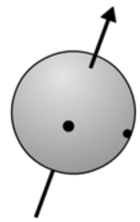
The NMR Phenomenon

Magnetic Field and *Nuclear Spin*



(on display in NMR facility)

1. Nuclear Spin

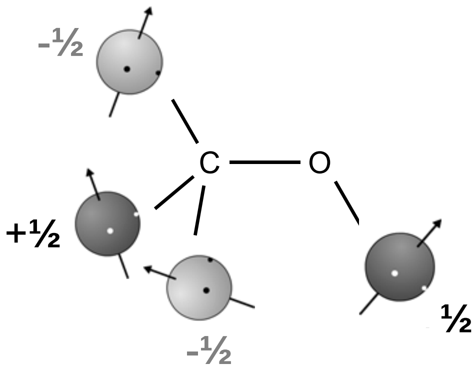
Total nuclear spin is analogous to electron spin, but does not follow "Aufbau" principle—so convenient to look up in tables.

Three main types of nuclei:

- I = 0 (^{12}C, ^{16}O, ^{32}S). No spin, no NMR.
- I = ½ (^{1}H, ^{13}C, ^{19}F, ^{29}Si, ^{31}P; "dipolar nuclei"). Simplest and most common nuclei studied by NMR.
- I ≥ 1 (^{2}H, ^{14}N; "quadrupolar nuclei"). Less frequently studied, but have important coupling behavior with I = ½ nuclei.

1. Nuclear Spin

^{1}H (I = ½) in CH_3OH as an example.



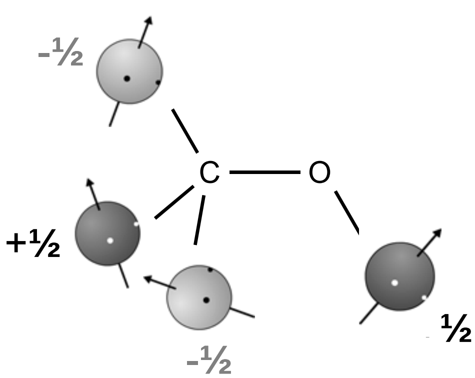
I = ½

total spin states = $2I + 1$
= 2

M_I = +½, -½

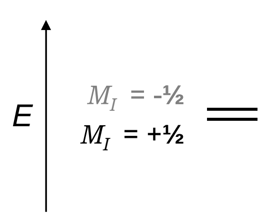
1. Nuclear Spin

^{1}H (I = ½) in CH_3OH as an example.



In the absence of an applied field, nuclei are randomly oriented.

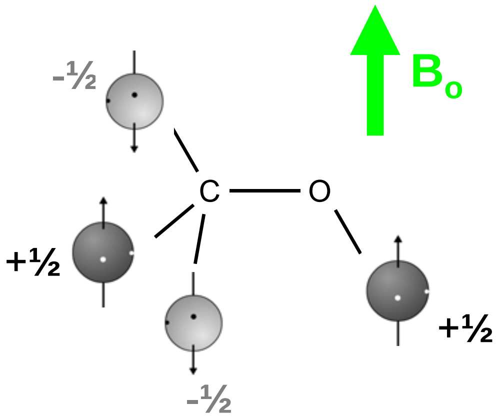
Energies of all nuclei are equivalent.



Spins do interconvert periodically.

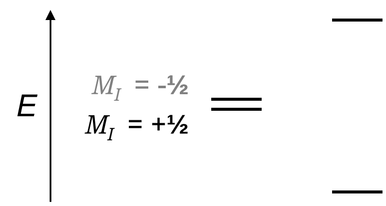
2. Applied Static Magnetic Field

^{1}H (I = ½) in CH_3OH as an example.

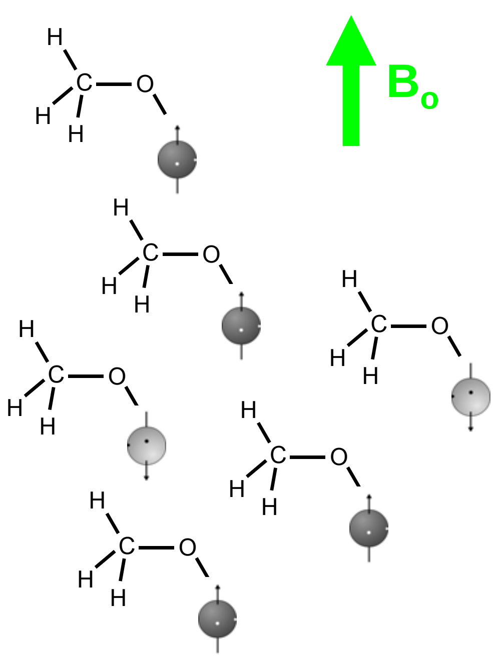


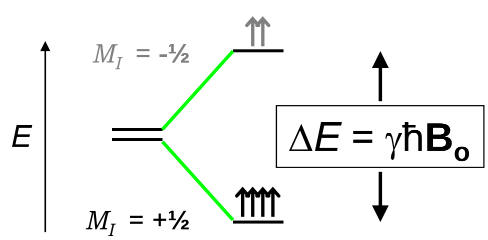
In the presence of an applied field $\mathbf{B_o}$, nuclei are oriented by the field.

Energies of nuclei are split by the field.



2. Applied Static Magnetic Field





Sensitivity of NMR is dependent on population distribution. So, sensitivity depends on:

1. Applied field strength $\mathbf{B_o}$;

2. Magnetogyric ratio of nucleus γ;

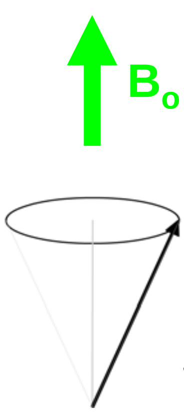
3. Abundance of spin in population.

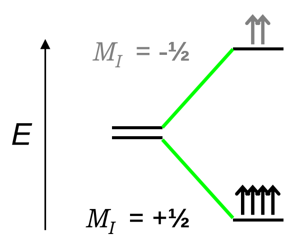
Nuclei of Major Interest to NMR Spectroscopists

	Isotope	Abundance (%)	Z	Spin	μ[a]	$\gamma \times 10^{-8}$[b]	Relative[c] sensitivity	ν_0 at 1T (MHz)
great nucleus.	^{1}H	99.9844	1	1/2	2.7927	2.6752	**1**	42.577
	^{2}H	0.0156	1	1	0.8574	0.4107		6.536
	^{10}B	18.83	5	3	1.8006	0.2875		4.575
	^{11}B	81.17	5	3/2	2.6880	0.8583		13.660
not so great.	^{13}C	1.108	6	1/2	0.7022	0.6726	**1.76×10^{-4}**	10.705
	^{14}N	99.635	7	1	0.4036	0.1933		3.076
poor.	^{15}N	0.365	7	1/2	−0.2830	−0.2711	**3.85×10^{-6}**	4.315
also great.	^{19}F	100	9	1/2	2.6273	2.5167	**0.83**	40.055
	^{29}Si	4.70	14	1/2	−0.5548	−0.5316		8.460
also great.	^{31}P	100	15	1/2	1.1305	1.0829	**6.65×10^{-2}**	17.235

[a] Magnetic moment in units of the nuclear magneton, $eh/(4\mu M_p c)$.
[b] Magnetogyric ratio in SI units.
[c] For equal numbers of nuclei at constant field.

2. Applied Static Magnetic Field





$$\Delta E = \gamma \hbar \mathbf{B_o}$$

$$\Delta E = h\nu$$

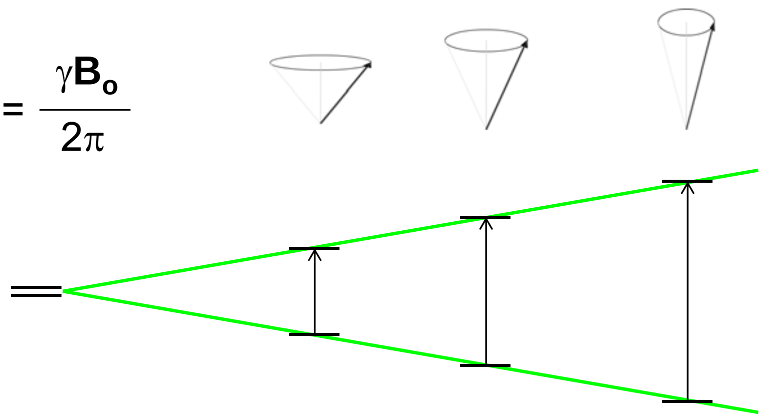
Nuclei precess at the **Larmor frequency.** →

$$\nu_o = \frac{\gamma \mathbf{B_o}}{2\pi}$$

- Different for different nuclei
- Depends on field strength

2. Applied Static Magnetic Field

$$\nu_o = \frac{\gamma B_o}{2\pi}$$



B_o	4.73 T	9.46 T	11.75 T
ν_o (^{1}H)	200 MHz	400 MHz	500 MHz
ν_o (^{13}C)	50 MHz	100 MHz	125 MHz

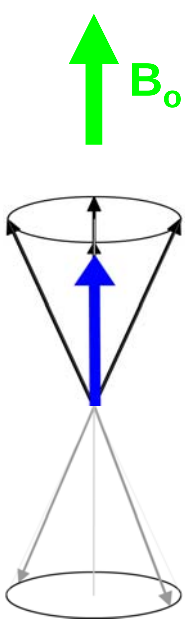
Big Fields Means Big Magnets

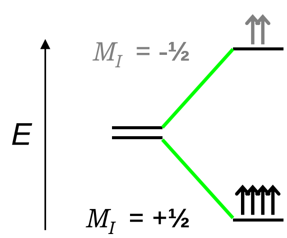
Interior of a 4.73 T magnet (on display in NMR Facility, Smith Hall)

Installation of 16.45 T magnet in Hasselmo Hall.

An NMR Facility

2. Applied Static Magnetic Field

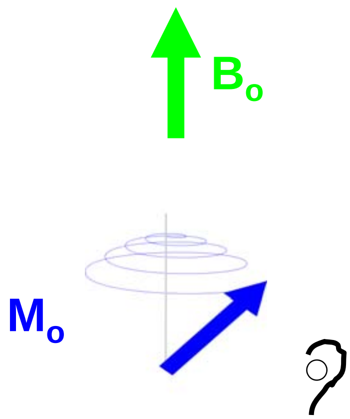




$$\nu_o = \frac{\gamma B_o}{2\pi}$$

M_o = "bulk magnetization", sum of all spin vectors precessing about **B_o**

3. Applied Radiofrequency Pulse



Transient M_{xy} is detected by radiofrequency coil.

- Oscillating applied field
- Frequency matched to Larmor frequency of precessing nucleus
- B_1 makes individual precessing vectors follow oscillation
- As a result, M_o also follows oscillation
- If B_1 is halted, M_o relaxes back to original state