The world of "tiny nuclear magnets"

T. G. Ajithkumar
Scientist, Central NMR Facility
National Chemical Laboratory


NMR FACILITY
BRUKER
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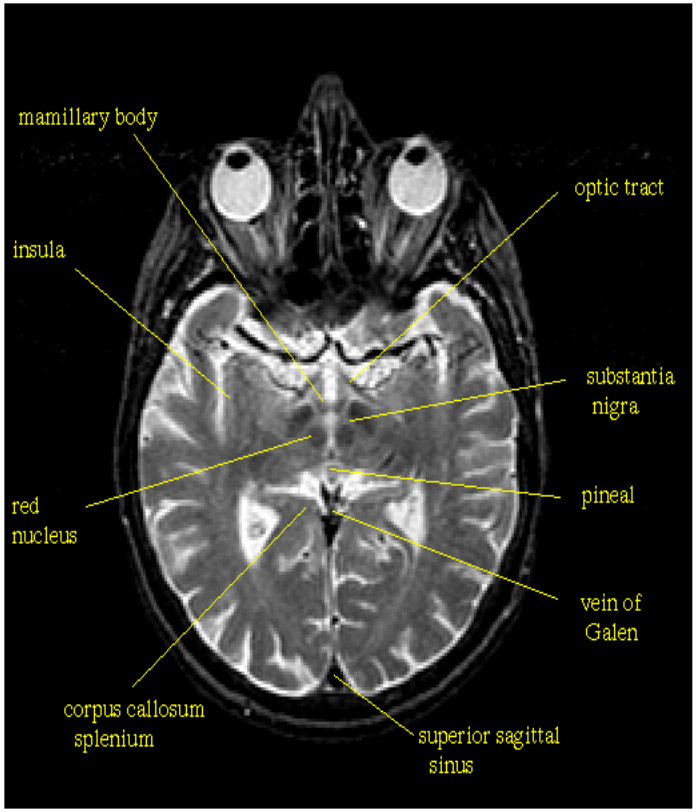
Why Nuclear Magnetic Resonance Spectroscopy (NMR) ?

- The most powerful analytical tool for synthetic chemists.
- Study of reaction kinetics.
- Three dimensional structural studies (protiens, RNA/DNA complexes).
- Structure function relationships for drug design.
- In medicine, magnetic resonance imaging (MRI) has become a very important diagnostic tool.
- Solids state NMR to study structure and dynamics of a variety of materials like polymers, catalysts, nanomaterials.

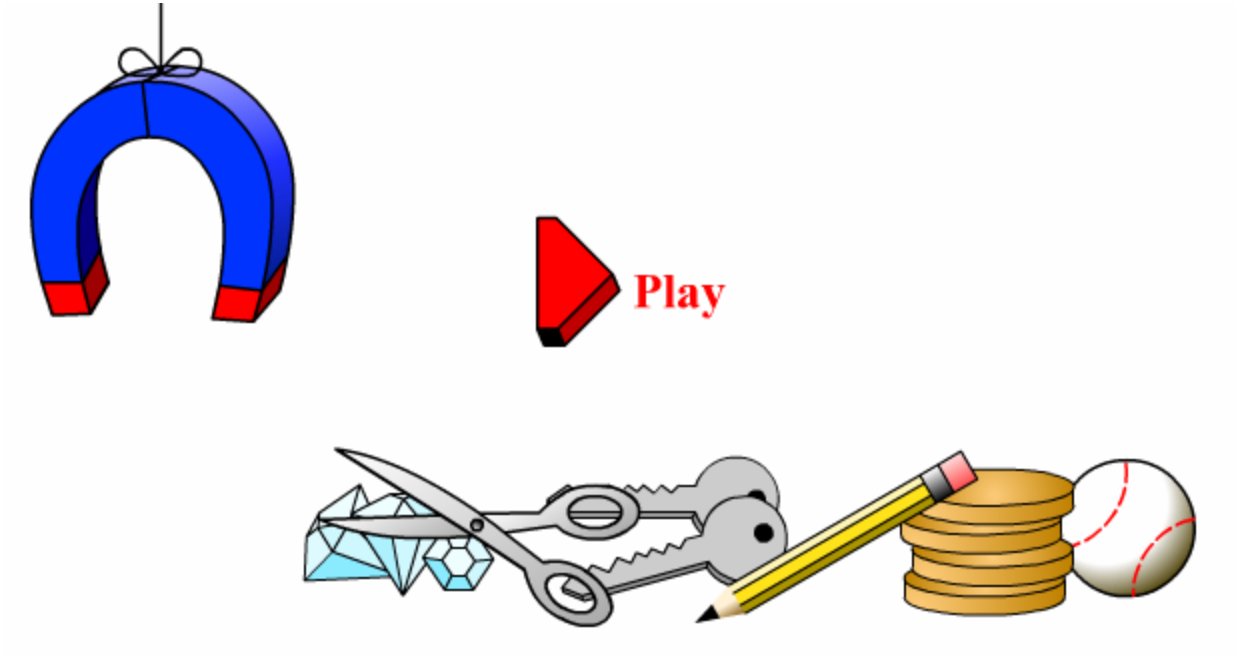
MRI

MRI of human brain



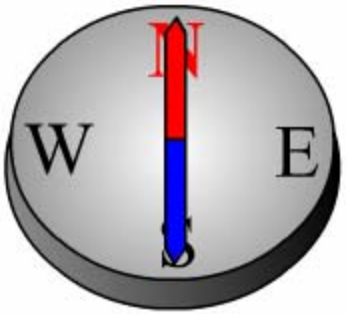
Data sources : Left - The Whole-brain Atlas, K. A. Johnson and J. A. Becker, Harvard; Right - SMIS UK Ltd.

Magnetism

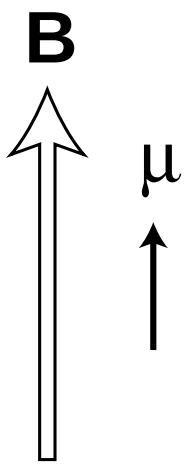


Magnetic Field

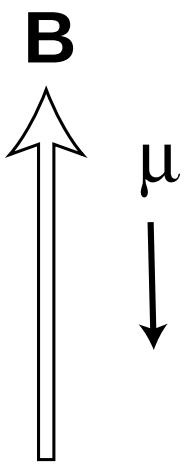
In this demonstration we will use an ordinary bar magnet and a regular compass.



We will demonstrate the magnetic field of the bar magnet by circling the compass around the bar magnet and watching the needle of the compass.

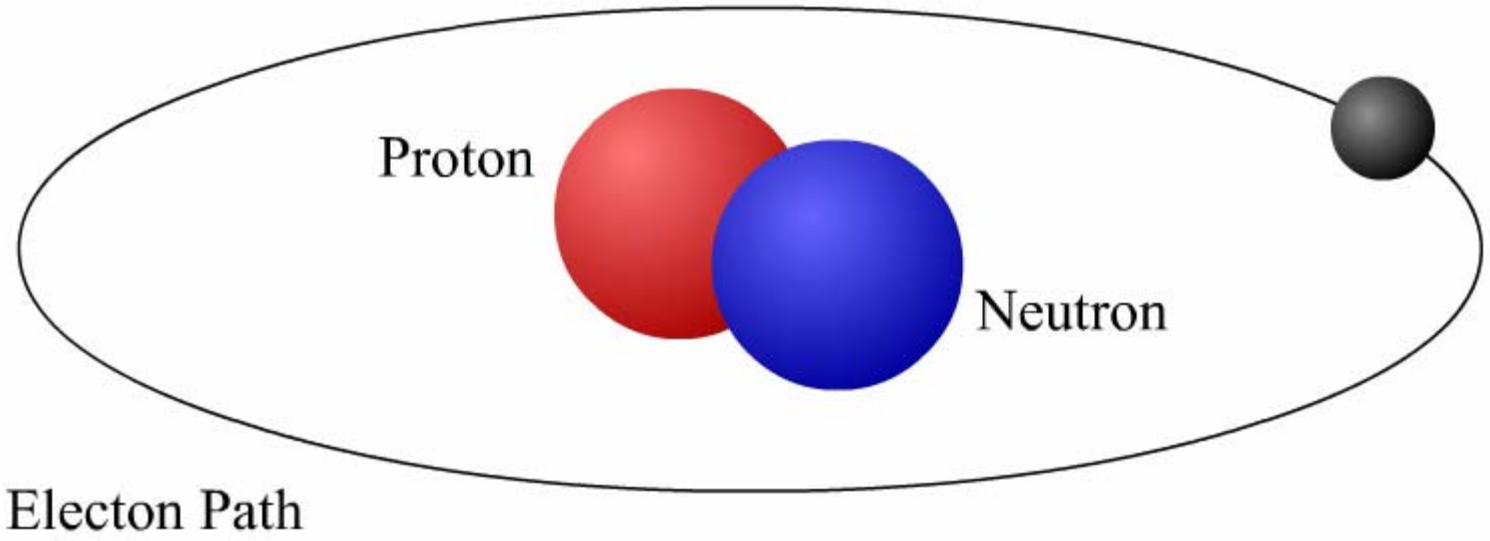


Low Energy

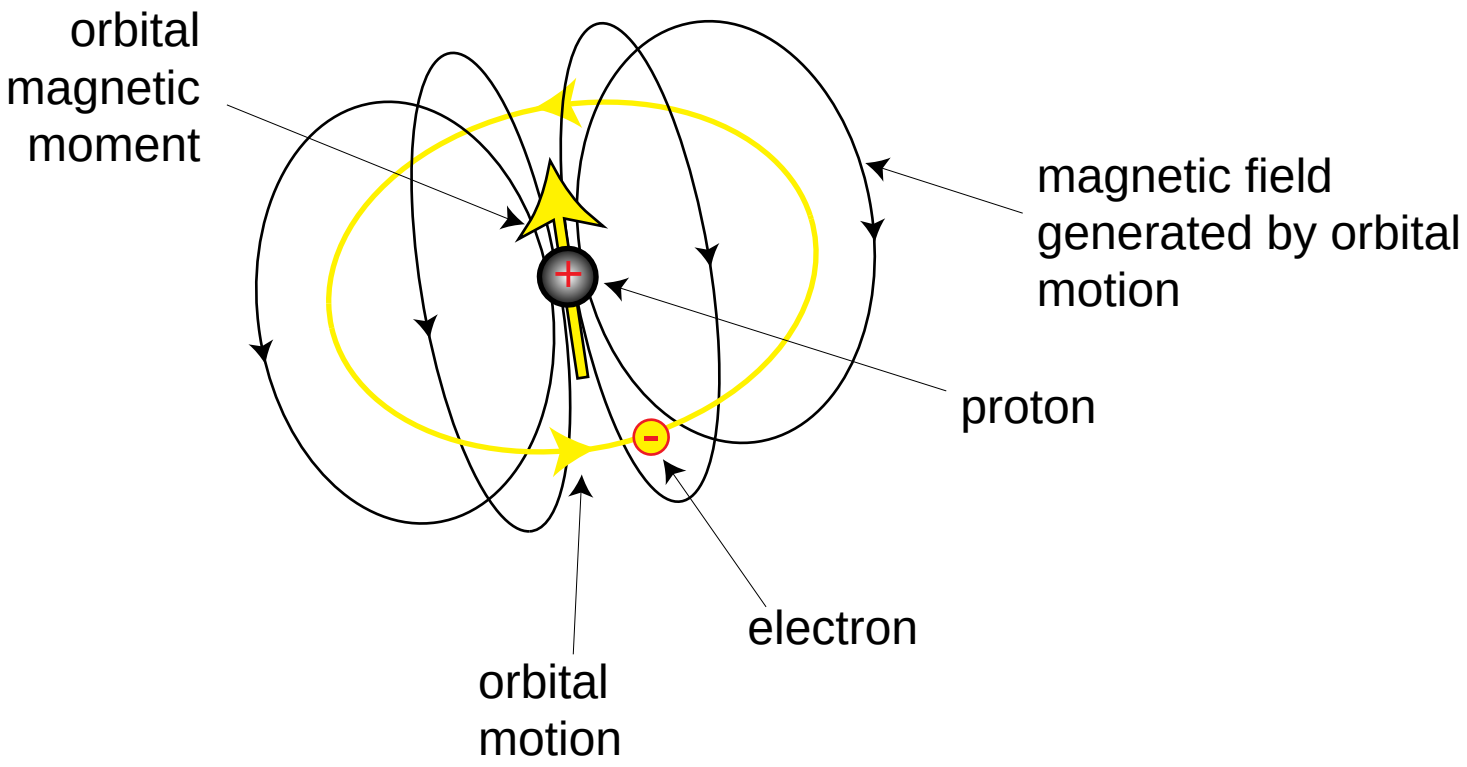


High Energy

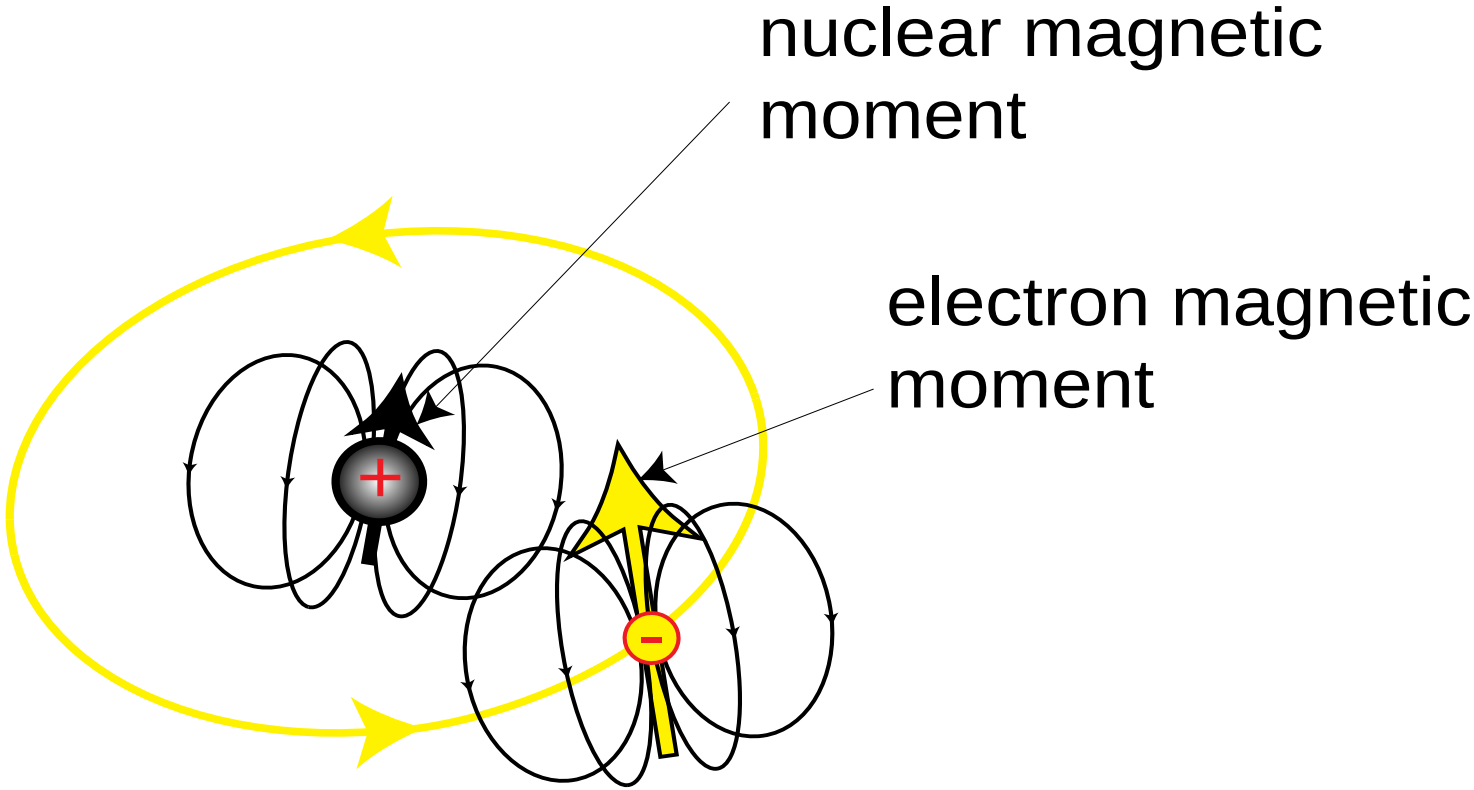
The atom



The origin of magnetism

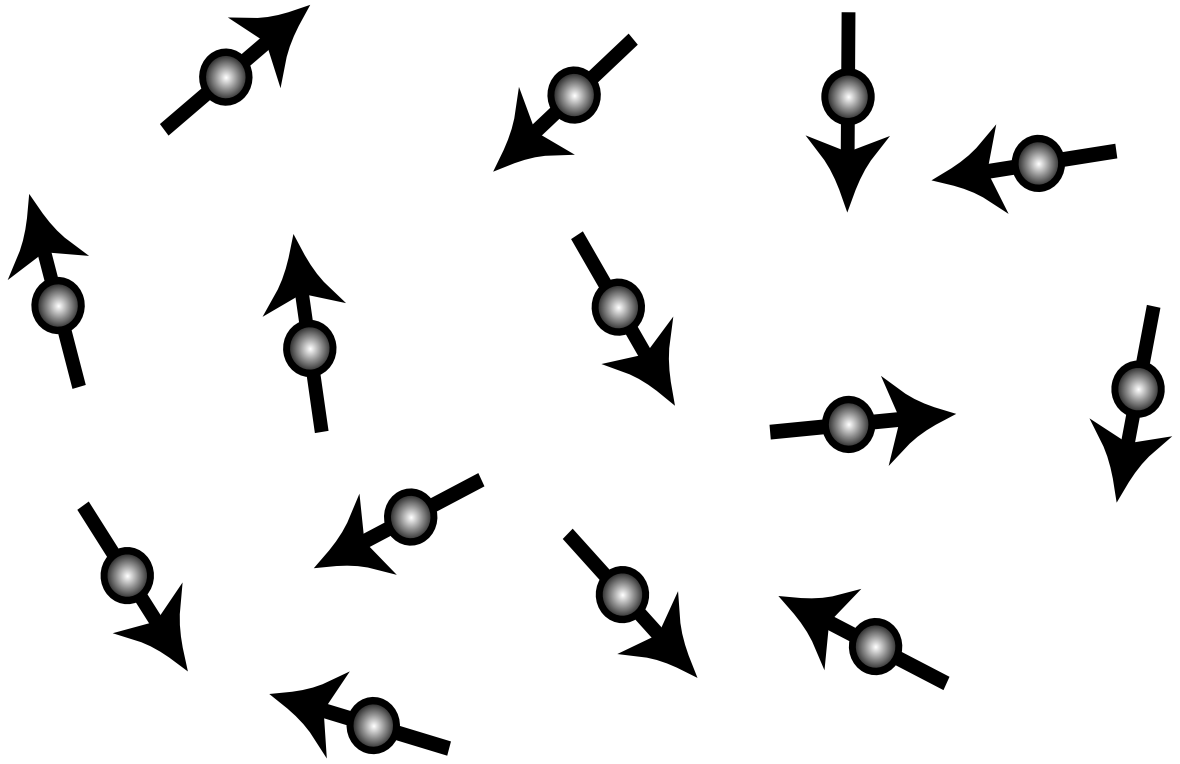


Magnetic moments



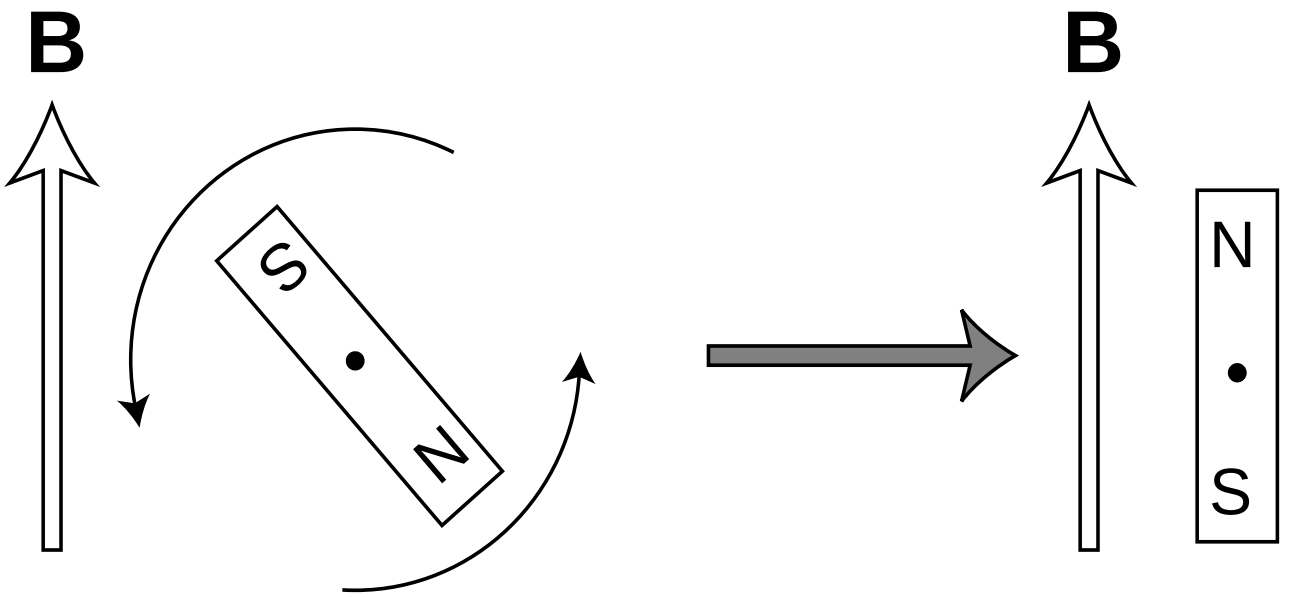
The nuclear magnetic moment is many orders of magnitude weaker than the electron magnetic moment.

No external Field



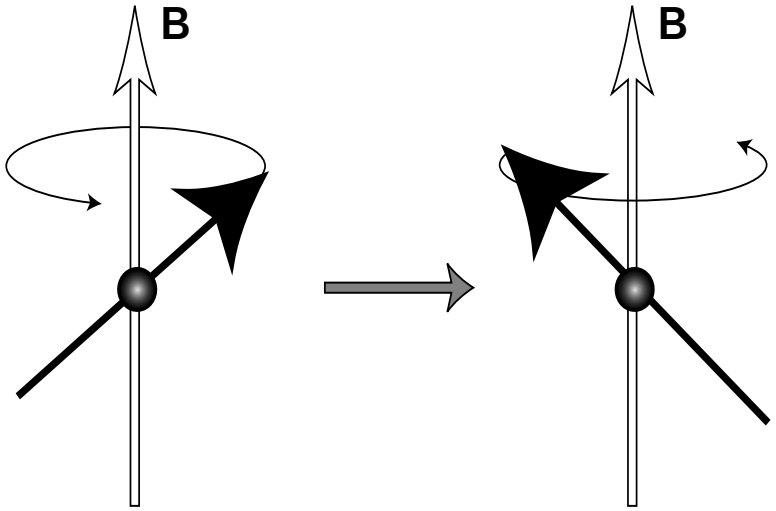
In the absence of a Magnetic Field, the magnetic moments are aligned in all random directions and thus the net magnetic moment is zero

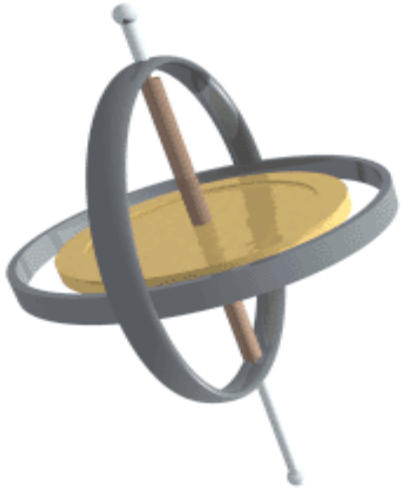
On application of external Field



A bar magnet aligns itself in the direction of the magnetic field !

Larmour Precession





Precession/Larmour Frequency $\nu = -\gamma B$

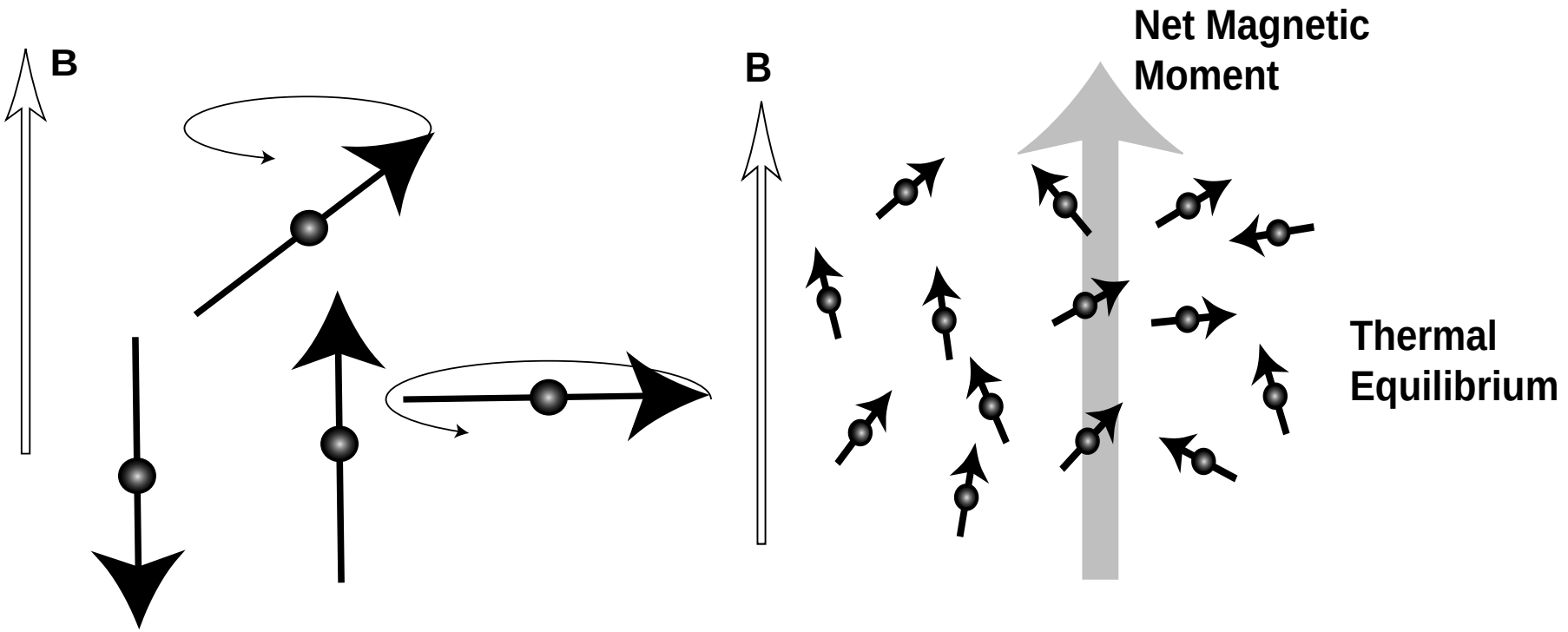
Larmour Frequency (MHz/T) of important nuclei

^{1}H 42.576

^{13}C 10.705

^{31}P 17.235

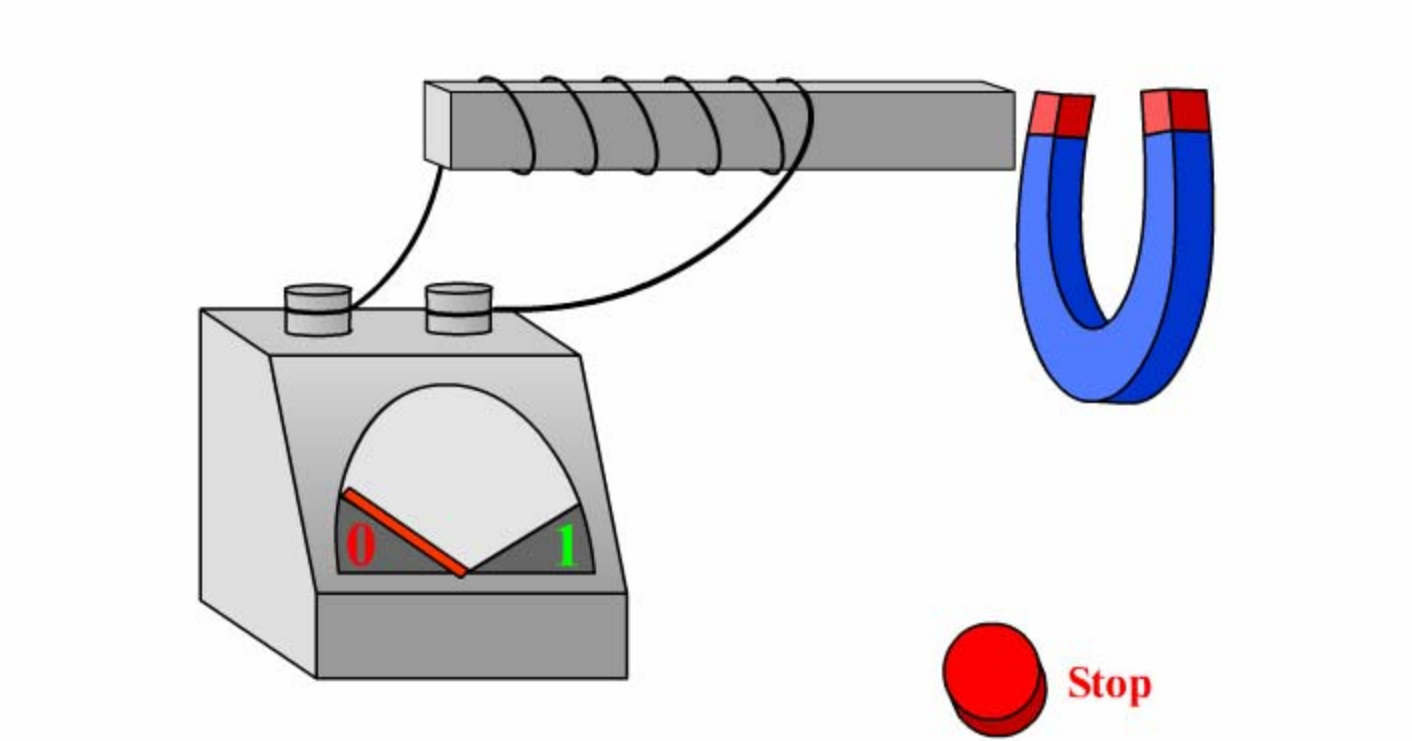
Usually, an NMR spectrometer is named based on the ^{1}H Larmour Frequency
Thus, a spectrometer which has a field of 7.05 T is called a 300MHz spectrometer
9.4 T is called the 400 MHz spectrometer, 11.74T called a 500MHz spectrometer


B
B
Net Magnetic
Moment
Thermal
Equilibrium

Resonance

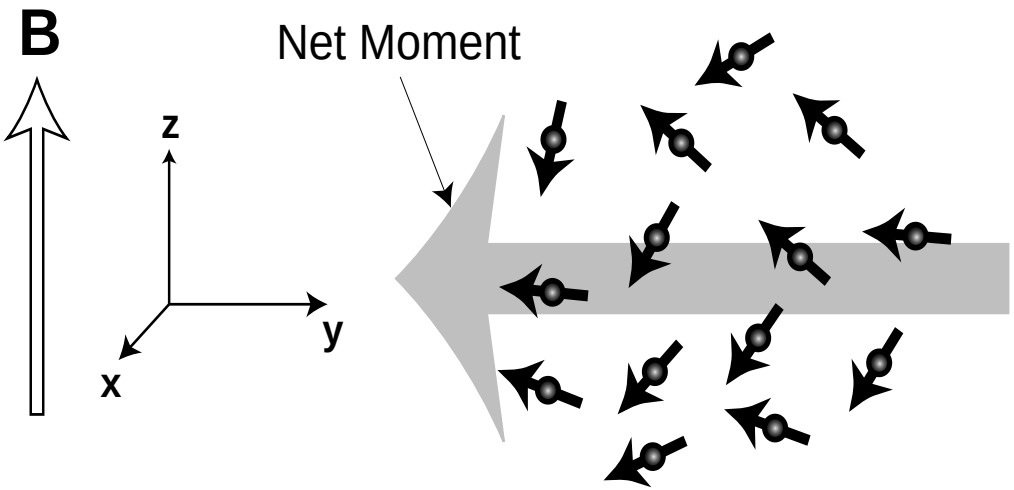
- An experiment to demonstrate Resonance using a spring and motor.
- The Larmour Frequency is in the Radio Frequency Range.

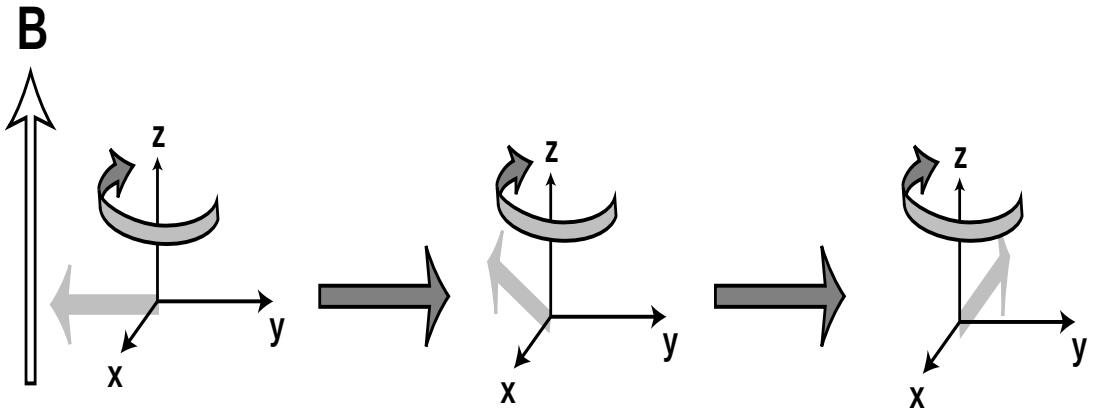
Electricity from magnetism



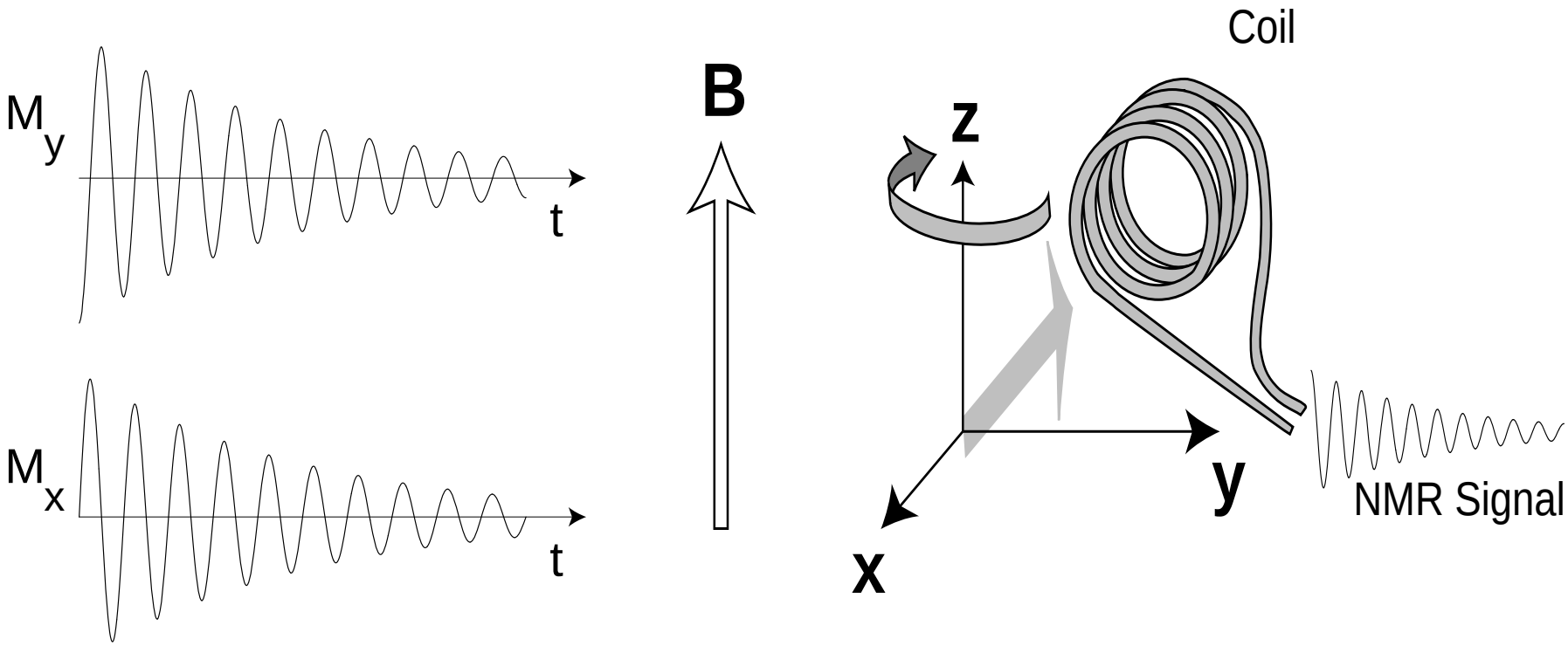
The experiment where an oscillation magnet in a coil generates a alternating current..
Very similar to the NMR signal !!!

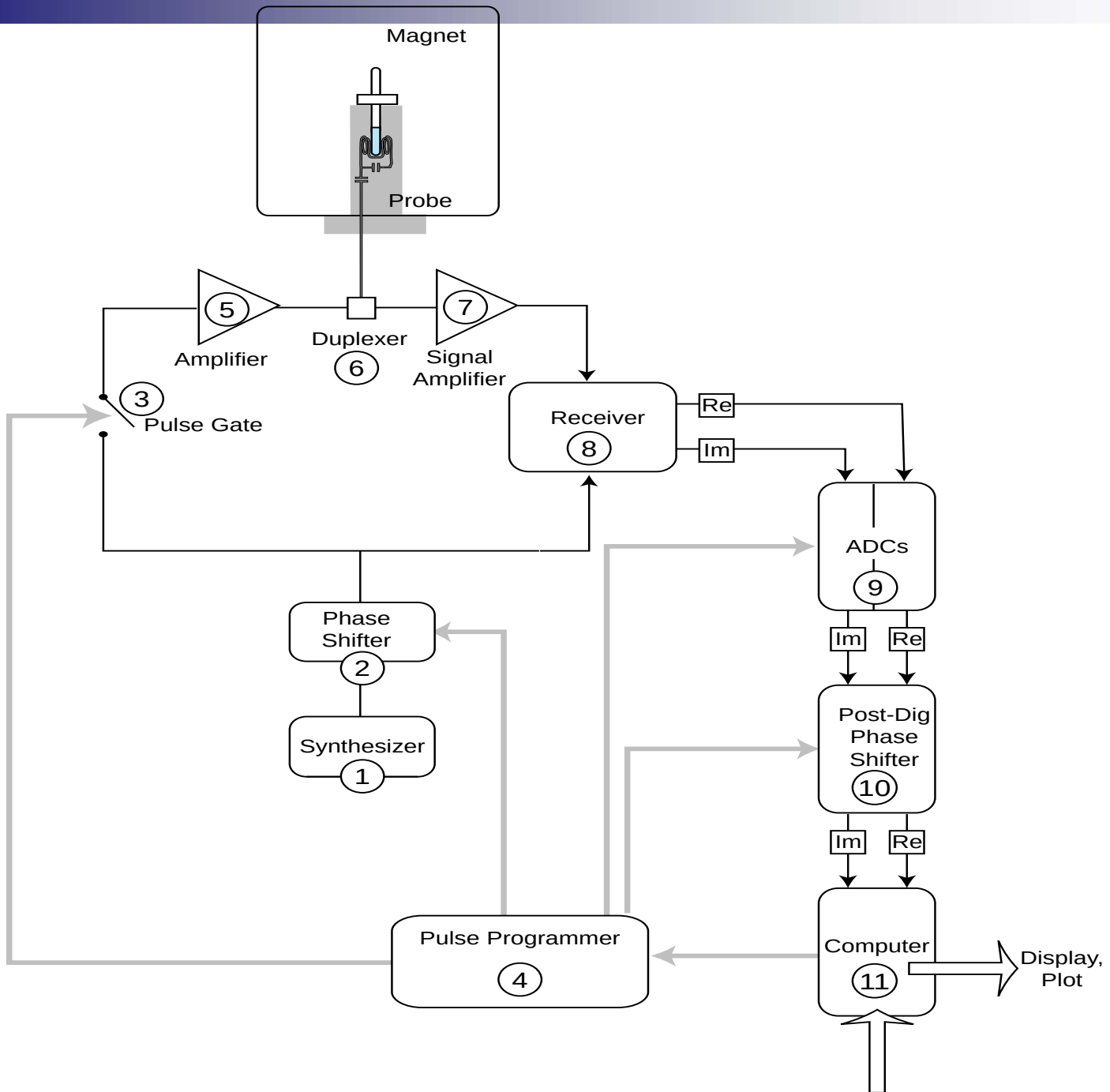
Application of Radio Frequency



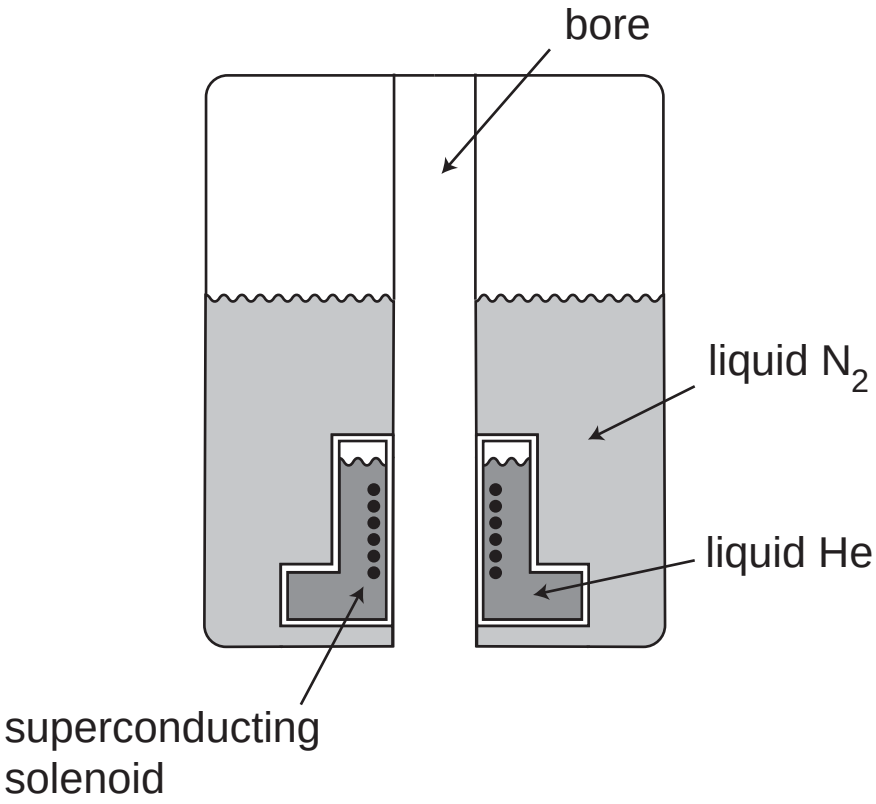


NMR signal

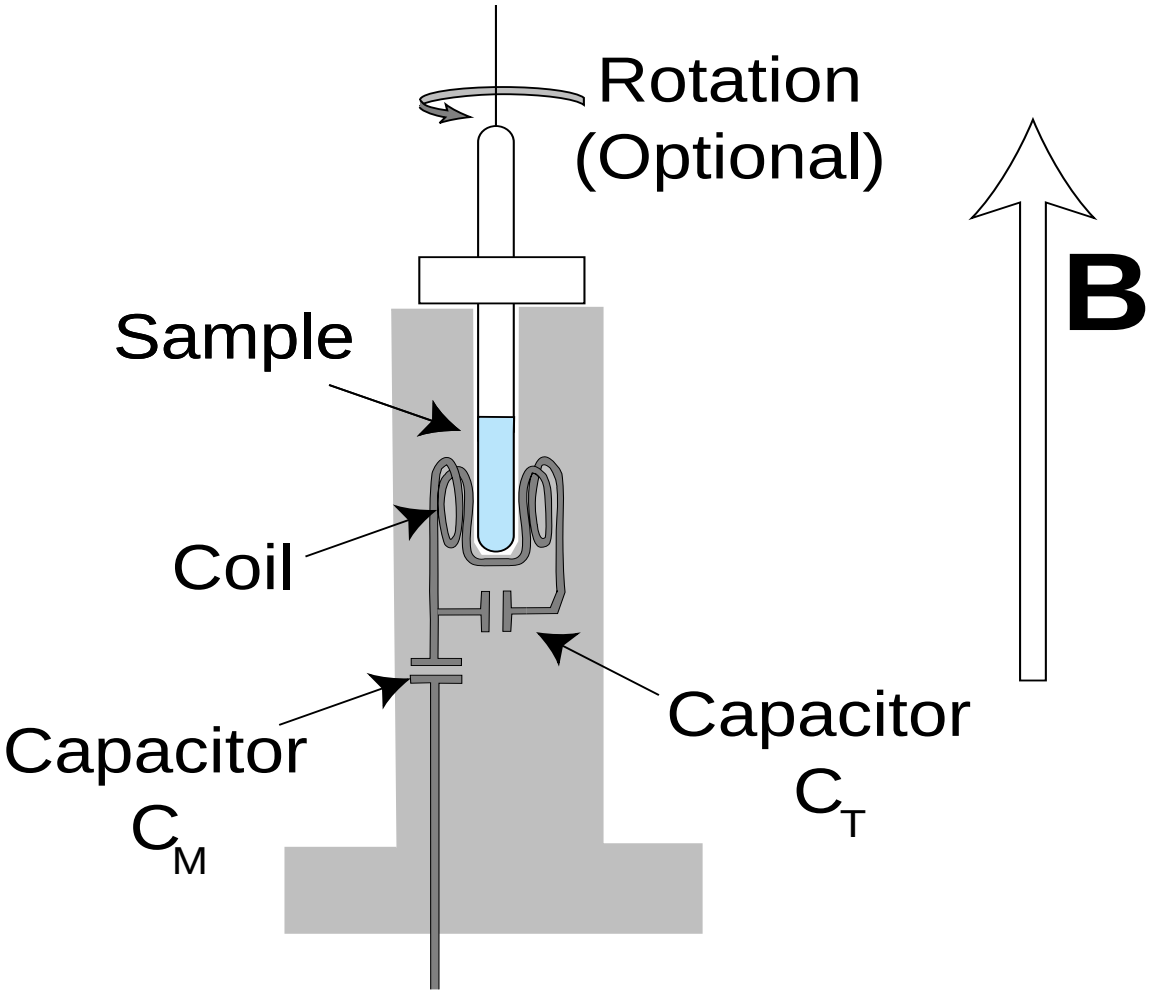



Magnet
Probe
5
Amplifier
Duplexer
6
7
Signal
Amplifier
3
Pulse Gate
Receiver
8
Re
Im
ADCs
9
Phase
Shifter
2
Synthesizer
1
Im
Re
Post-Dig
Phase
Shifter
10
Im
Re
Pulse Programmer
4
Computer
11
Display,
Plot

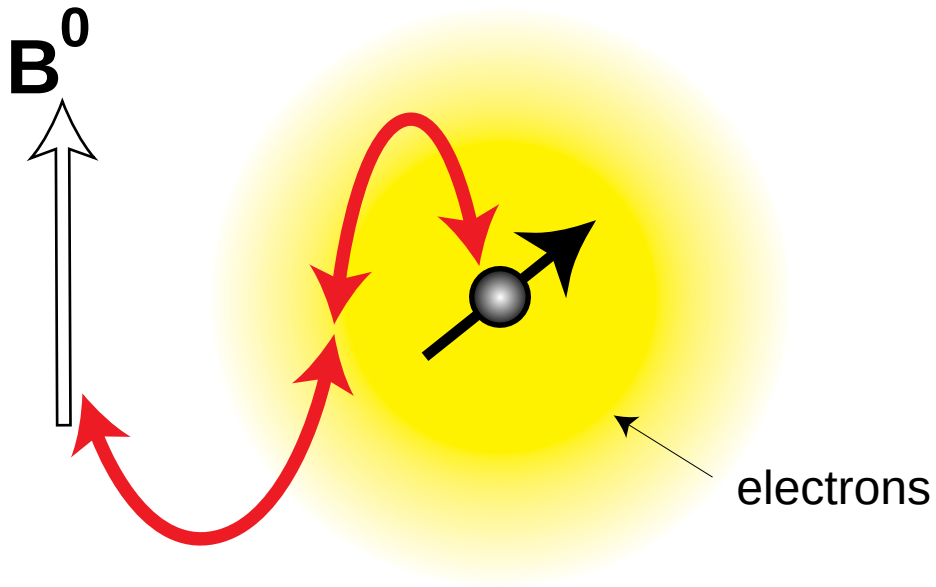
Magnet



Probe



Chemical Shift



The field experienced by the nucleus in a molecule will depend on the electron environment..

Fourier transform NMR

How to efficiently detect a range of NMR frequencies (in a spectrum)

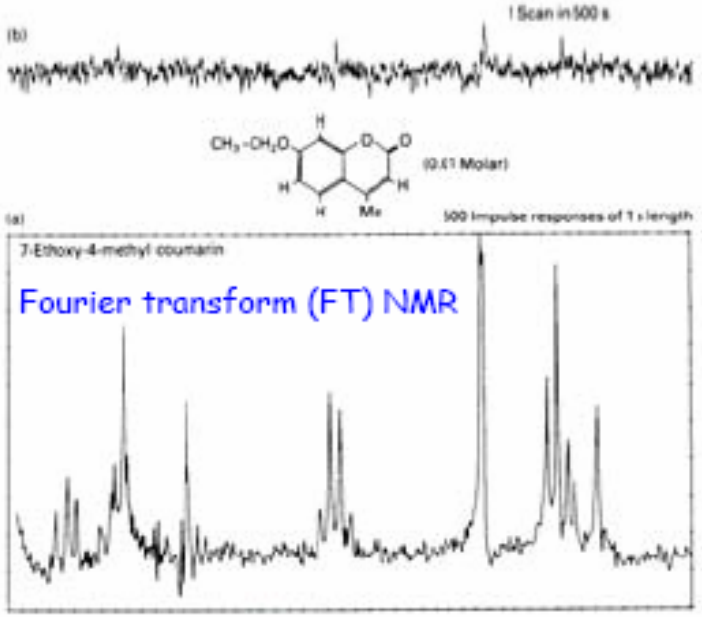
CW

FT

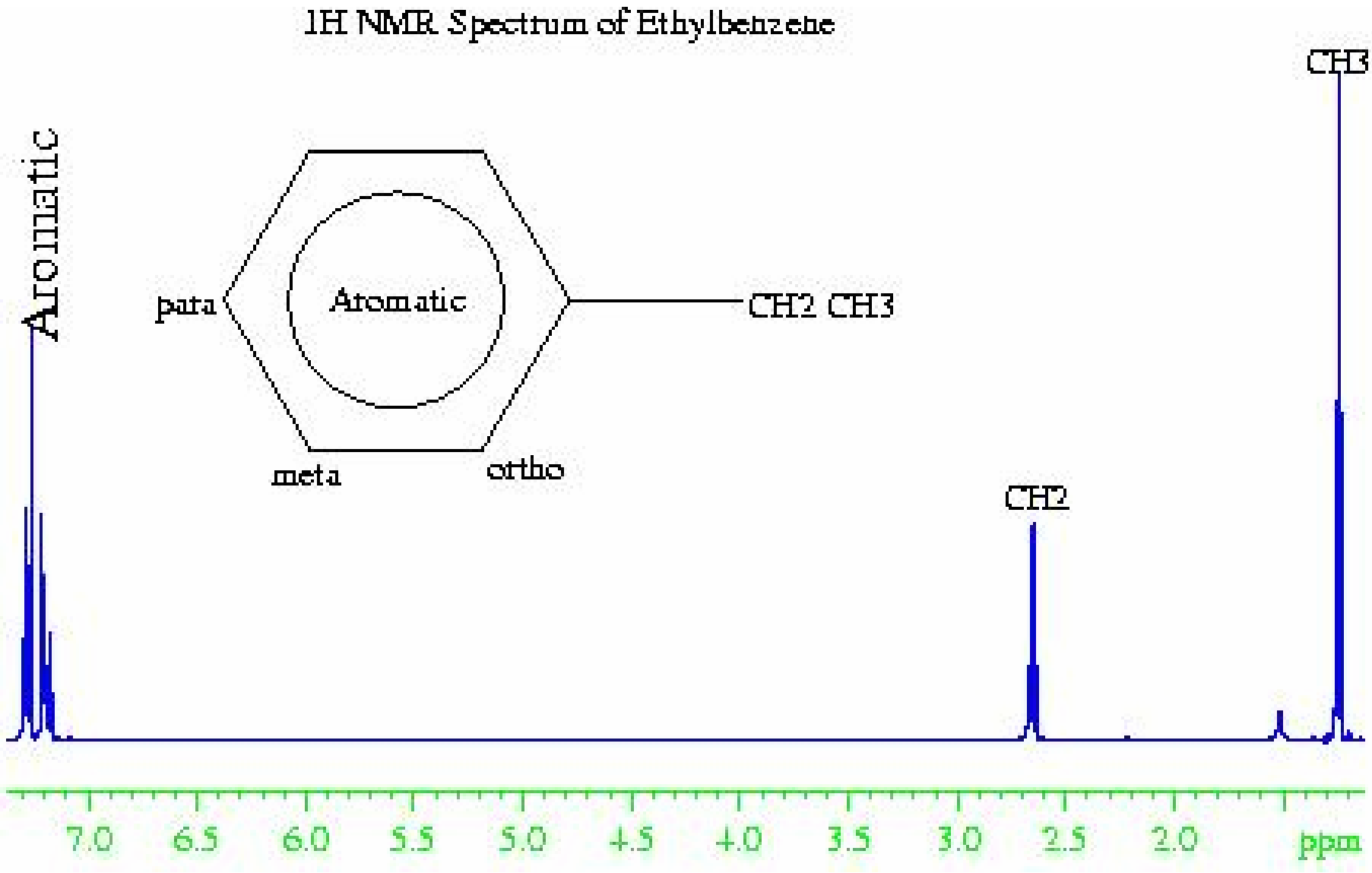
$$f(t) \underset{IFT}{\overset{FT}{\rightleftharpoons}} F(\omega)$$

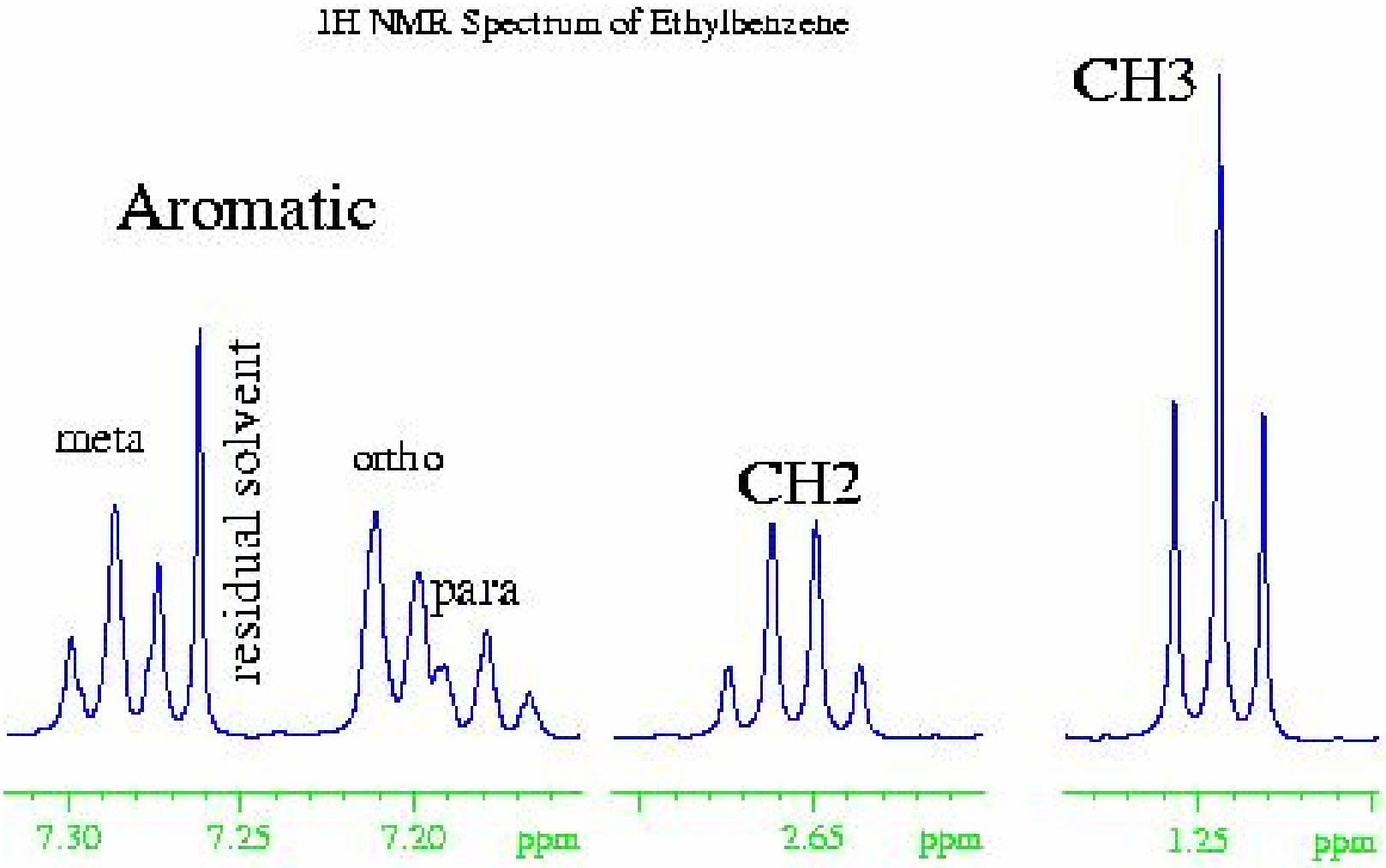
time domain — frequency domain

Continuous Wave (CW) NMR

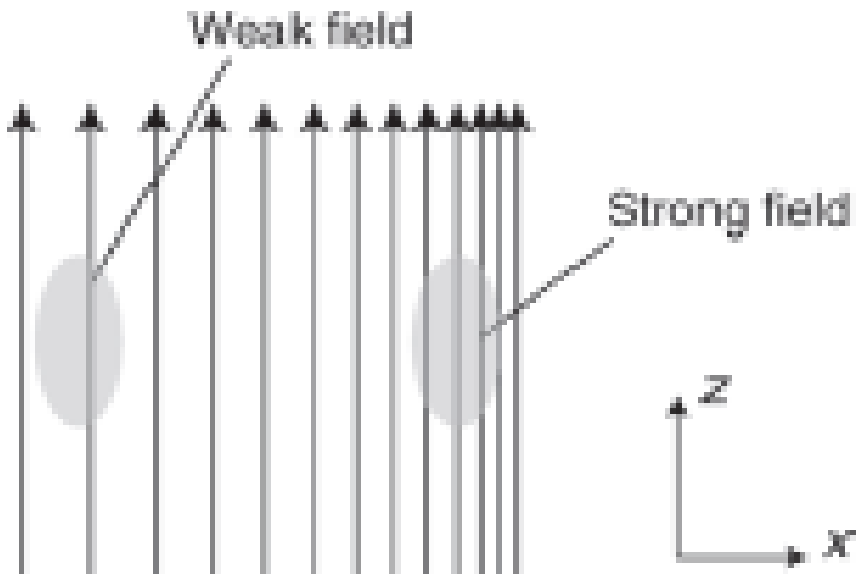


(Ernst, et al. "Principles of Nuclear Magnetic Resonance")


1H NMR Spectrum of Ethylbenzene
Aromatic
para
Aromatic
CH2 CH3
meta
ortho
CH3
CH2
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm


1H NMR Spectrum of Ethylbenzene
Aromatic
meta
residual solvent
ortho
para
CH2
CH3
7.30
7.25
7.20
ppm
2.65
ppm
1.25
ppm

NMR Imaging



Along with the external field, a field gradient which is propotional to the geometry is applied

Nobel Glories of NMR

1954 **Physics**

Bloch

Purcell

1990 **Chemistry**

Ernst

2002 **Biology**

Wuthrich

2003 **Medicine**

Lauterbur

Mansfield

In the winter of our first experiment….looking on snow with new eyes. There the snow lay around my door step….great heaps of protons quietly precessing in the Earth's magnetic field. To see the world for a moment as something rich and strange is the private reward of many a discovery.

Ed Purcell, 1946

Acknowledgements

- Dr. T. S. Mahesh, IISER for his help in setting up the demo experiments.

Thank you…