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FAST FIELD CYCLING NMR RELAXOMETRY

THE BASIC PRINCIPLES OF NUCLEAR RELAXATION AND ITS APPLICATIONS IN ENVIRONMENTAL SCIENCE

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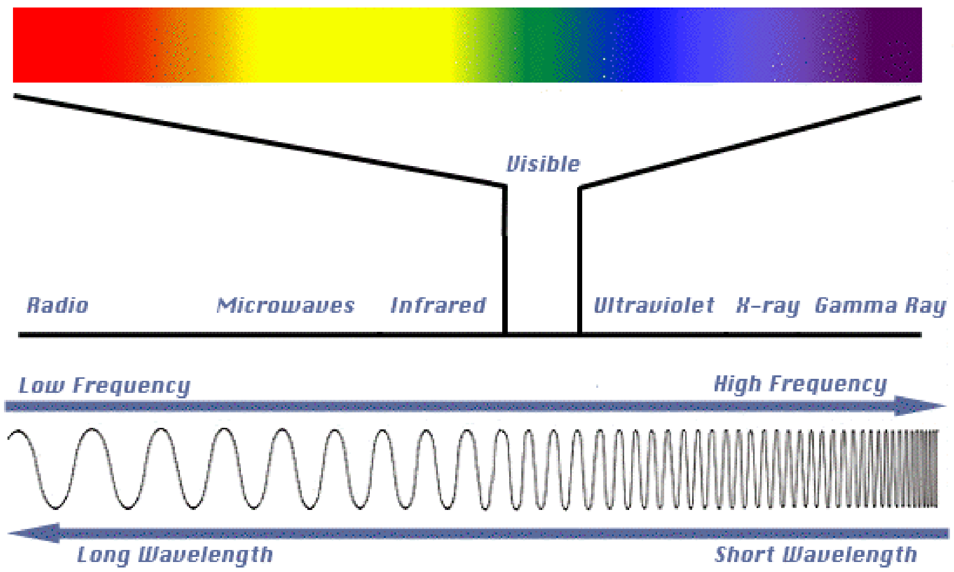
NMR Spectroscopy

NMR spectroscopy is a form of ***absorption*** spectrometry.



Most absorption techniques (*e.g.* – Ultraviolet-Visible and Infrared) involve the electrons… in the case of NMR, it is the ***nucleus*** of the atom which determines the response.

An applied (magnetic) field is necessary to "develop" the energy states (produce a separation of the energy states) necessary for the absorption to occur.

Application of NMR

NMR is utilized widely not only Physics and/or chemistry but also medical diagnostics (MRI) and so on.

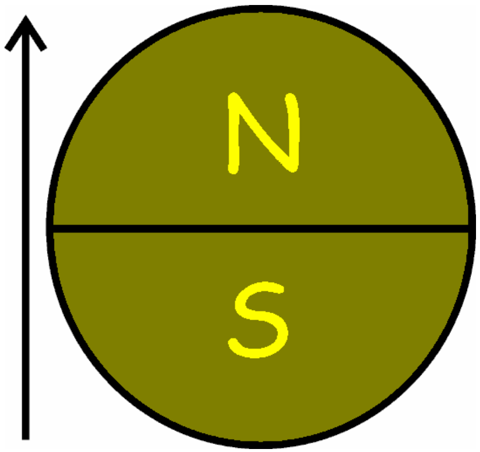
For example;

- Physics
  - Condensed matter physics、Magnet, Superconductor、and so on
- Chemical
  - Analysis and/or identification of material
- Biophysics
  - Analysis of Protein structure
- Medical
  - MRI (Magnetic Resonance Image)

Brain tomograph

Why The Interest In Dynamics?

- Function requires motion/kinetic energy
- Entropic contributions to binding events
- Protein Folding/Unfolding
- Uncertainty in NMR and crystal structures
- Effect on NMR experiments- spin relaxation is dependent on rate of motions → know dynamics to predict outcomes and design new experiments
- Quantum mechanics/prediction (masochism)



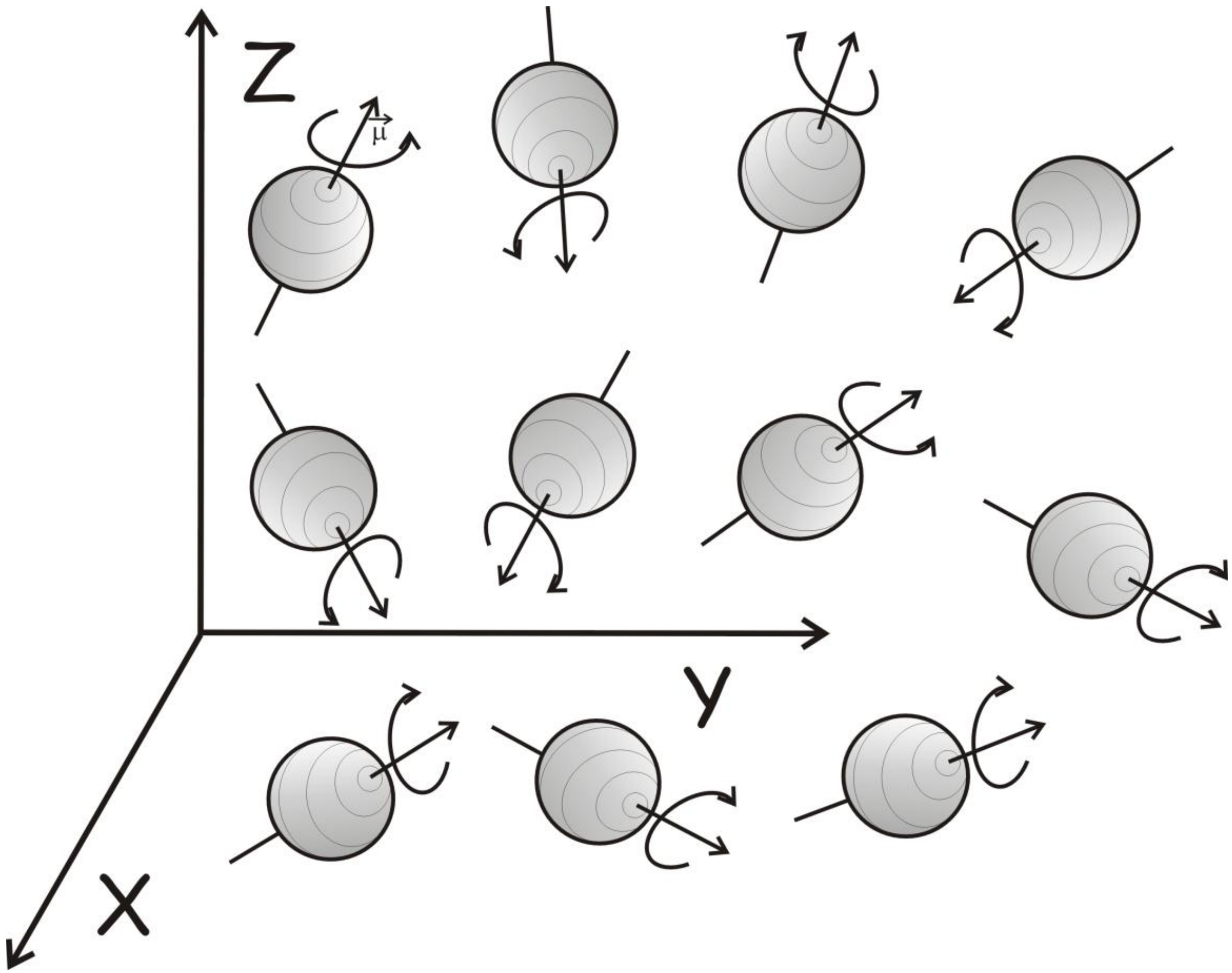
Magnetic moment $\bar{\mu} = \frac{\gamma \bar{I} h}{2\pi} = \gamma \hbar \bar{I}$

γ gyromagnetic ratio

$\hbar = \frac{h}{2\pi}$ Planck constant

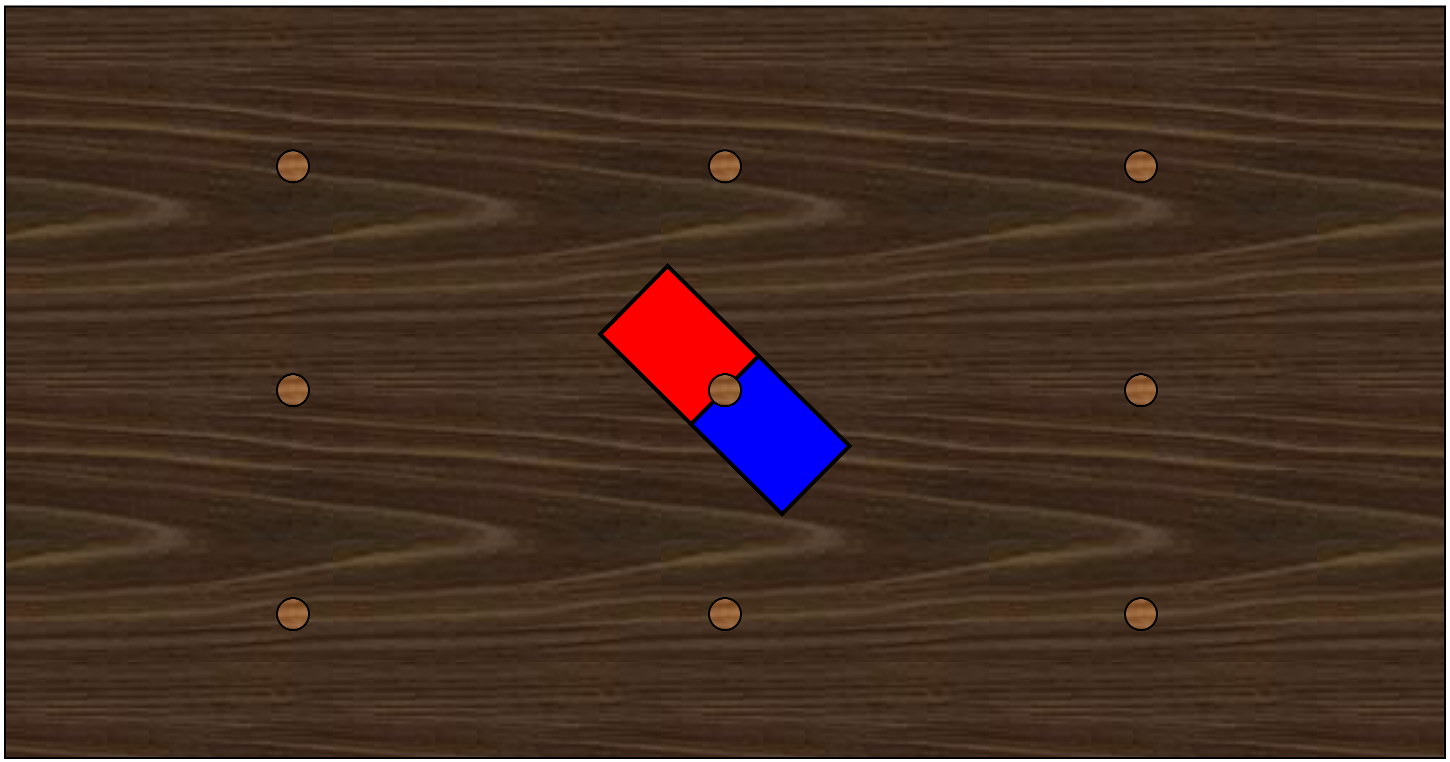
Table 1: properties of NMR-active nuclei (from Bruker Almanac 2005)

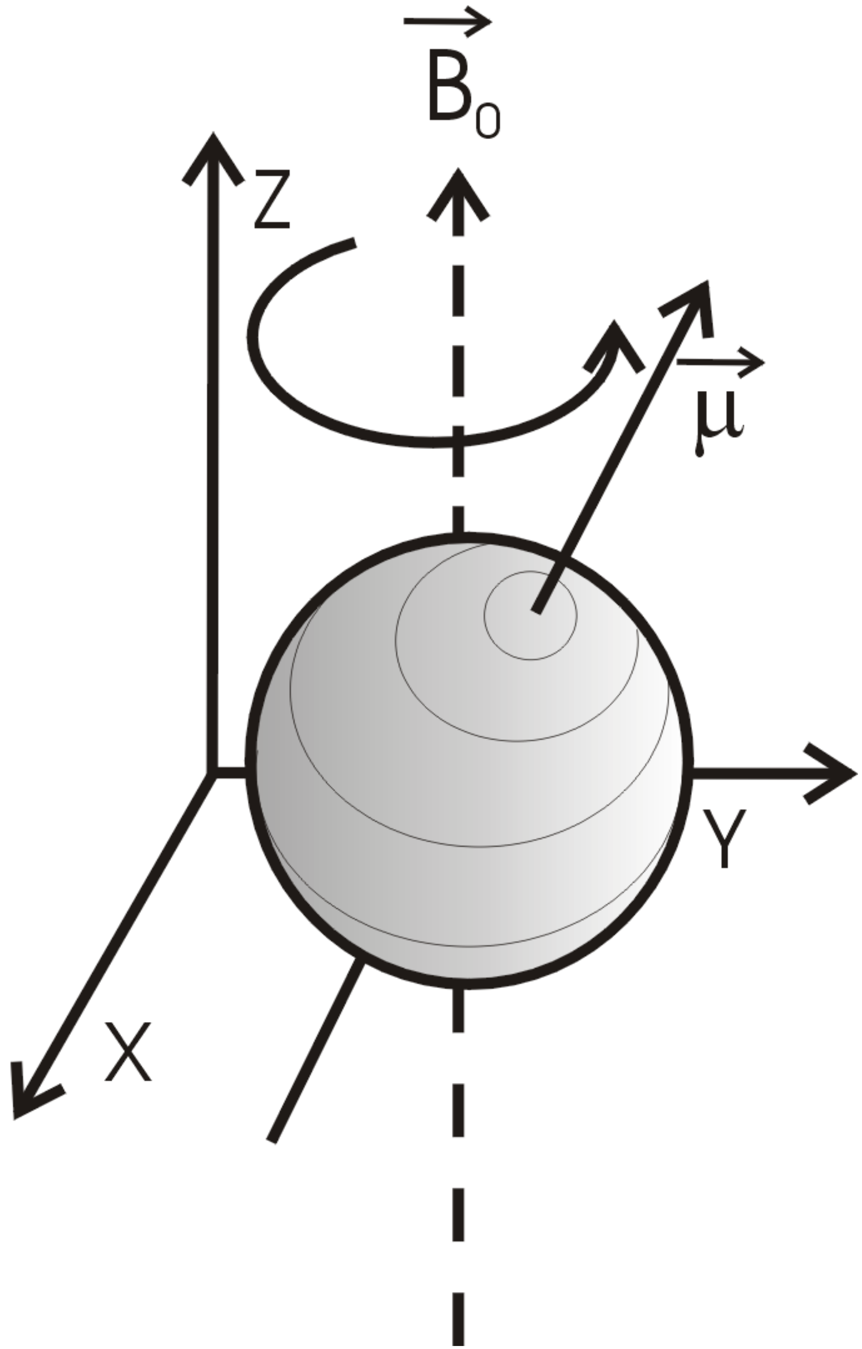
Nucleus	I	γ (x10^7 rad $T^{-1}s^{-1}$)	Natural abundance (%)
^{1}H	1/2	26.8	99.99
^{13}C	1/2	6.7	1.10
^{15}N	1/2	-2.7	0.37
^{17}O	5/2	-3.6	0.04
^{19}F	1/2	25.2	100.00
^{23}Na	3/2	7.1	100.00
^{25}Mg	5/2	-1.6	10.00
^{27}Al	5/2	7.0	100.00
^{29}Si	1/2	-5.3	4.67
^{31}P	1/2	10.8	100.00
^{55}Mn	5/2	6.6	100.00
^{113}Cd	1/2	-6.0	12.22
^{119}Sn	1/2	-10.0	8.59


Z
μ
y
X

Development of Energy States of Nuclei in an Applied Magnetic Field

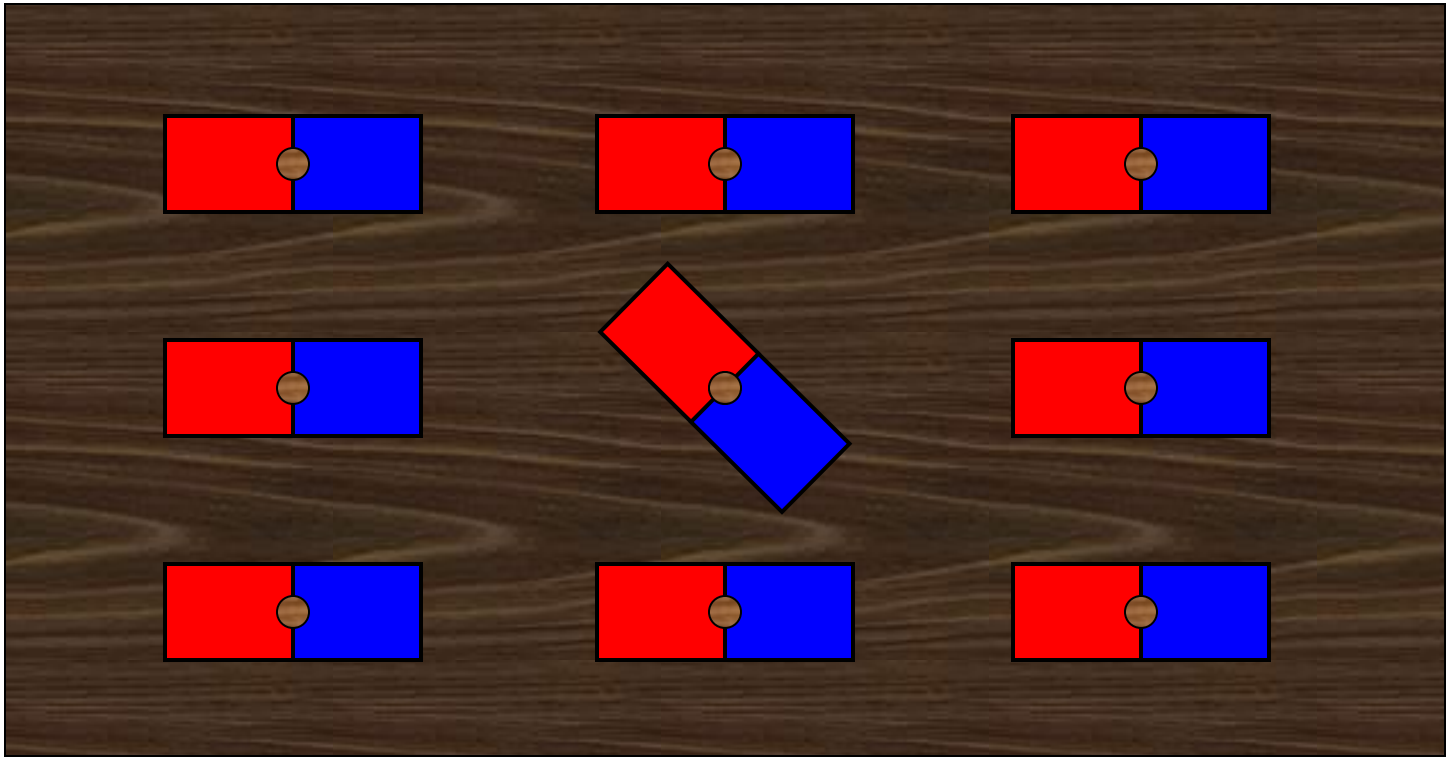
Spin ½ Nucleus = "Bar Magnet"

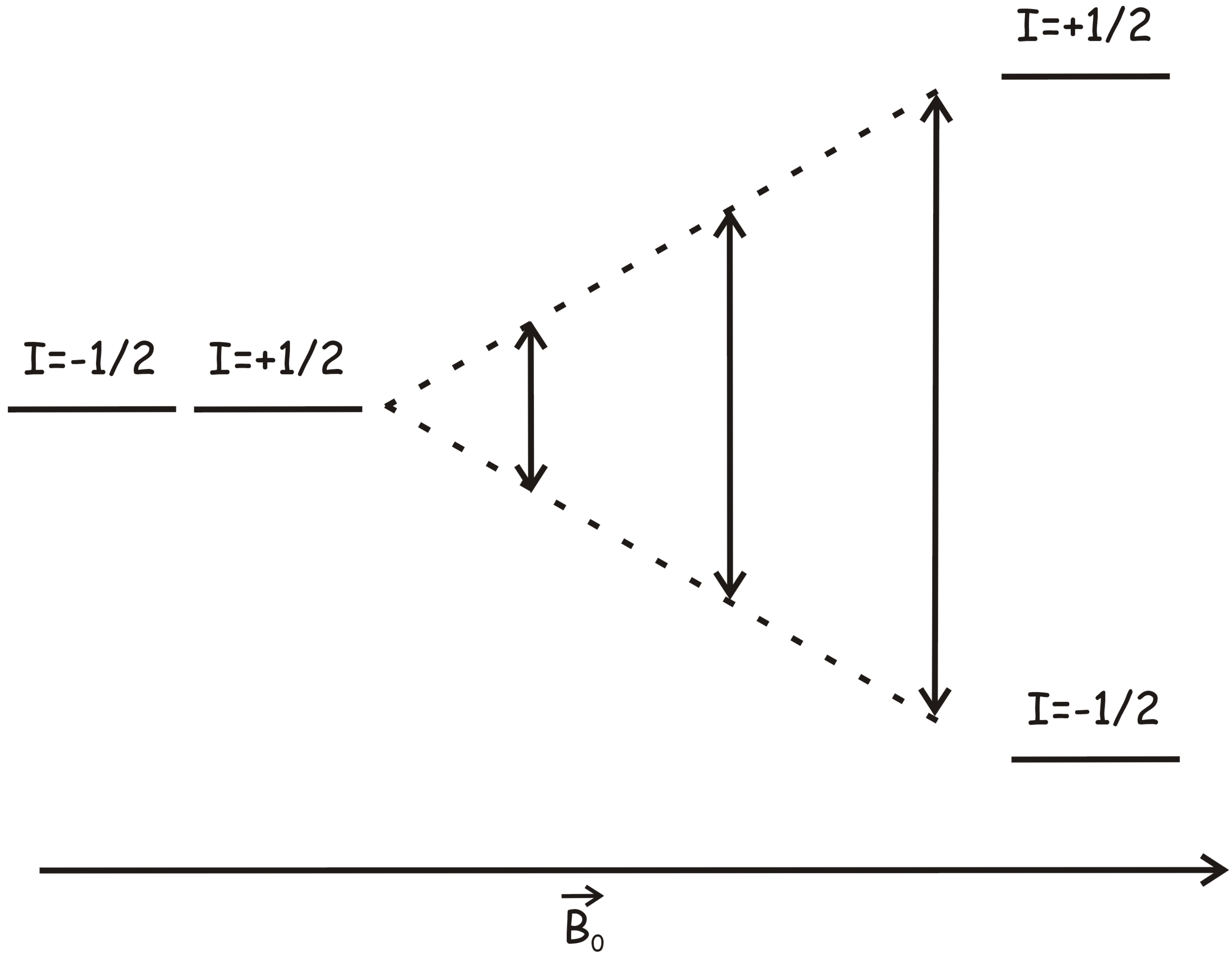



$\vec{B}_0$
Z
$\vec{\mu}$
Y
X

Development of Energy States of Nuclei in an Applied Magnetic Field

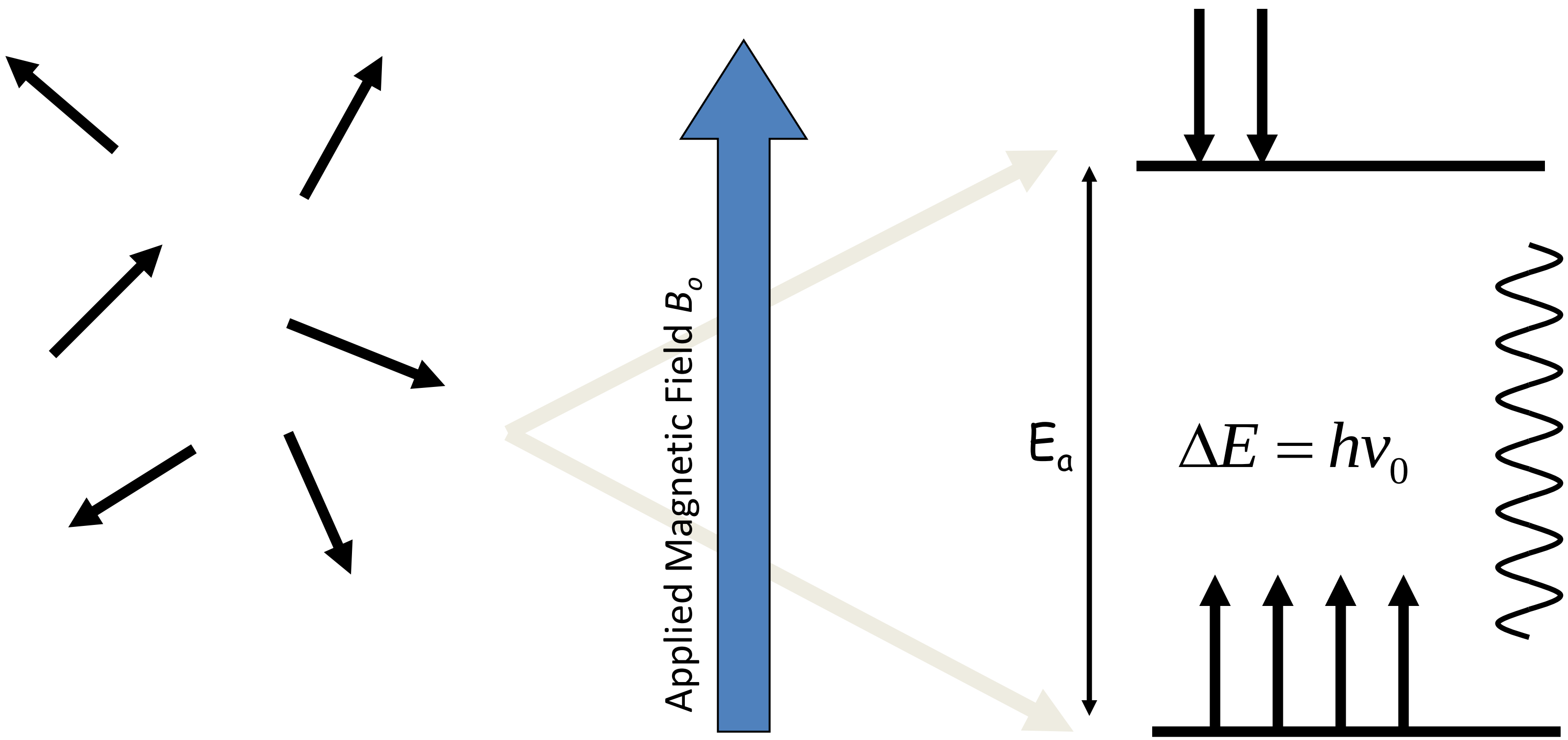
Spin ½ Nucleus = "Bar Magnet"





I=+1/2
I=-1/2
I=+1/2
I=-1/2
$\vec{B}_0$

Populations of the Energy States of Hydrogen Nuclei (Spin ½ Nuclei) in a Magnetic Field



Without an applied magnetic field, there is no division of energy states to discuss.

Development of Energy States of Nuclei in an Applied Magnetic Field

Potential energy, *E*, and the energy difference between two given states:

In general, the potential energy, *E*, of a given energy state/orientation is related to the magnetic quantum number by:

$$E_m = -\frac{\gamma m h}{2\pi} B_0$$

Transition of Nucleus from One Energy State to Another

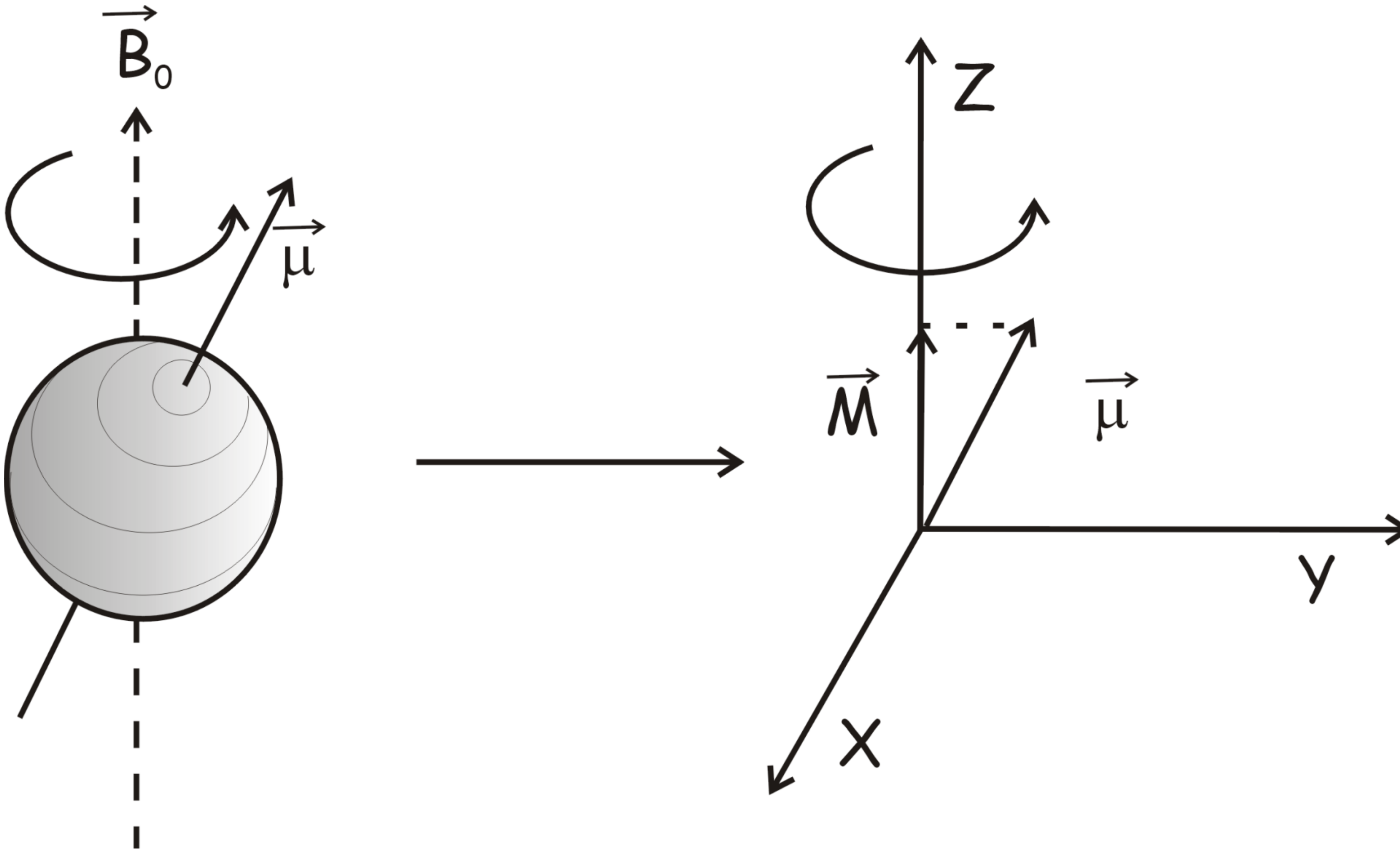
Planck relationship, between ΔE and an applied radio frequency, v_0 is:

$$\Delta E = hv_0$$

$$v_0 = \frac{\Delta E}{h}$$

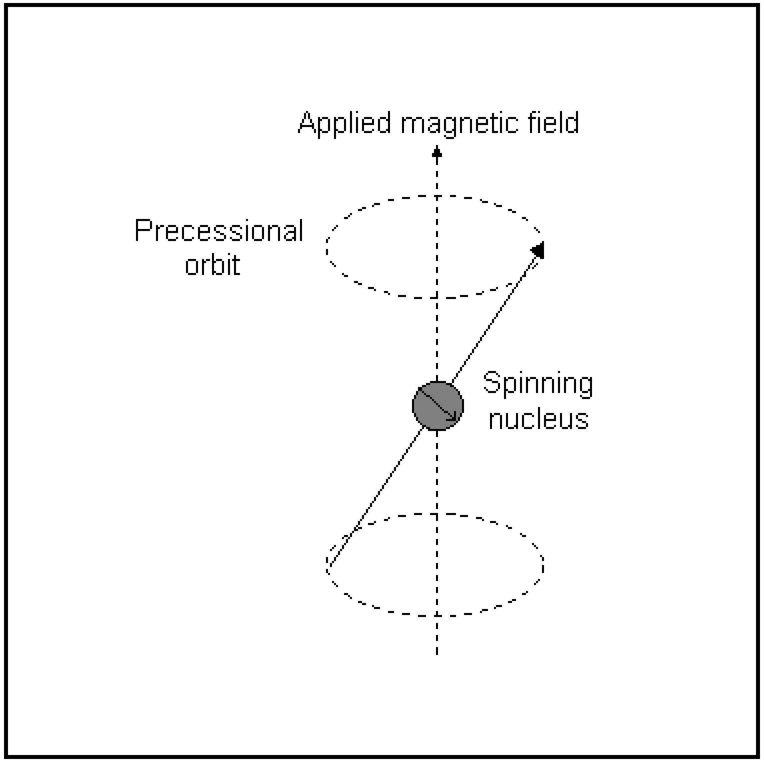
$$v_0 = \frac{\left(\frac{\gamma h}{2\pi} B_0\right)}{h} = \frac{\gamma}{2\pi} B_0 \text{ or } v_0 = \frac{\gamma B_0}{2\pi}$$

$$v_0 \propto \Delta E \propto B_0$$

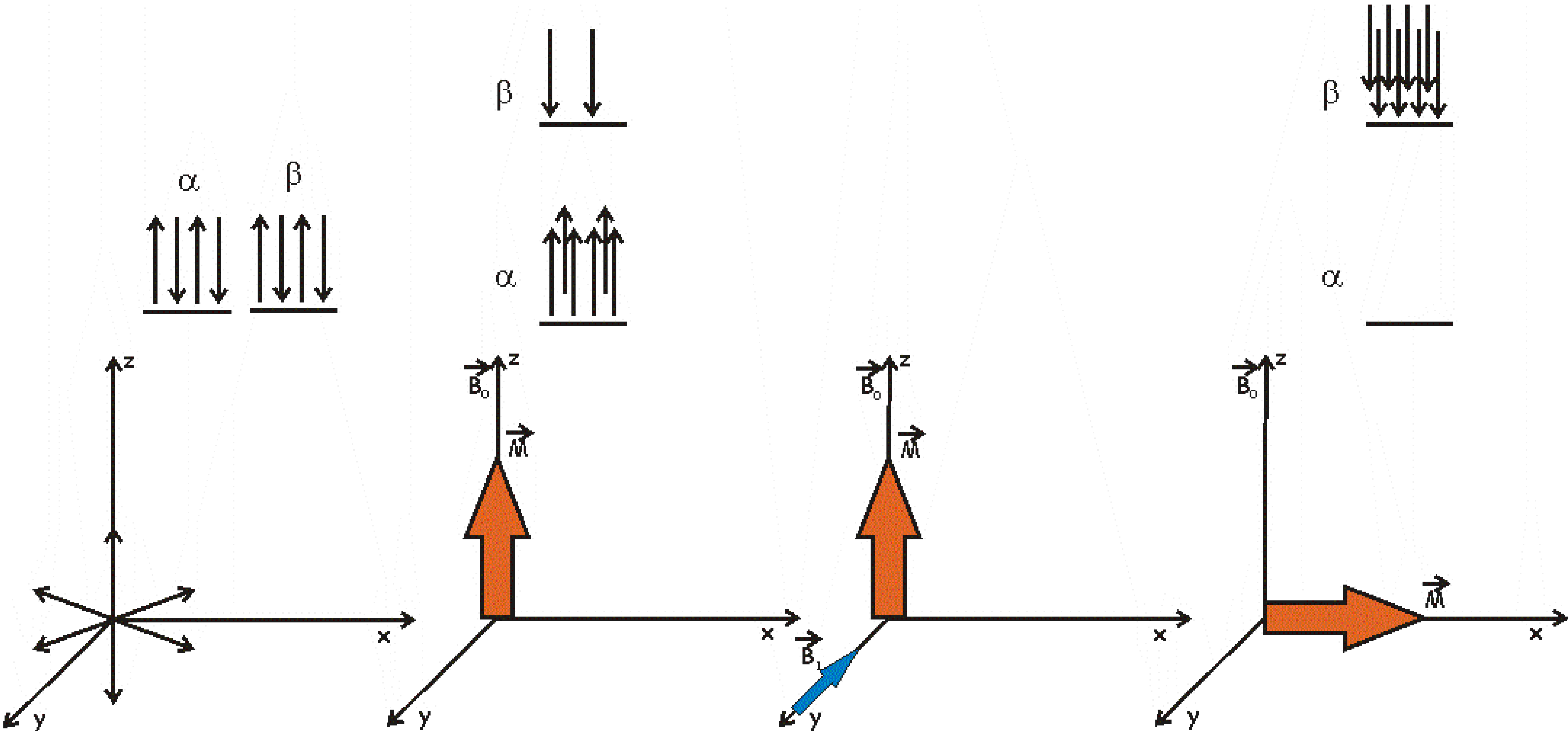


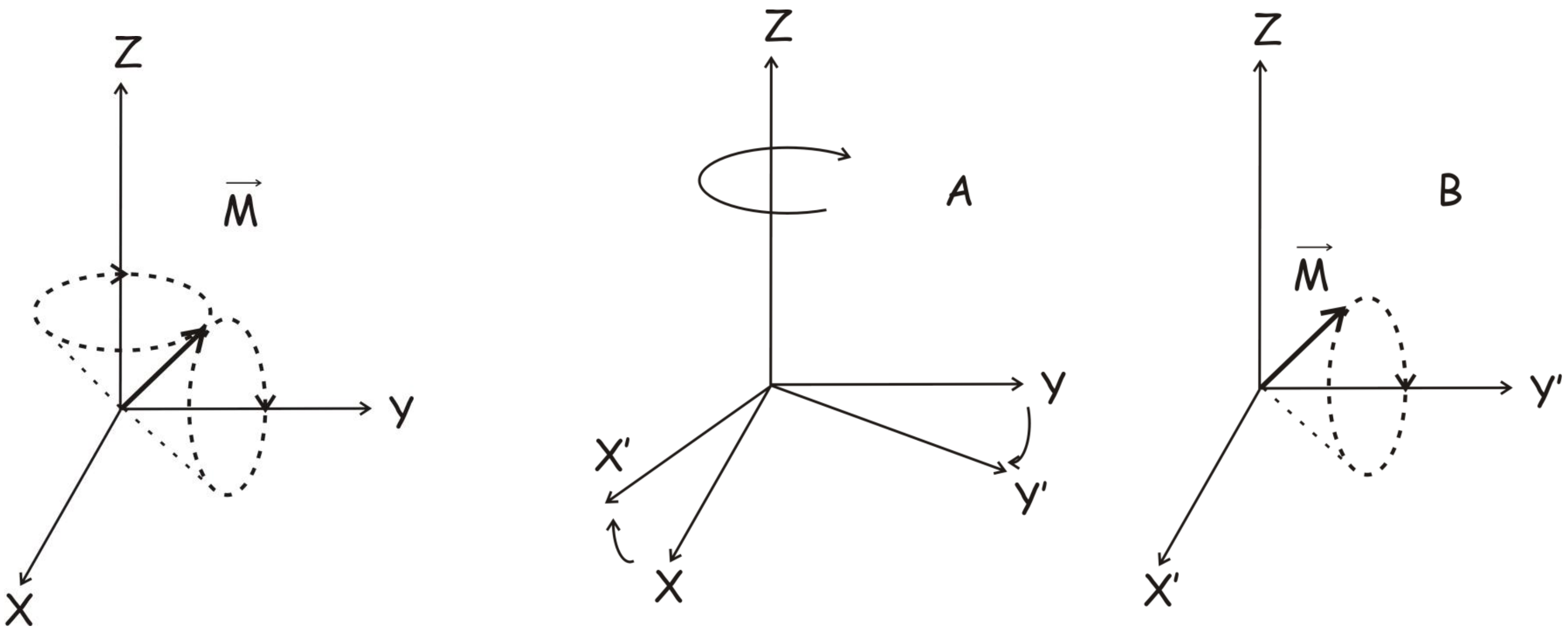
$\vec{B}_0$
$\vec{\mu}$
Z
$\vec{M}$
$\vec{\mu}$
y
X

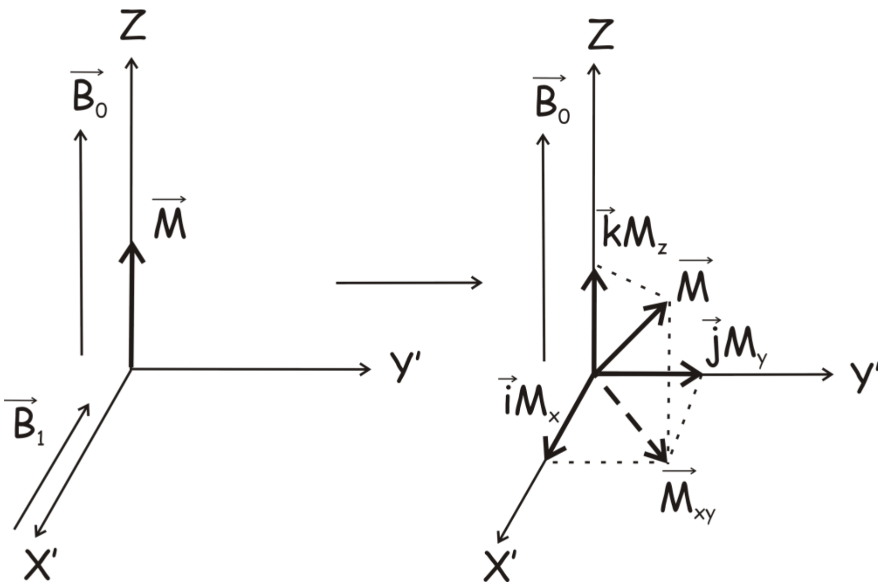
NMR: Relying on Radio Frequencies and Nuclear Precession



NMR phenomenon




Z
$\vec{M}$
Y
X
Z
A
Y
X'
Y'
X
Z
B
$\vec{M}$
Y'
X'



$$\frac{\partial M_z(t)}{\partial t} = \gamma\left(\overline{M}(t)\times\overline{B_0}(t)\right)_z - R_1\left(M_z(t) - M_0\right)$$

$$\frac{\partial M_x(t)}{\partial t} = \gamma\left(\overline{M}(t)\times\overline{B_0}(t)\right)_x - R_2 M_x(t)$$

$$\frac{\partial M_y(t)}{\partial(t)} = \gamma\left(\overline{M}(t)\times\overline{B_0}(t)\right)_y - R_2 M_y(t)$$

$R_1=1/T_1$ spin lattice relaxation time

$R_2=1/T_2$ spin-spin relaxation time