PHY127 FS2026

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Lecture 12

May 22nd, 2026

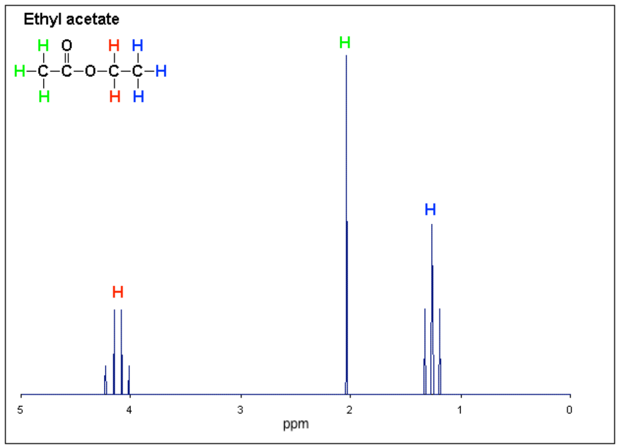
Today:

1) NMR: Nuclear Magnetic Resonance
   → useful for determining molecular structure, functional groups, dynamic processes (exchange + rotation)

2) MRI: Magnetic Resonance Imaging
   → useful for medicine: creating detailed, non-destructive, images of soft tissue (brain, heart, organs)

3) intro to nuclear physics

NMR



NMR: we seek to determine molecular structure, typically by measuring the hydrogen (proton) nuclear magnetic moments.

Using radiofrequency (RF) photons tuned to values of magnetic moment and magnetic field, we cause energy transitions in spin states that are measurable: condition: $h\nu = \Delta E = 2\mu_z B_z$

Typically, we use f_{armor}, resonance frequency, or W_{armor}

$$W_{armor} = 2\pi f_{armor} = \gamma \cdot B_z$$

where γ: gyromagnetic ratio

$$\gamma = \frac{q\,g}{2m}$$

m: mass of nucleus
g: strength factor
q: charge

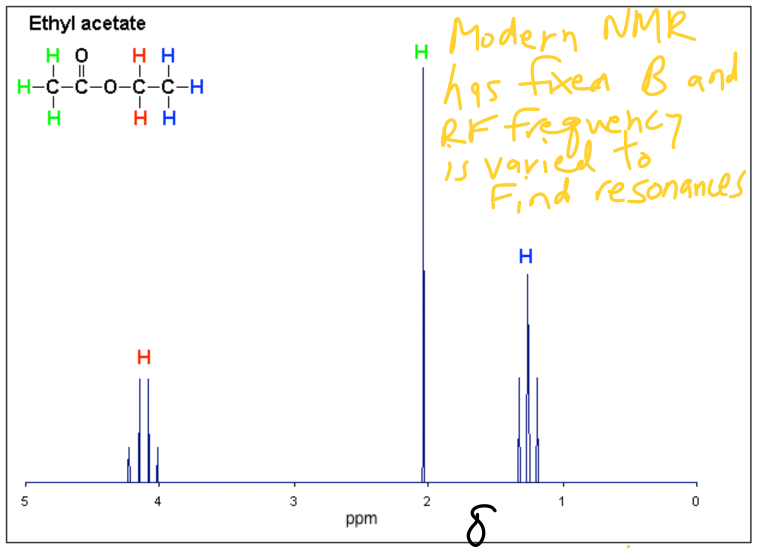
This value for ^1H is:

$$\gamma = 2\pi\ 42.58\ \frac{MHz}{T}$$

(T: Tesla)

e.g. For ^1H in 1.5 T magnetic field

$$f_{armor} = \frac{\gamma B_z}{2\pi} = \left(42.58\frac{MHz}{T}\right)\left(\frac{\cancel{2\pi}}{\cancel{2\pi}}\right) 1.5\,T = 63.87\ MHz$$



Modern NMR has fixed B and RF frequency is varied to Find resonances

δ

Resonances occur when RF frequency matches local Larmor

(Electron shielding changes local Larmor frequency)

← δ: position of peaks is measured as a shift.

$$\delta = \frac{f_{sample} - f_{reference}}{f_{external}} \times 10^6$$

δ (units: parts per million)

δ is measured through induced currents in detecting solenoid.

f_{sample}: frequency measured in the sample

$f_{reference}$: reference sample, typically use TMS "tetra methylsilane" $(CH_3)_4Si$

It's chemically inert, & has a strong signal of 12 Hydrogen protons.

$f_{external} = \nu$ where $\Delta E = h\nu$ excites transitions between spin states.

NMR spectra encode molecular structure through local magnetic environments & spin interactions

δ features: 1) number of peaks is # of hydrogen groups

2) peak splitting (singlet, doublet, triplet) from nearby H atoms

3) position of peaks depends on nearby electron density

4) peak area tells relative number of H atoms

5) peak width can reveal molecular motion & exchange

peak area $\propto$ # of H atoms

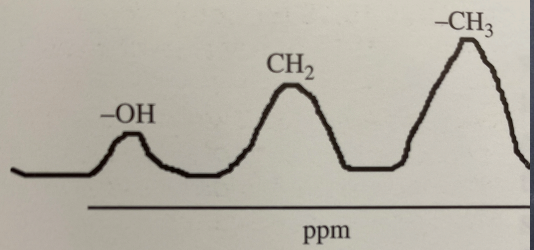


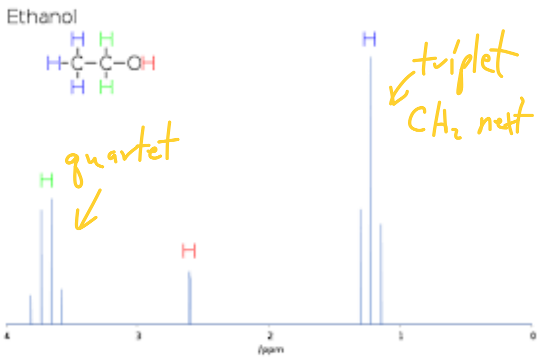
FIGURE 18.16 *Low resolution NMR spectrum of ethanol showing the 3:2:1 ratio of peak areas.*

Ethanol: $\underbrace{CH_3}\,\underbrace{CH_2}\,\underbrace{OH}$

expected peak area ratios:

3 : 2 : 1

Examples of NMR spectra   x-axis is δ (ppm)



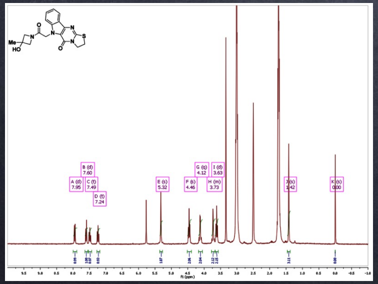
quartet

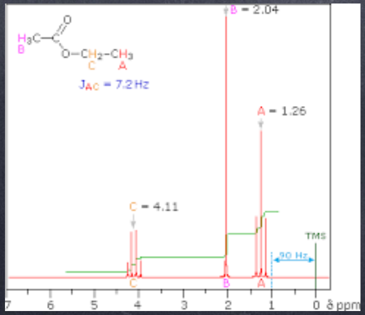
triplet
CH_2 next to CH_3

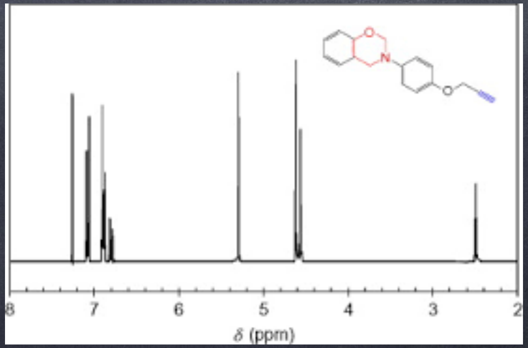
multiple peaks are from protons that have been split by neighboring protons
"n+1 rule": 3 neighbors → 3+1 = 4 peaks
(known as quartet)

e.g.
quartet: 3 neighbors,
typical of CH_2 next to CH_3

Other examples







Another measurable effect in NMR:

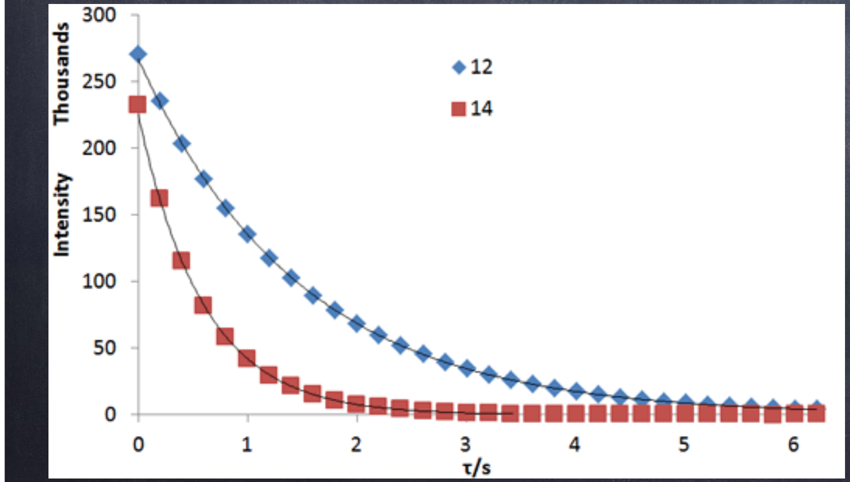
when we put in pulse of RF radiation into sample, the magnetization of the sample changes, but the magnetization relates to equilibrium

$$U_{ind} = U_{ind}^{max}\, e^{-t/T_2}$$

induced energy in the measuring solenoidal coil.

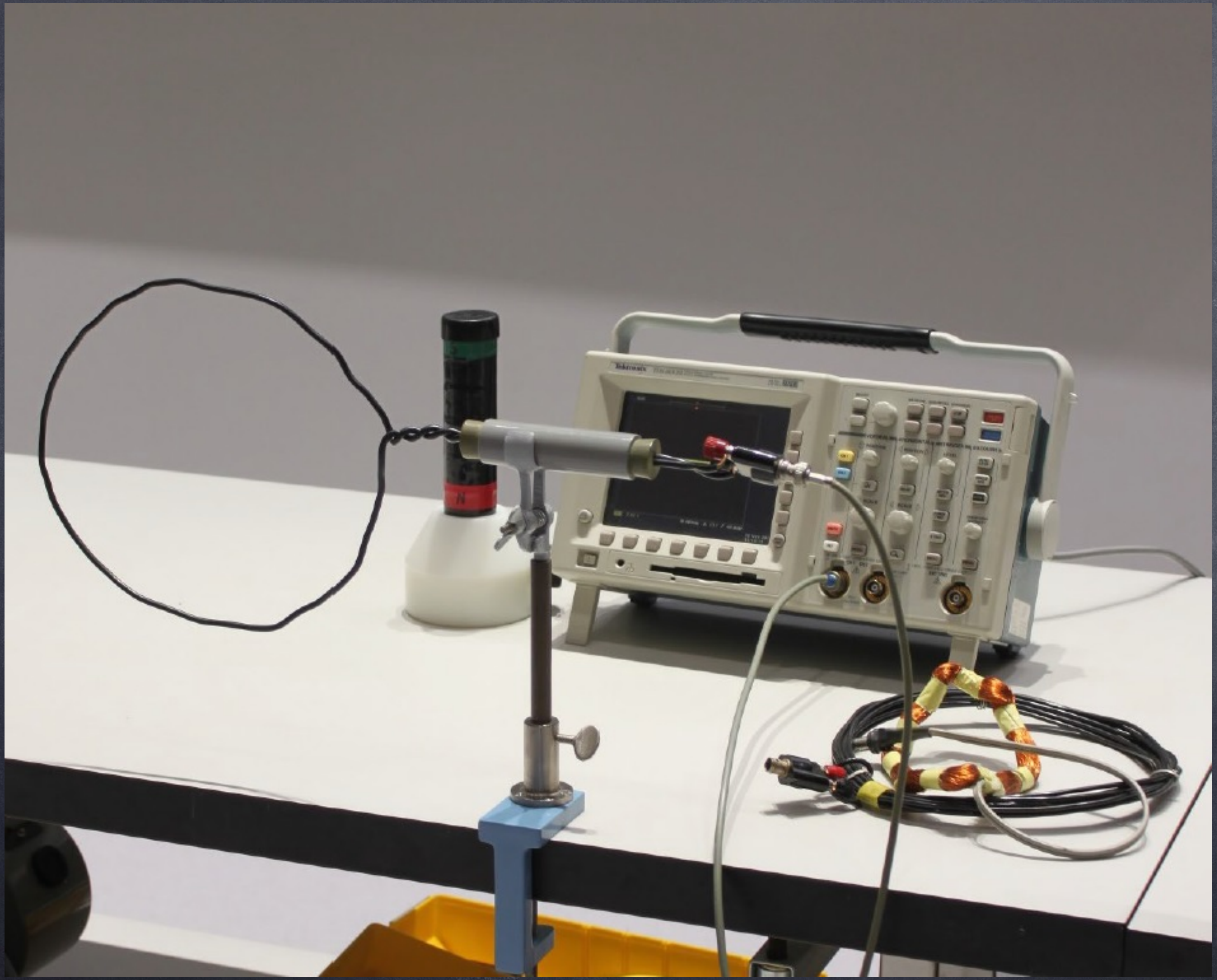
Max value

T_2 : spin-relaxation time



← example of T_2 for 2 different ^{t}butyl protons from

12,14-di ^{t}butyl benzo[g] chrysene



In our class experiment, we change magnetic field, + measure the induced current in a solenoid.

In NMR, we instead use a radiofrequency pulse, tuned in ν, to the resonance frequency f_{larmor} to change the magnetic moment of our sample, and measure the induced current with a solenoid.

Now, we talk about MRI (magnetic resonance imaging)

Our goal is to do a 3-D scan of a human body, non-destructively

we use NMR to map out the location of hydrogen (protons) in the human body.

If the magnetic field were constant over the body, there would be no way to tell where the NMR signal is coming from.

In MRI,

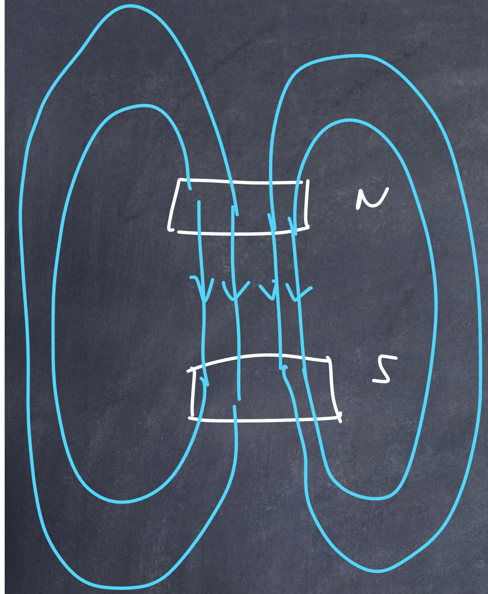
we apply a magnetic field gradient to our body in 3 dimensions. The magnetic field will vary in 3-D as a function of x, y, z

Gradients of typically 10^{-2} T/m are used so that the resonance condition $\Delta E = 2\mu_z B_z = h\nu$ will vary along each direction according to B.

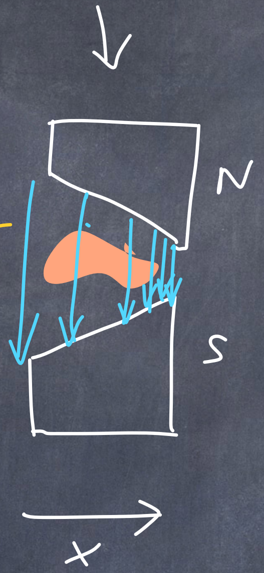
If an RF pulse matches the resonance condition for a particular slice (or plane), then only protons in this slice will be detected.

The x, y, z positions of the body are encoded in the RF frequency.

Magnetic field gradient



In figures, $\bar{B}$ is stronger when lines are closer together



$$B(x) = B_0 + B_{gr}(x)$$

↑ nominal constant value

$$\omega(x) = \gamma B(x)$$

Larmor frequency varies with x

Different positions resonate at different frequencies.

The level of the NMR signal at a frequency ω_i is a measure of the density of hydrogen nuclei at the location x.

we would have gradients in x, y, + z

$$B(y) = B_{0y} + B_{gr}(y)$$

$$B(z) = B_{0z} + B_{gr}(z)$$

1) Apply the gradients sequentially in 3 directions.

2) While we do this, we transmit RF pulses.

3) As we do this, we measure the induced current (in our solenoid)

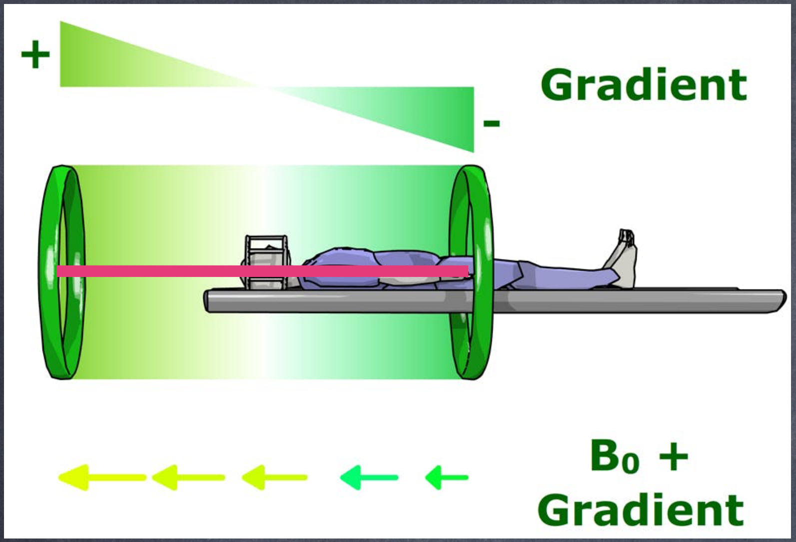
→ determines the magnetization at a specific location

→ density of hydrogen nuclei at that location.

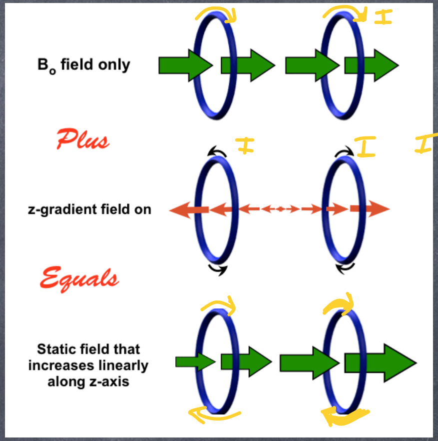
(the measured signal is proportional to the # of hydrogen nuclei at a specific x, y, z)

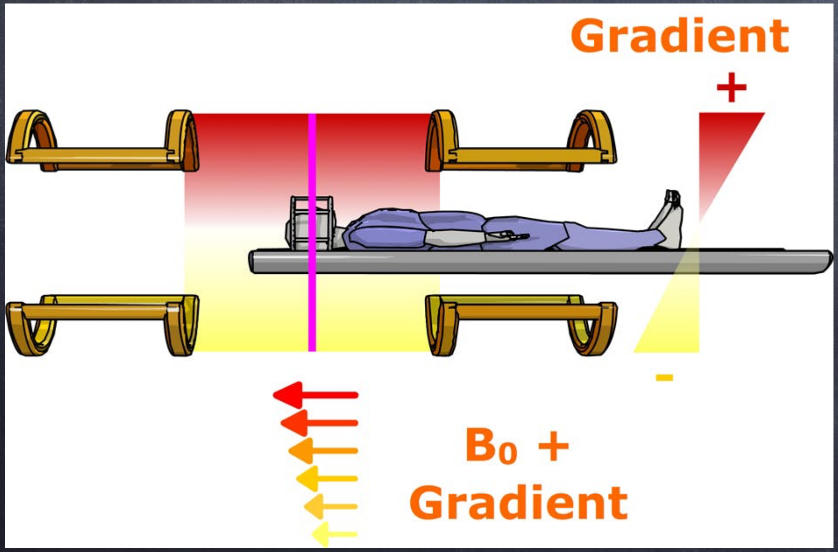
Then a computer reconstructs the image in 3-D.

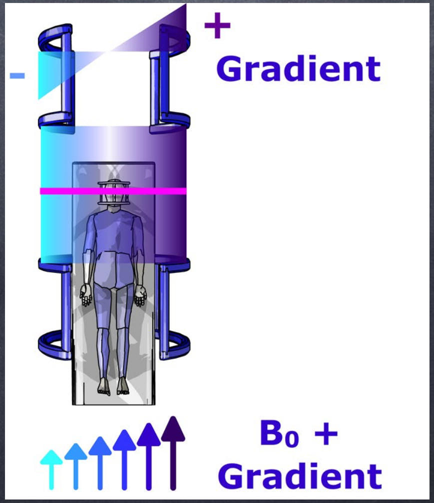
How to make a B-field gradient :

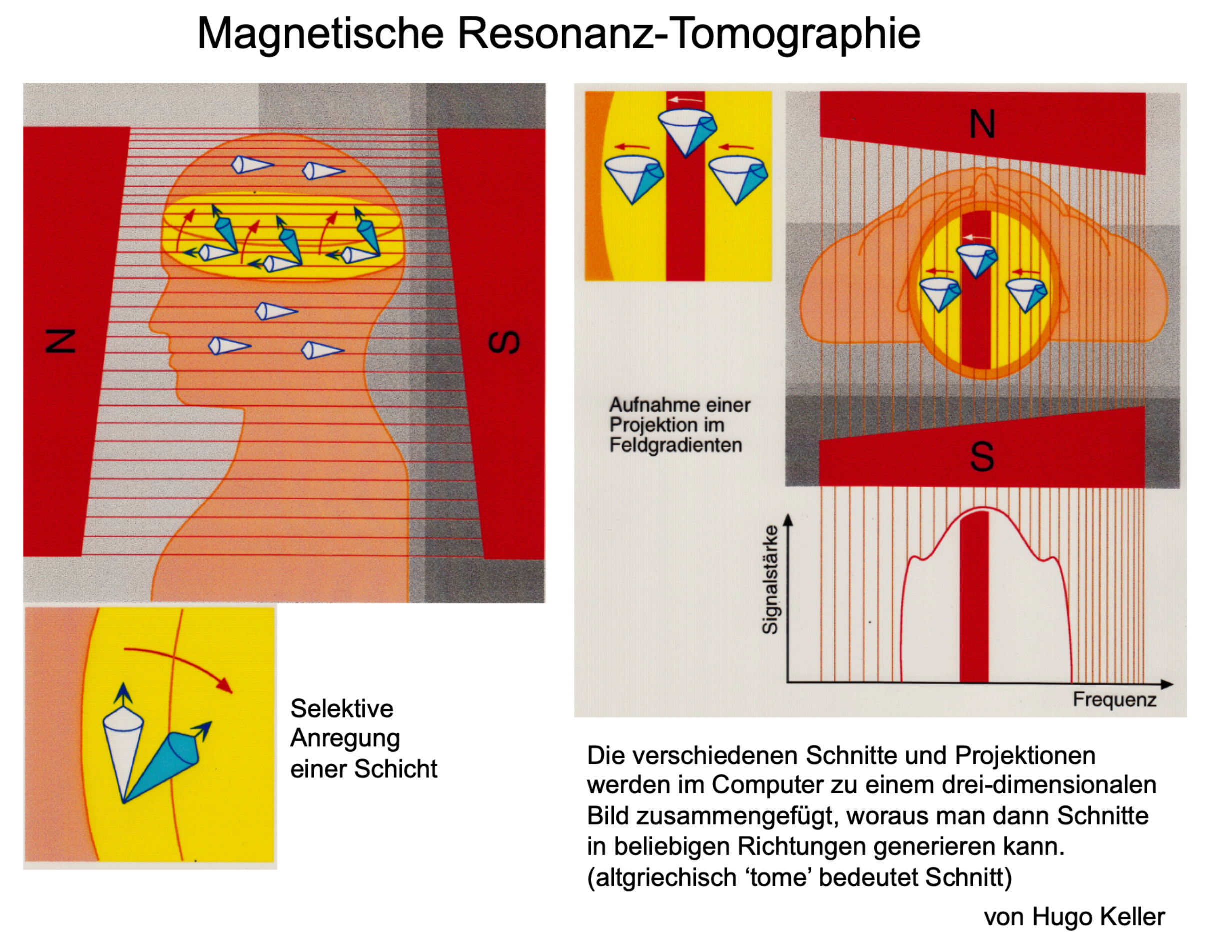


we add extra gradient coils :









Magnetische Resonanz-Tomographie

Selektive
Anregung
einer Schicht

Aufnahme einer
Projektion im
Feldgradienten

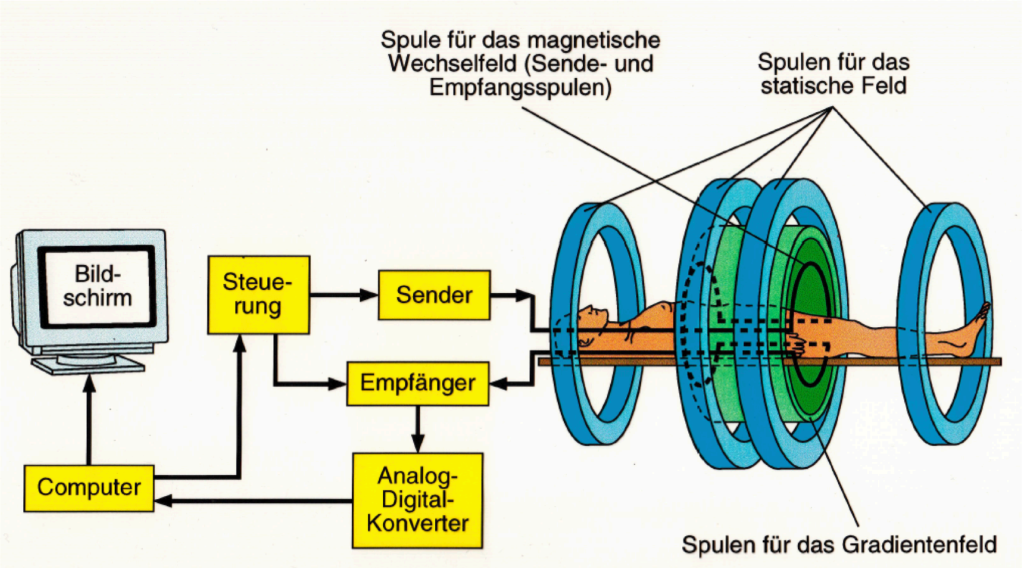
Die verschiedenen Schnitte und Projektionen werden im Computer zu einem drei-dimensionalen Bild zusammengefügt, woraus man dann Schnitte in beliebigen Richtungen generieren kann. (altgriechisch ‘tome’ bedeutet Schnitt)

von Hugo Keller

MRI

RF excites
spin transitions
when the
RF frequency
matches the
local
Larmor
frequency

Aufbau einer MRT-Anlage

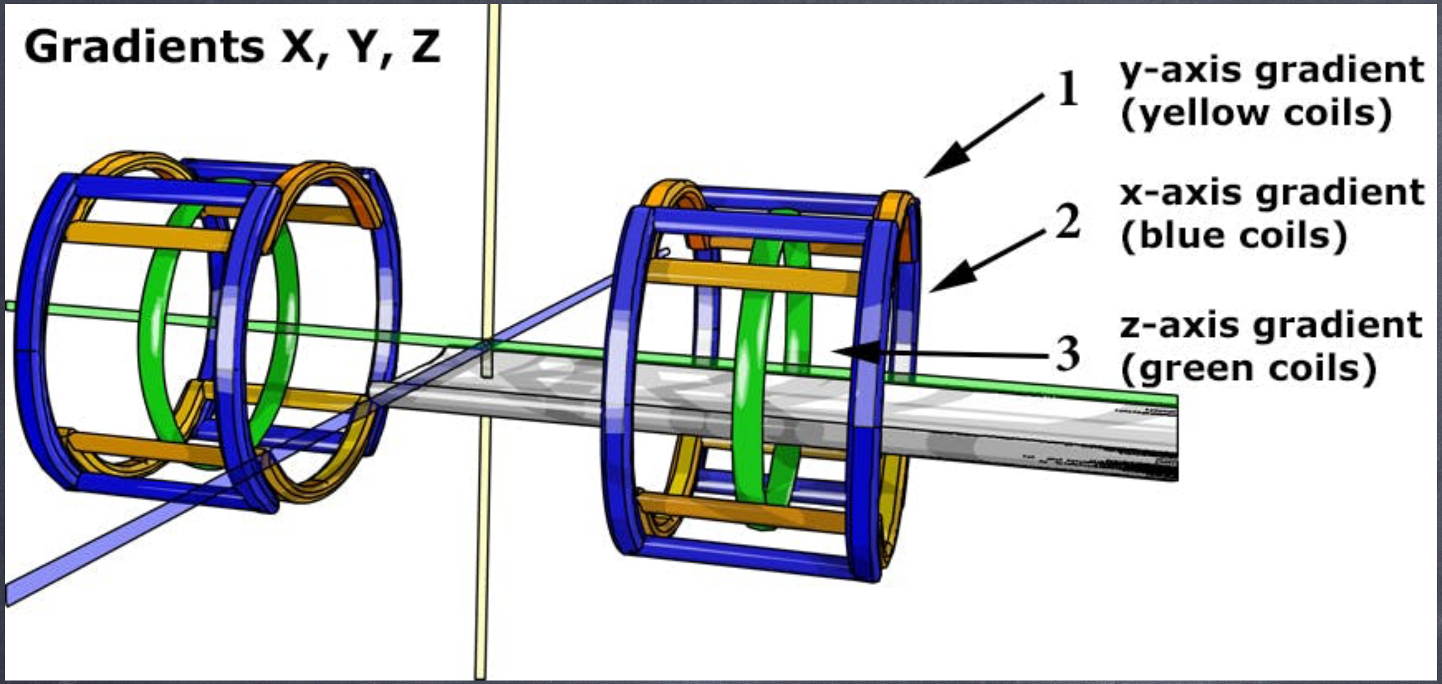


von Hugo Keller

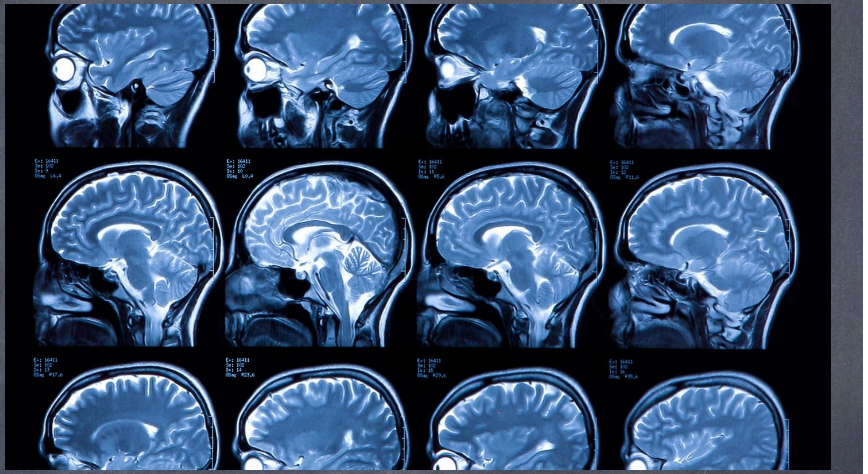
Blue coils:

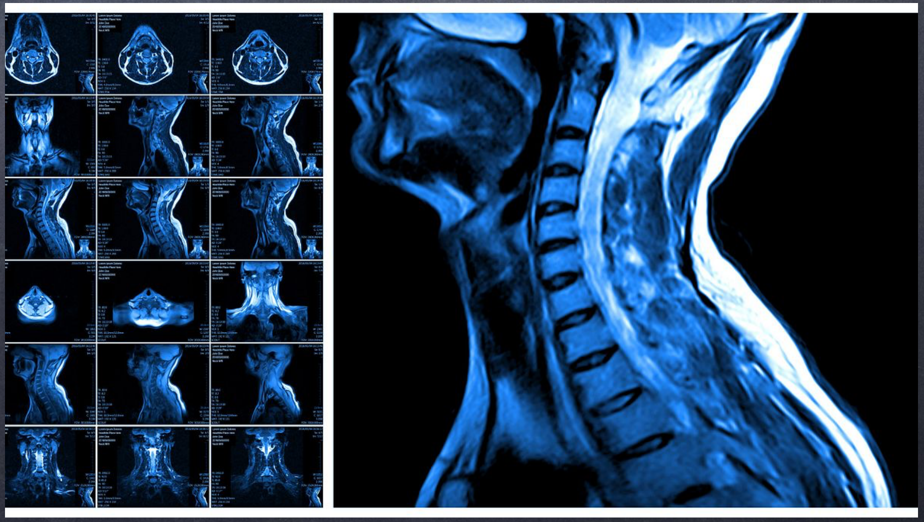
← $\bar{B}$ is static (constant)

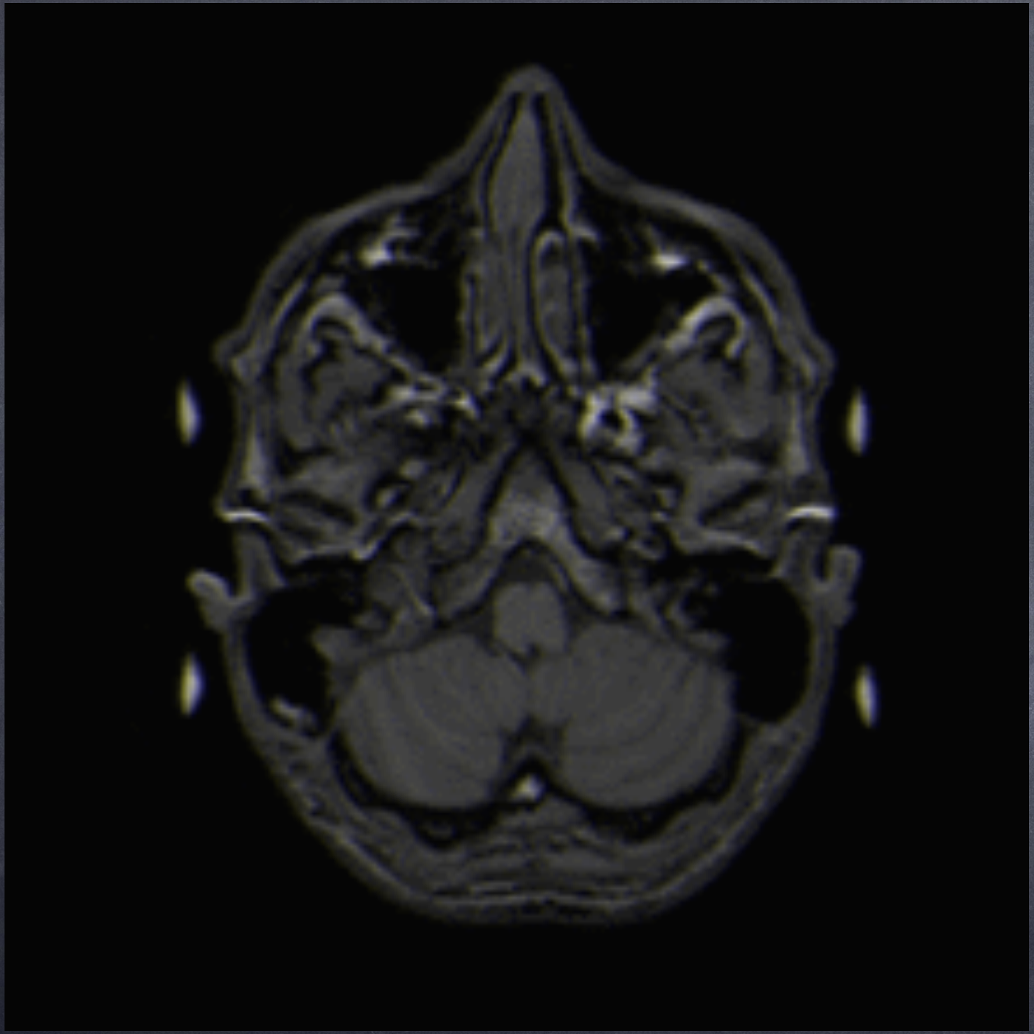
← green coil generates gradient field $\bar{B}(x)$


Gradients X, Y, Z
1
y-axis gradient
(yellow coils)
2
x-axis gradient
(blue coils)
3
z-axis gradient
(green coils)

Examples of MRI







Contrast between tissues in MRI comes from two processes. One is that different tissues have different water content (H_2O)

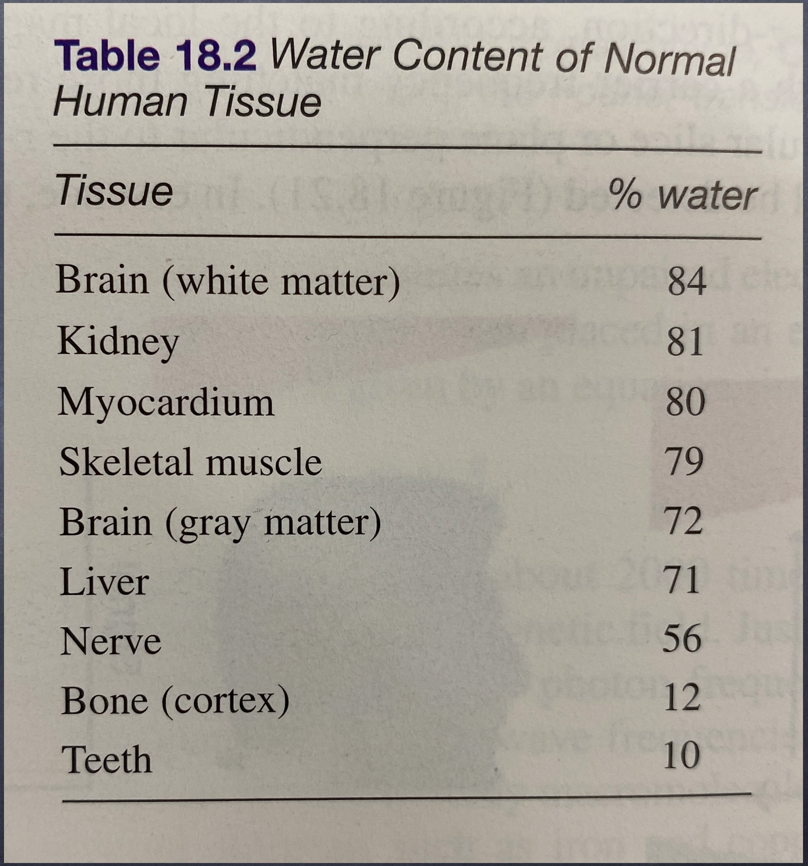


Table 18.2 *Water Content of Normal Human Tissue*

Tissue	*% water*
Brain (white matter)	84
Kidney	81
Myocardium	80
Skeletal muscle	79
Brain (gray matter)	72
Liver	71
Nerve	56
Bone (cortex)	12
Teeth	10

The second differentiation of tissue is from the relaxation time, T_2

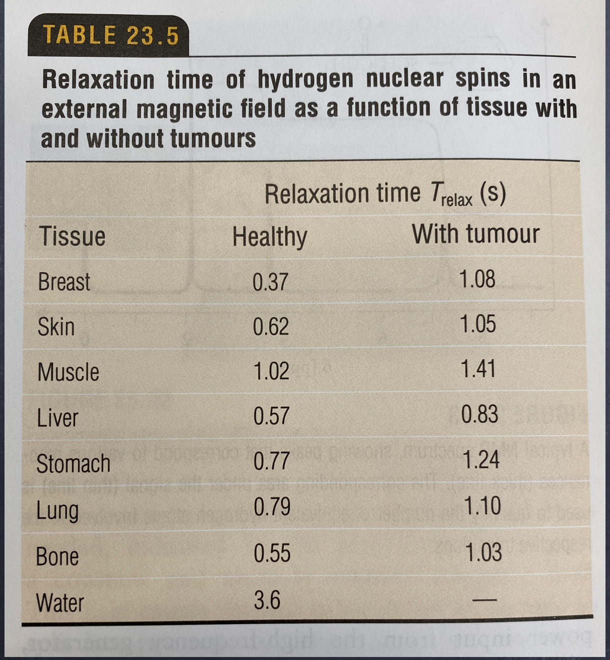


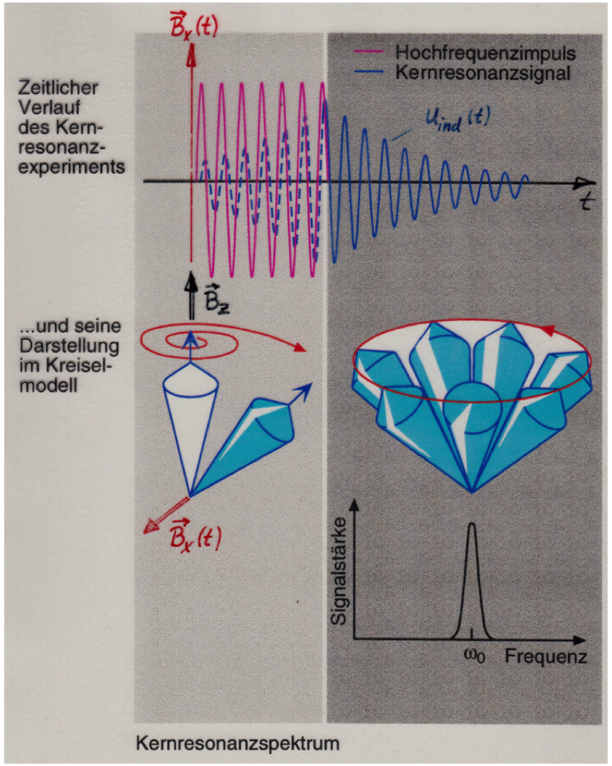
TABLE 23.5

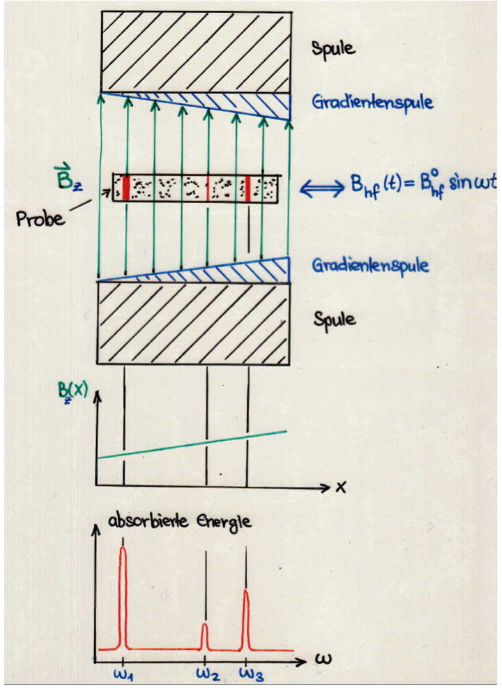
Relaxation time of hydrogen nuclear spins in an external magnetic field as a function of tissue with and without tumours

	Relaxation time T_{relax} (s)	
Tissue	Healthy	With tumour
Breast	0.37	1.08
Skin	0.62	1.05
Muscle	1.02	1.41
Liver	0.57	0.83
Stomach	0.77	1.24
Lung	0.79	1.10
Bone	0.55	1.03
Water	3.6	—

MRS uses the same scanner as MRI

Magnetische Resonanz-Spektroskopie





Die Ortsinformation, von woher ein Signal stammt, wird über die bekannte Ortsabhängigkeit des B-Feldes kodiert, welche in die Resonanzfrequenz eingeht.

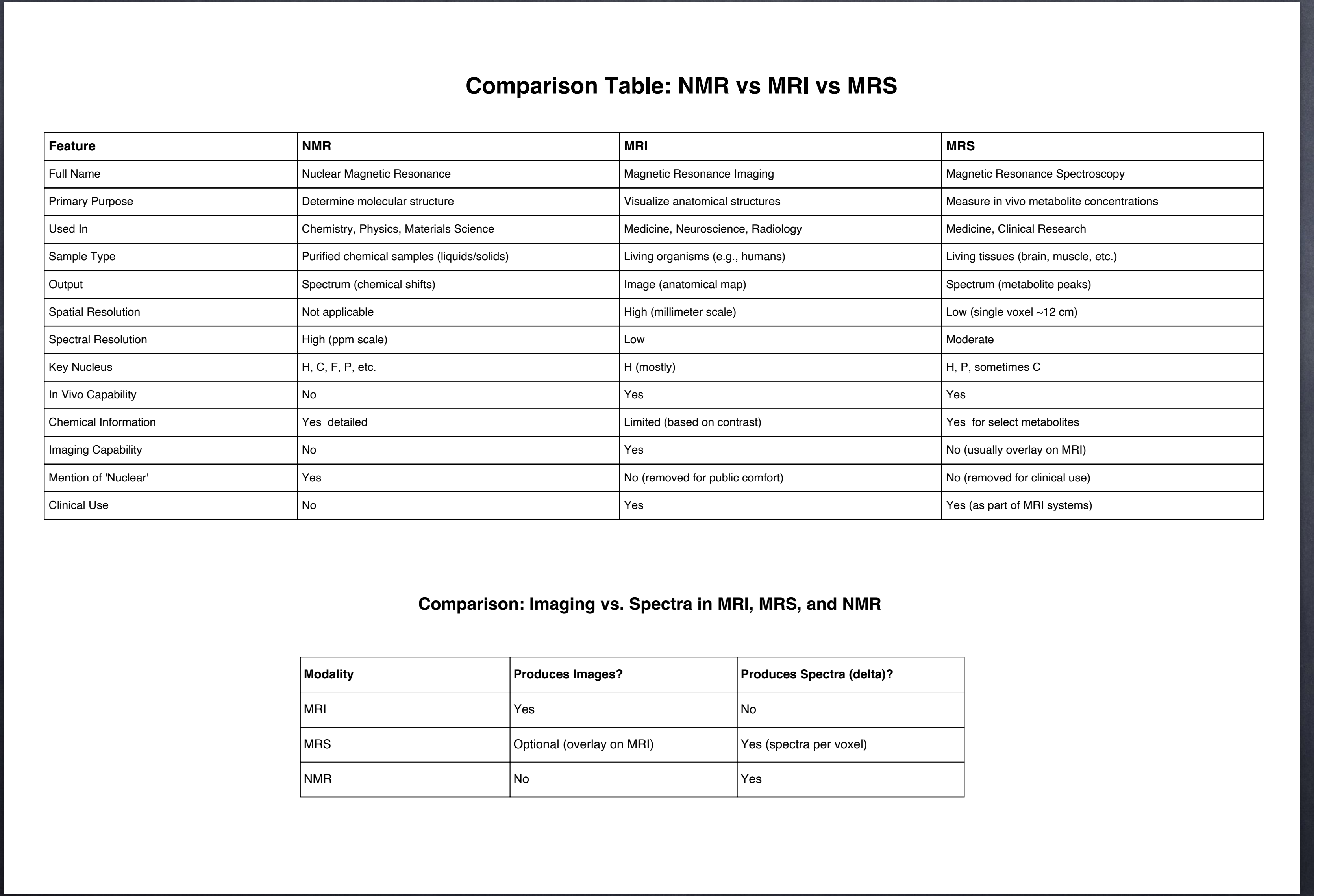
von Hugo Keller

MRS can be used to do chemical/metabolic analysis

MRI tells you "where is the problem?"

MRS tells you "is there altered metabolism?"

Summary :



Comparison Table: NMR vs MRI vs MRS

Feature	NMR	MRI	MRS
Full Name	Nuclear Magnetic Resonance	Magnetic Resonance Imaging	Magnetic Resonance Spectroscopy
Primary Purpose	Determine molecular structure	Visualize anatomical structures	Measure in vivo metabolite concentrations
Used In	Chemistry, Physics, Materials Science	Medicine, Neuroscience, Radiology	Medicine, Clinical Research
Sample Type	Purified chemical samples (liquids/solids)	Living organisms (e.g., humans)	Living tissues (brain, muscle, etc.)
Output	Spectrum (chemical shifts)	Image (anatomical map)	Spectrum (metabolite peaks)
Spatial Resolution	Not applicable	High (millimeter scale)	Low (single voxel ~12 cm)
Spectral Resolution	High (ppm scale)	Low	Moderate
Key Nucleus	H, C, F, P, etc.	H (mostly)	H, P, sometimes C
In Vivo Capability	No	Yes	Yes
Chemical Information	Yes detailed	Limited (based on contrast)	Yes for select metabolites
Imaging Capability	No	Yes	No (usually overlay on MRI)
Mention of 'Nuclear'	Yes	No (removed for public comfort)	No (removed for clinical use)
Clinical Use	No	Yes	Yes (as part of MRI systems)

Comparison: Imaging vs. Spectra in MRI, MRS, and NMR

Modality	Produces Images?	Produces Spectra (delta)?
MRI	Yes	No
MRS	Optional (overlay on MRI)	Yes (spectra per voxel)
NMR	No	Yes

Nuclear physics

Atomic sizes ~ 0.1 nm $(10^{-10}\,m)$

nuclear sizes ~ 10^{-15} m

If an atom has the size of a football field, the nucleus would be the size of a pin head (1 mm)

proton mass ~ 1800 * electron mass

Elements: $$\underset{\substack{\uparrow\\ \text{atomic}\\ \text{number}}}{A} = \underset{\substack{\uparrow\\ \#\\ \text{protons}}}{Z} + \underset{\substack{\uparrow\\ \#\text{ neutrons}}}{N}$$

Notation for element, E : ${}^{A}_{Z}E \to {}^{A}E$

example ${}^{13}C \equiv {}^{13}_{6}C$

units $1\,u \equiv \frac{1}{12}\,C^{12}$ atom

Nuclide refers to a particular Z + N combination

Nuclides with the same Z but different N, are called <u>isotopes</u>

Some isotopes are <u>stable</u>, and some are <u>radioactive</u>

Structure of isotopes has been determined by scattering electrons on the isotope.

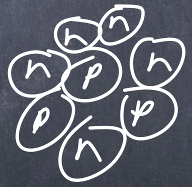
$$\lambda = \frac{h}{p}$$

For an electron with $p = 200\ \frac{\text{MeV}}{c}$ $\qquad c = 3E8\ \frac{m}{s}$

$$\lambda = \frac{h}{p} = \frac{4.1357E\text{-}15\ \text{eV.s}}{200\ \frac{\text{MeV}}{c}} = \frac{4.1357E\text{-}15\ \cancel{\text{eV.s}}}{200E6\ \cancel{\text{eV}}} \cdot 3E8\ \frac{m}{\cancel{s}}$$

$$= 6E\text{-}15\ m = 6\ \text{fm}$$

This is small enough to probe nuclear sizes.



Note: formula for energy relates to momentum and mass

$$E^2 = (cp)^2 + \underbrace{(mc^2)^2}_{\text{can be neglected if } p \gg m}$$

Then $p = \frac{E}{c}$

Example: for an electron with $p = 200\,\frac{\text{MeV}}{c}$

$$E^2 = (200\text{ MeV})^2 + (0.511\text{ MeV})^2$$

$$E = 200.0007\text{ MeV}$$

units: $E\,[\text{eV}]$

$p\,\left[\frac{\text{eV}}{c}\right]$

$m\,\left[\frac{\text{eV}}{c^2}\right]$

Nuclear size $R \cong R_0 A^{1/3}$ $R_0 \sim 1.2$ fm

density is almost the same for all nuclei

density of a proton = $\rho_{proton} = \frac{m_p}{\frac{4}{3}\pi r^3} = \frac{1.67E-27\,kg}{\frac{4}{3}\pi(1.2E-15m)^3}$

$\rho_{proton} = 2E17 \frac{kg}{m^3}$

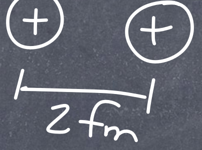
$\rho_{nucleus}$ is 10^{14} times larger than the density of an atom

(Nuclei are mostly spherical, but some are more eliptical )

Why is the nucleus ever stable?

It is densely packed with protons that repel each other.

Coulomb force $= F = \frac{e^2}{4\pi\varepsilon_0 r^2}$



For $r = 2\text{fm}$, 2 protons repel each other with a force of $F = 60\ \text{N}$ (equivalent to a 6 Kg weight)

Answer: the nucleus is held together by the strong nuclear force.

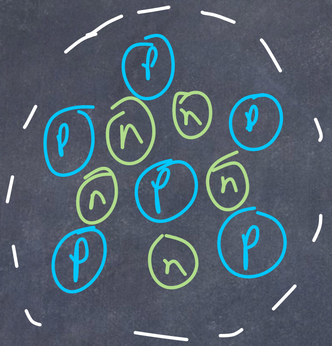
This is an attractive force more than 200 times stronger than the Coulomb force repulsion.

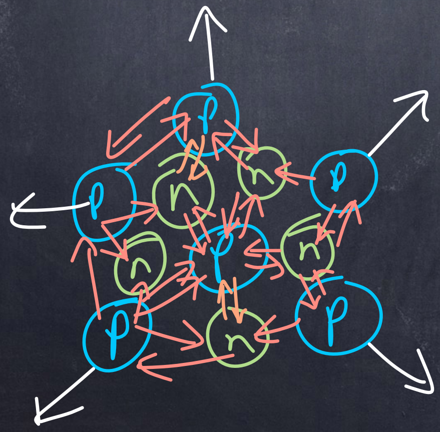
↓

only true when the protons are close to each other (like in a nucleus) nucleon = proton or a neutron

→ nucleons are all attracted by the strong nuclear force.

Nucleus

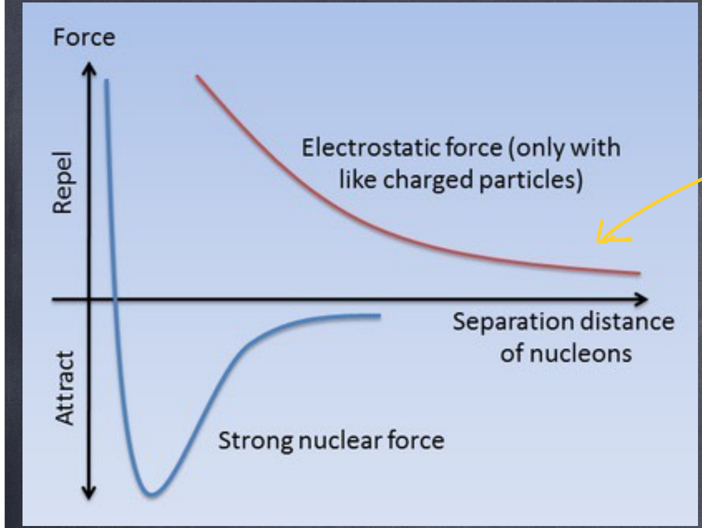




strong force

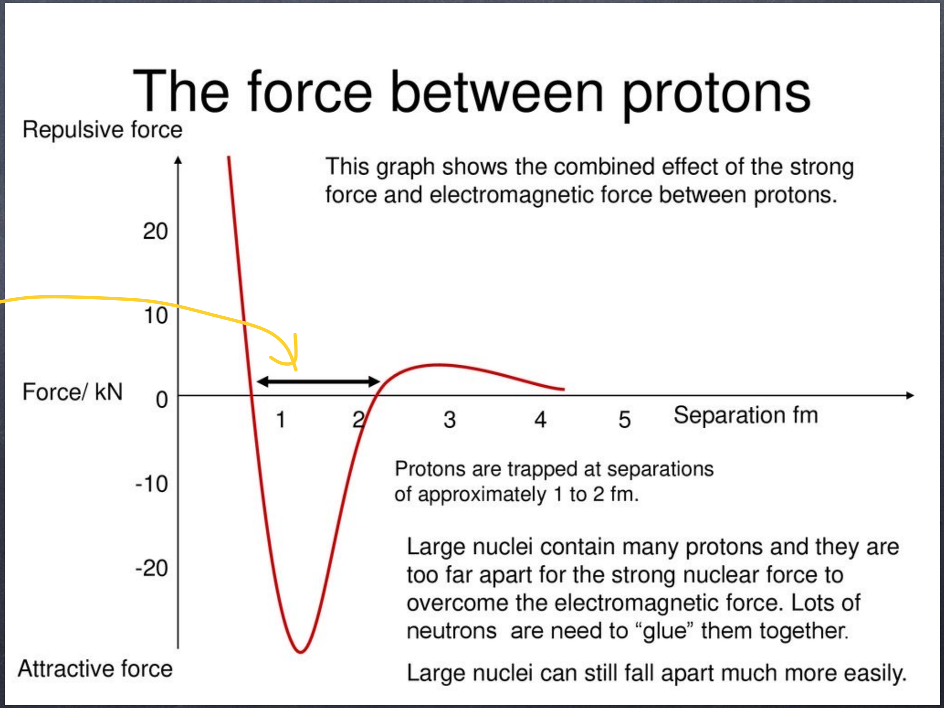
electrostatic repulsion
(coulomb repulsion)

Force between protons : two separate forces



Coulomb force

The combined effect of the two forces



The force between protons

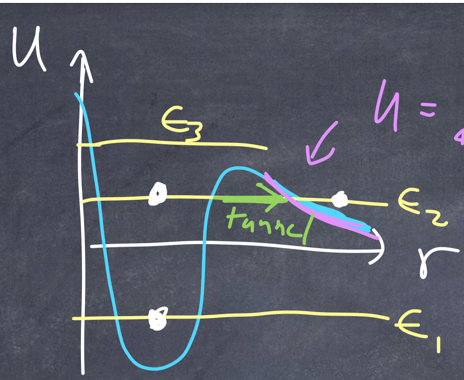
This graph shows the combined effect of the strong force and electromagnetic force between protons.

Protons are trapped at separations of approximately 1 to 2 fm.

Large nuclei contain many protons and they are too far apart for the strong nuclear force to overcome the electromagnetic force. Lots of neutrons are need to “glue” them together.

Large nuclei can still fall apart much more easily.

where protons would be trapped in the potential well



$$U = \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} = \frac{ke^2}{r}$$

U: potential energy of a proton at a given radius

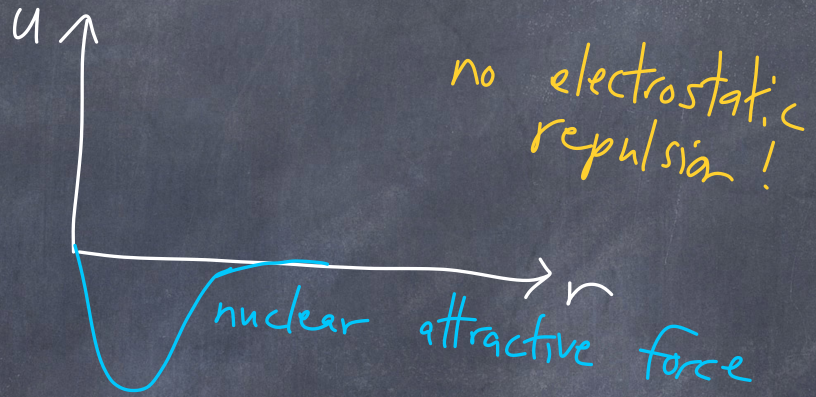
Imagine a proton of different energies in a nuclear potential well.

ϵ_1: stuck in the potential, not enough energy to escape (stable nuclei)

ϵ_2: meta-stable, quantum mechanics lets the proton tunnel out of the well, since it has enough energy to exist outside the nucleus.

ϵ_3: unstable, immediately escapes the nucleus.

For a neutron
it is very different:



Easier for a neutron to get captured (or escape) a nucleus (than a proton)

"Liquid drop model" of a nucleus

The nucleus is often thought of as a liquid drop.

nucleus	drop

both are incompressible & have uniform density.

nucleus	drop
↓	↓
held together by the nuclear force	held together by surface tension

useful analogy because
a drop can break into smaller drops

The total energy of a nucleus is the sum of the kinetic & potential energy of the constituents (nucleons). The potential energy is negative and larger than the kinetic energy, so the total energy is negative.

The total energy of the individual nucleons is larger than the energy of the assembled nucleus. The difference is due to the binding energy of the nucleus.

$$\text{Nuclear binding energy} = Z\left(m_p c^2\right) + N\left(m_n c^2\right) - \underbrace{mc^2}_{\text{mass of the assembled nucleus}}$$

m_p : mass of proton
m_n : mass of neutron

The binding energy is about 1% of the total mass.

$$\frac{8\ \text{MeV}}{1\ \text{u}} = \frac{8\ \text{MeV}}{930\ \text{MeV}} \sim 1\%$$