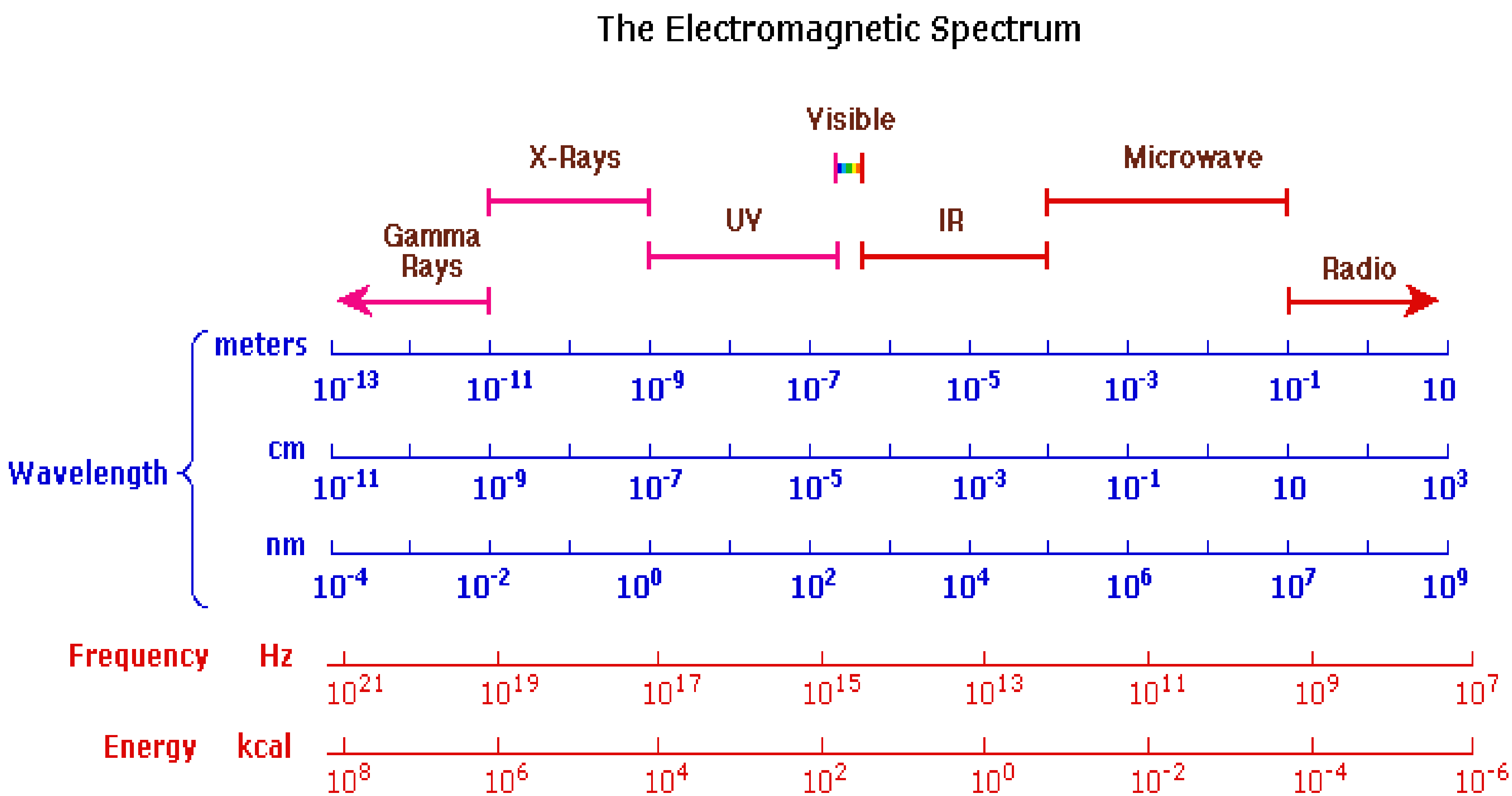
Outline

- Introduction to Spectroscopy
- Properties of Spin
- The Nuclear Magnetic Moment
- The Nuclear Spin Quantum Number
- Magnetic Properties of atomic Nuclei
- Nuclear precession in Magnetic field
    - Semi-Classical Description
    - Quantum mechanical Description
    - Quantum- classical correspondence

Introduction to Spectroscopy

Spectroscopy is the study of the interaction of electromagnetic radiation (light) with matter.



NMR uses electromagnetic radiation in the radio frequency range

- •Long wavelength, very low energy
- •Low energy has significant consequences:
- •Sharp signals (Good)
- •Poor sensitivity (Bad)
- •Longer experiment time (Bad)

Properties of Spin

Spin is a fundamental property of nature

- Any unpaired electron, proton, or neutron will possess a spin of ½
- Atomic nuclei, which are composed of protons and neutrons, may also possess spin

The spin of an atomic nucleus is determined by the number of protons and neutrons

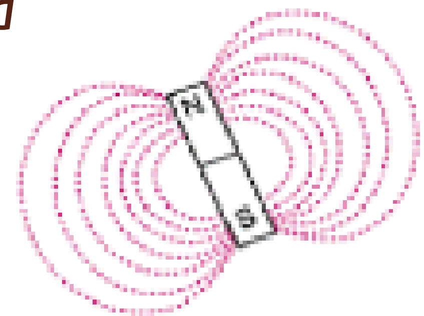
- Atoms with odd number of protons will have spin
- Atoms with odd number of neutrons will have spin
- Atoms with EVEN number of protons and neutrons will not have spin

The value of the nuclear spin is defined by **I, the *nuclear spin quantum number and can have values of (I = 0, 1/2, 1, 3/2, 2, 5/2, …)***

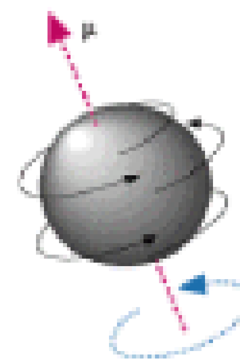
A nucleus of spin **I can exist in (2I+1) spin states.**

The Nuclear Magnetic Moment

•All atomic nuclei can be characterized by a nuclear spin quantum number, *I. I can be ≥0 and any multiple of ½*



•*Nuclei with I= 0 do not possess nuclear spin and consequently are termed 'NMR silent'.*



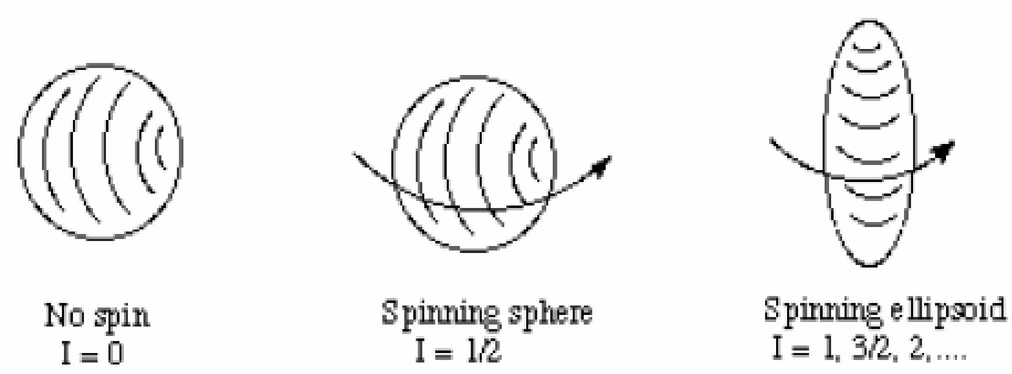
•*All nuclei with I≠0 possess spin, charge and angular momentum P, resulting in a nuclear magnetic moment μ.*

$$\mu = \gamma P$$

Where γ is the gyromagneticratio of the nucleus.

Values of γ can be positive or negative and determine the sense of precession and thus the direction of the magnetic moment.

I = the nuclear spin quantum number



For Nuclei of:	I =	Example
Odd Mass	Half Integer	^{1}H, ^{13}C
Even Mass/Even Charge	Zero	^{12}C, ^{16}O
Even Mass/Odd Charge	Integer	^{2}H, ^{14}N

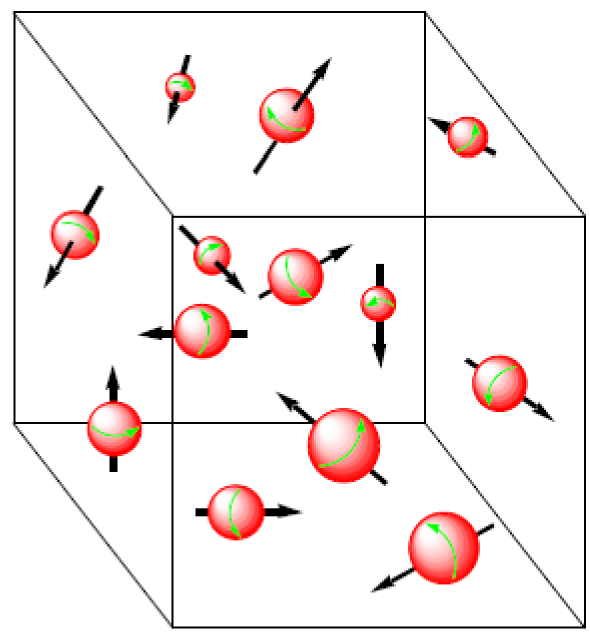
If I = 0, NMR Inactive

If I ≥1, Quadrupolar (non-spherical nuclear charge distribution)

Magnetic properties of atomic nuclei

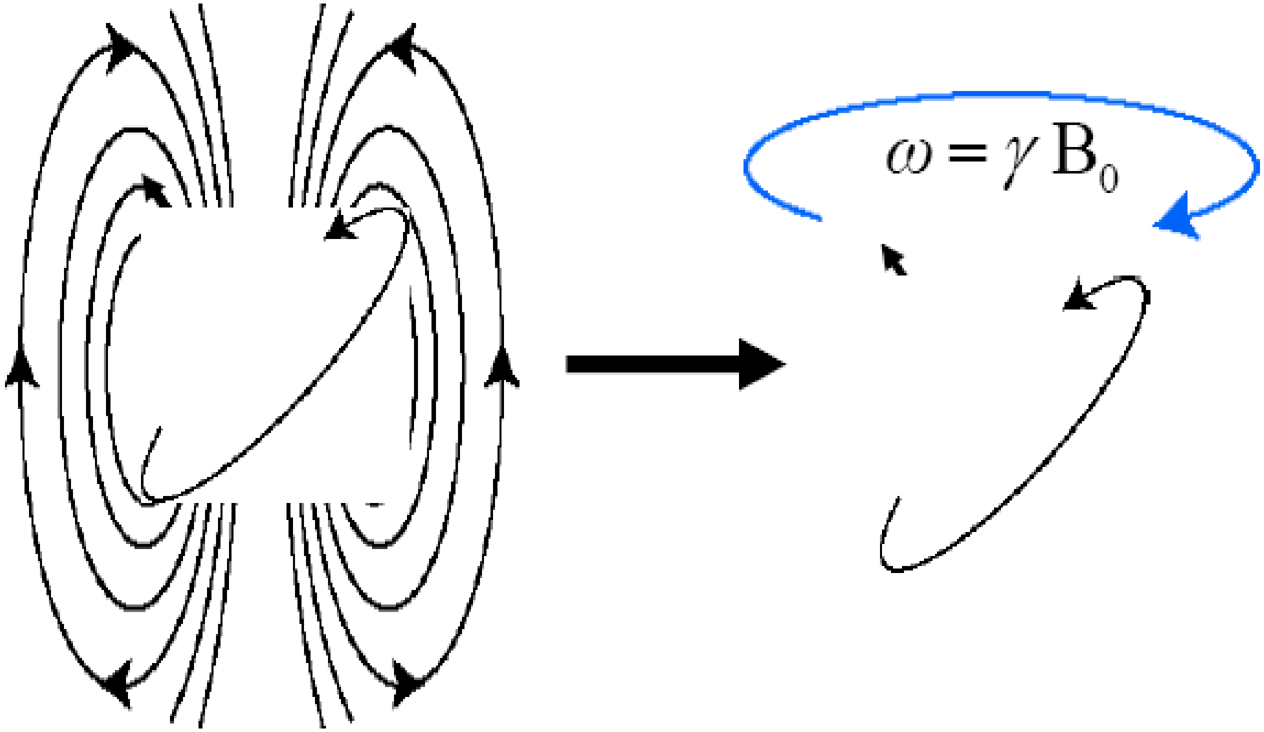
- The magnetic moment (**μ)is a vector quantity that has both magnitude and direction**

- •In the absence of an external magnetic field the magnetic moments **(μ)are randomly orientated.**



Nuclear Precession in a Magnetic Field

Semi-Classical Description



Magnetic Field B_0

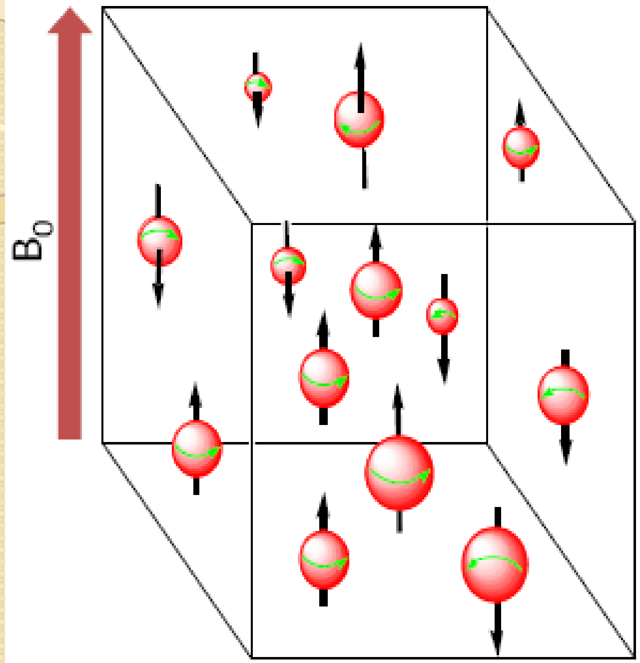
Example:

For ^{1}H nuclei (protons)
(γ=2.68x10^8 rad T^{-1} s^{-1})
in a magnetic field of
11.74 Tesla
ω=3.15 x 10^9 rad s^{-1}
or
$\nu=\omega/2\pi$=5x10^8 s^{-1}
= 500 MHz

The Magnetic Field (**B_0**) exerts torque on angular momentum (**L**) and causes Nuclear Precession, analogous to precession of spinning top. The frequency of the precession (**ω**), often called the Larmor frequency, is proportional to the gyromagnetic ration (γ) and the strength of the external magnetic field (**B_0**).

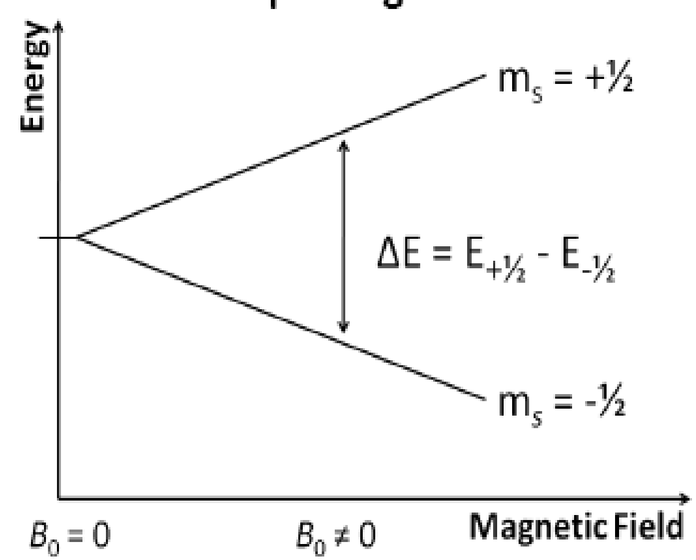
Nuclear Precession in a Magnetic Field

Quantum Mechanical Description



In the macroscopic world the two magnets can be aligned in an infinite number of orientations. At the atomic level, these alignments are **quantized** and the number of orientations (spin states) are equal to **2I+1**. We will only deal with spin ½ nuclei.

The different **quantized** orientations will each have an energy level determined by the Zeeman splitting

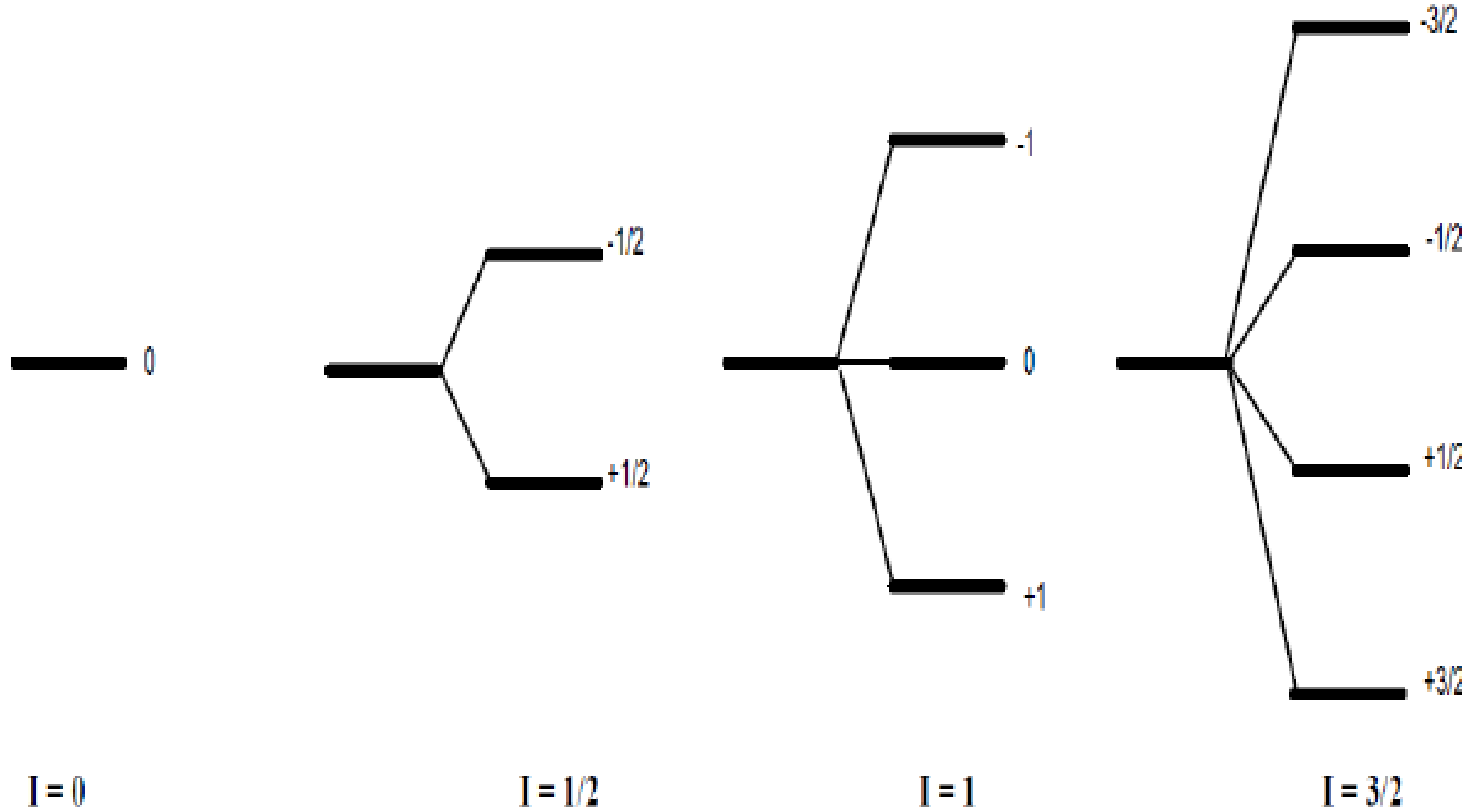


Nuclear Precession in a Magnetic Field

Quantum Mechanical Description

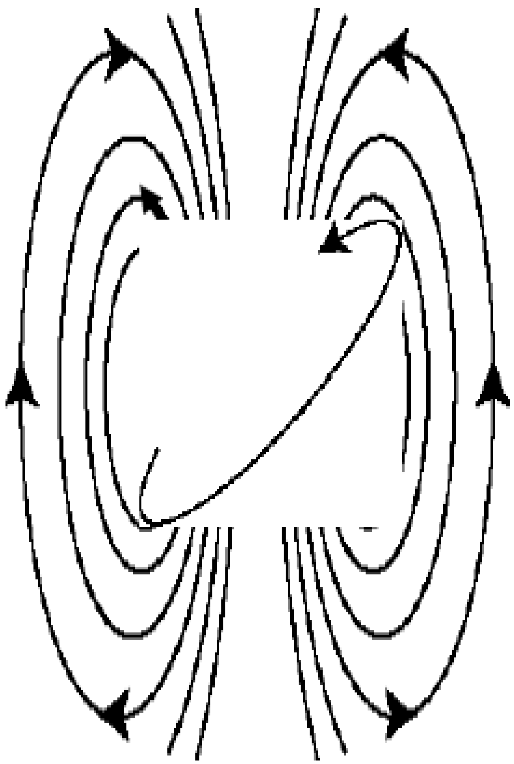
The energy levels are more complicated for I > 1/2

Zeeman Splitting

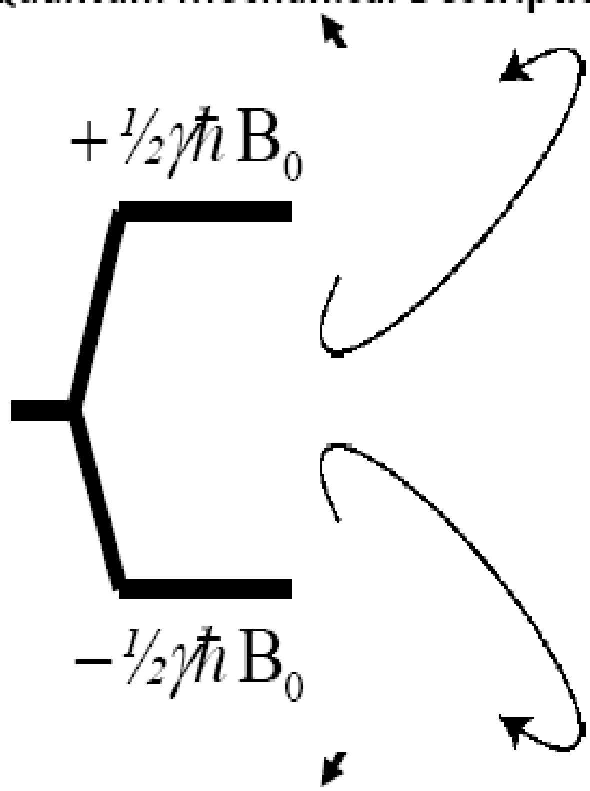


Nuclear Precession in a Magnetic Field

Quantum Mechanical Description



Magnetic Field B_0



Zeeman Splitting

$$\Delta E = \gamma\hbar B_0$$

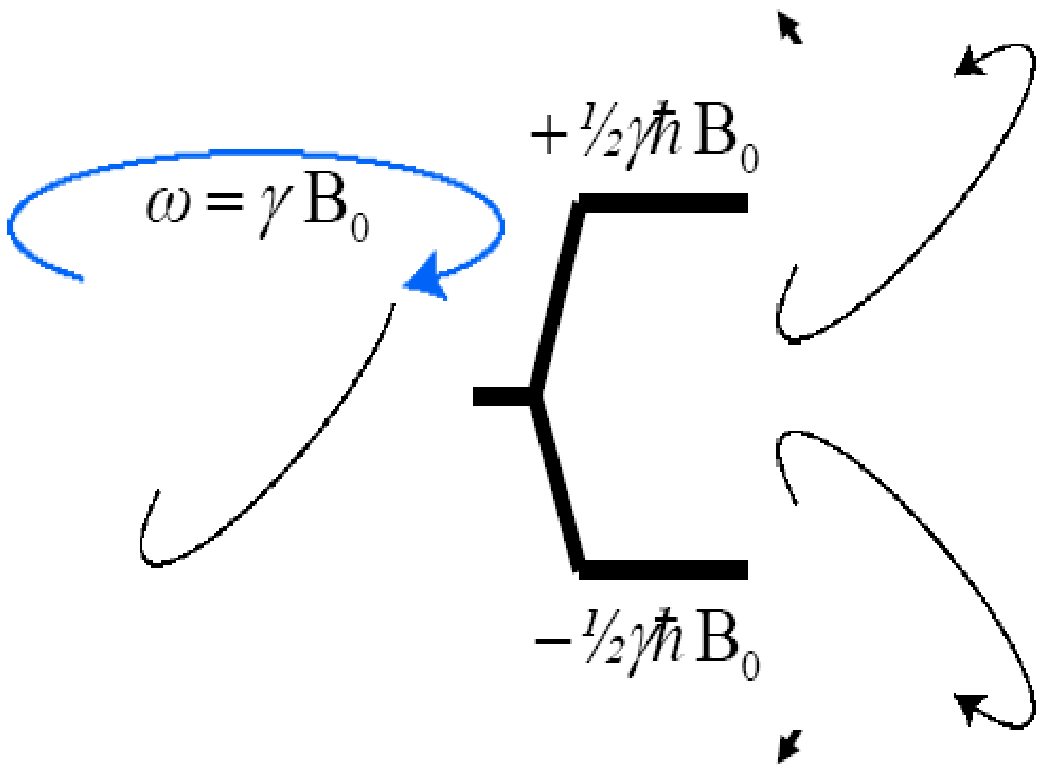
Knowing ΔE, we can stimulate the transition between these two states by applying an RF field such that:

$$E = h\nu = \hbar\omega$$

In NMR spectroscopy we are going to perturb the spin states by stimulating transitions between the energy levels.

Nuclear Precession in a Magnetic Field

Quantum-Classical Correspondence



$$\Delta E = \gamma\hbar B_0$$

Knowing ΔE, we can stimulate the transition between these two states by applying an RF field which satisfies the resonance condition:

$$E = \hbar\omega = \gamma\hbar B_0$$

Thank You