Nuclear Magnetic Resonance

Looking at magnetism from the inside !

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Spectroscopy of Quantum Materials

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MRI is NMR

MRI : Magnetic Resonance Imaging

NMR : Nuclear Magnetic Resonance

NMRI is NMR

NMRI : Nuclear Magnetic Resonance Imaging

NMR : Nuclear Magnetic Resonance

MRI is NMR with spatial resolution

What is a nucleus ?

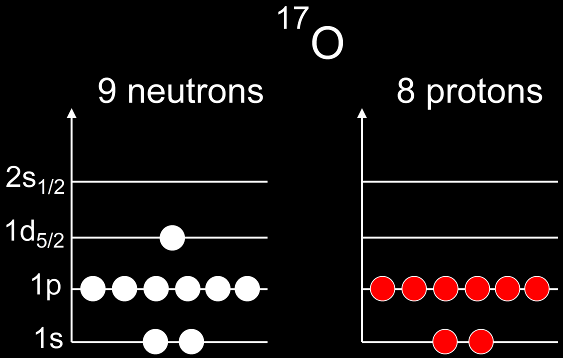
What is an atomic nucleus ?

Proton : opposite charge as electron and spin $1/2$

Neutron : not charged and spin $1/2$

Nuclear shell model

Like for electron around nucleus, nucleons (proton and neutron) are in shells.



S=5/2

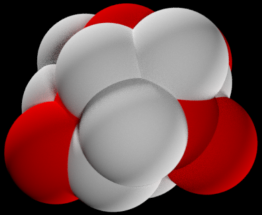
Properties of isotope

^{1}H	^{2}H	^{3}He	^{4}He	^{6}Li	^{7}Li	^{9}Be	^{10}B
1/2	1	1/2	0	1	3/2	3/2	3

^{11}B	^{12}C	^{13}C	^{14}C	^{14}N	^{15}N	^{16}O	^{17}O
3/2	0	1/2	0	1	1/2	0	5/2

Principle of NMR

Notation



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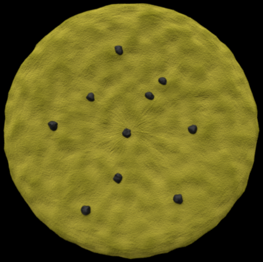
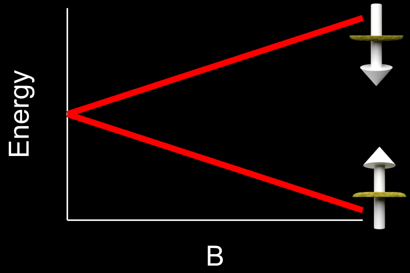


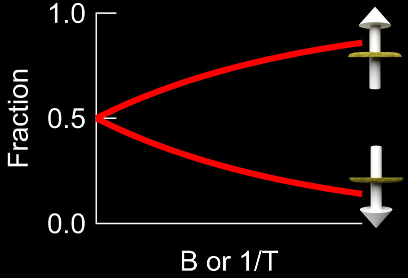
Spin 1/2 properties

A spin is like a magnetic dipole with quantized level. For spin 1/2 :

High magnetic field and low temperature

A macroscopique magnetic moment at thermal equilibrium

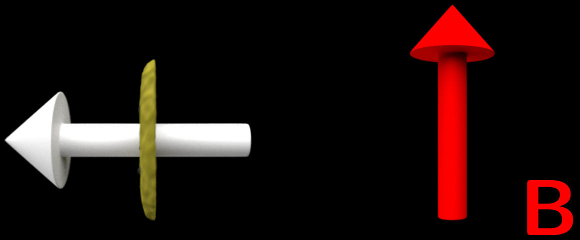




Precession

Macroscopic magnetic moment precesse around the external field

$$\frac{\partial \mathbf{M}(t)}{\partial t} = \gamma \mathbf{M}(t) \times \mathbf{B}(t) \qquad (1)$$



Frequency

$$f = \frac{\gamma}{2\pi}\mathbf{B} \tag{2}$$

B is not exactly the external field $\mathbf{B}_0$, electrons around the nucleus create a magnetic field $\mathbf{B}_{loc}$.
Static NMR consist to measure $\mathbf{B}_{loc}$ to extract wonderful information.

What can change B_{loc} ?

$$\mathcal{H} = \gamma_n \gamma_e \hbar^2 \mathbf{I} \cdot \left[\frac{\mathbf{L}}{r^3} + \left(3\frac{(\mathbf{S} \cdot \mathbf{r})\,\mathbf{r}}{r^5} - \frac{\mathbf{S}}{r^3} \right) + \frac{8\pi}{3}\mathbf{S}\delta(\mathbf{r}) \right] \tag{3}$$

In a dynamic phase (paramagnetic or diamagnetic), $\mathbf{B}_{loc} \propto \chi \cdot \mathbf{B}_0$ that depend of the density of state at the Fermi level

In frozen phase (ferromagnetic or spin glass), $\mathbf{B}_{loc} \propto \mu$

Cristal field

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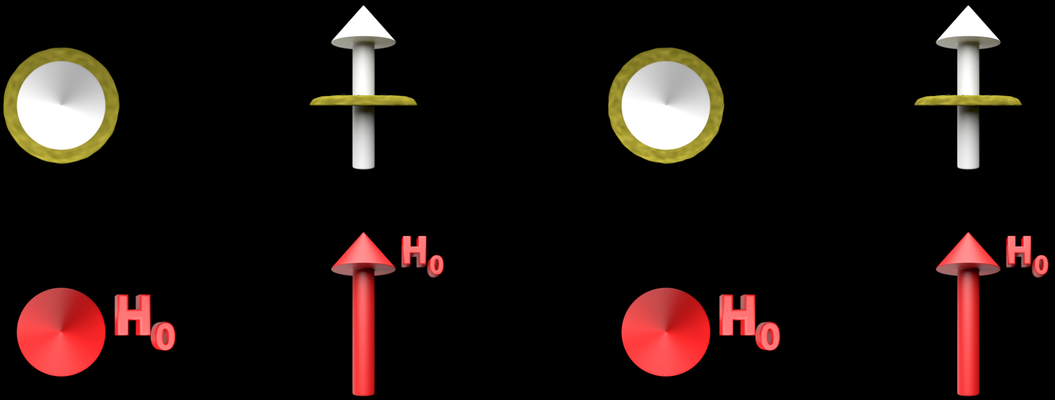
How mesure the frequency

How to manipulate spins

Laboratory frame

Rotating frame

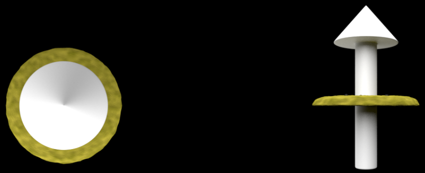
top side top side



Pulse echo

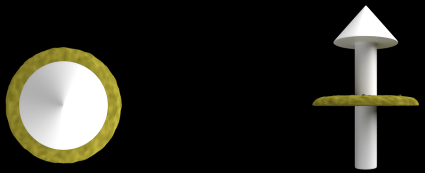
Laboratory frame

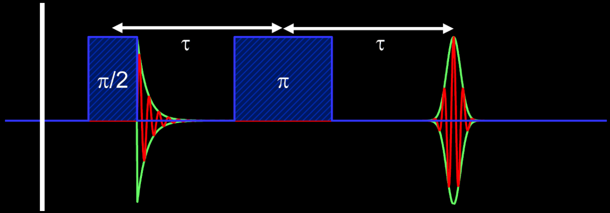
top side



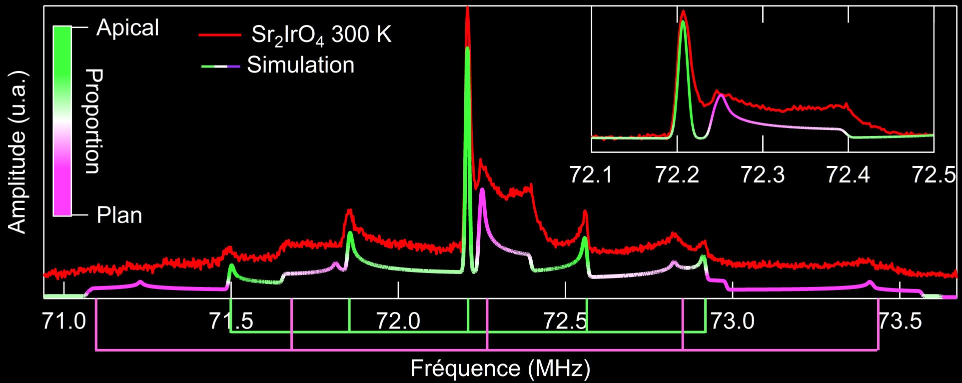
Rotating frame

top side





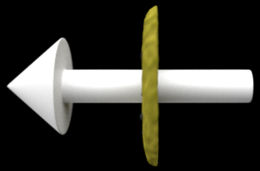
Sr_2IrO_4 at 300 K : ^{17}O spectrum



Dynamic NMR

The relaxation rate

Nuclei are linked to the environment and can exchange energy to go back at equilibrium. The characteristic time is called T_1 (spin-lattice relaxation)



The relaxation rate equation

General expression :

$$\frac{1}{T_1} = \gamma^2 \int_{-\infty}^{+\infty} \langle H_{loc}^{+}(t) H_{loc}^{-}(0) \rangle \, e^{-i\omega_0 t} dt \qquad (4)$$

If we assume that fluctuation are only electronic origin and by using the fluctuation-dissipation theorem

$$\frac{1}{T_1} = \frac{2\gamma^2}{g^2 \mu_B^2} k_B T \sum_{\vec{q}} |A(\vec{q})|^2 \frac{\chi''_{\perp}(\vec{q}, \omega_0)}{\omega_0} \qquad (5)$$

The Korringa law (in a metal)

$$\frac{1}{T_1 T K^2} = \frac{4\pi k_B}{\hbar} \left(\frac{\gamma_n}{\gamma_e} \right)^2 \qquad (6)$$

Conclusion

- local probe (can differentiate an impurity phase or different sites in one phase)

- sensible to electronic and magnetic properties (susceptibility, magnetic moment, ...)

- sensible to the environment configuration (quadrupolar electric effect)

- probe the fluctuations with **q** resolution

- probe the homogeneity of the properties (T_2, peak width, satellite width, ...)

...

You need an information ?

NMR can answer !

Not always but often