

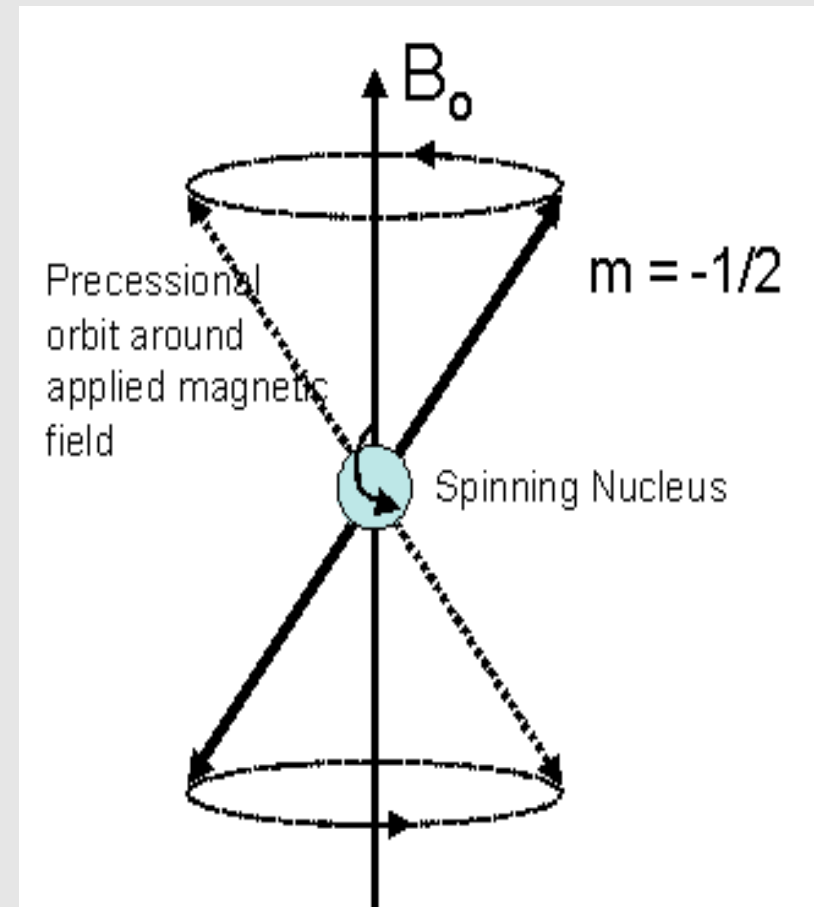
NMR EXPERIMENTS

NMR basics

- Nucleus with spin required
- External magnetic field

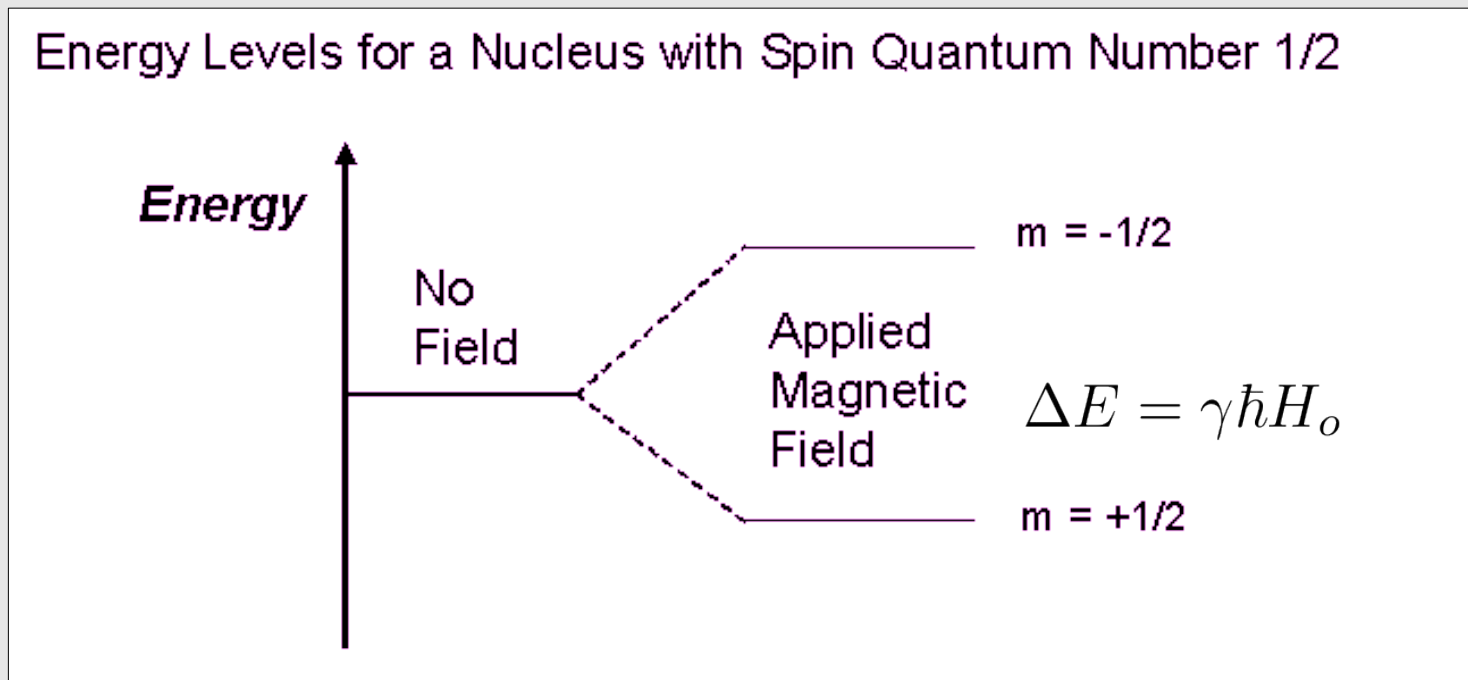
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- precession of magnetic moment
 - splitted energies

picture: www.process-nmr.com/



NMR basics

- Zeeman Hamiltonian: $\mathcal{H}_z = -\gamma\hbar \sum_i I_z^i H_0$
- $E = \pm\gamma\hbar\frac{H_0}{2}$



picture: www.process-nmr.com/

Continuous Wave NMR

- Excitation of nucleus with photons
- Frequency changed until resonance found
- Not up to date anymore

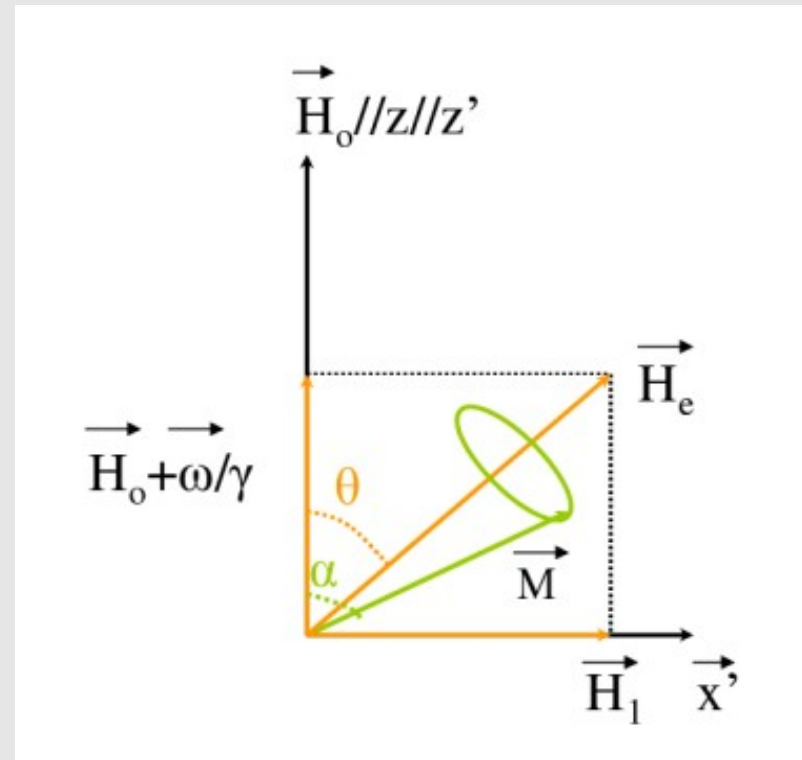
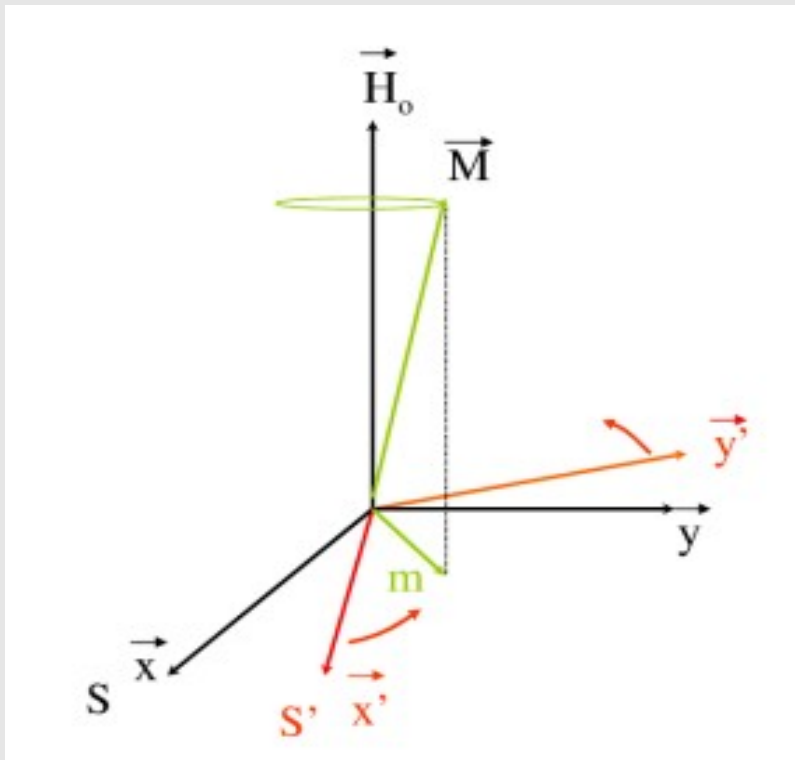
pulsed NMR

- Second rotating magnetic field
- Pulsed

NMR pulsed: rotating frame

- Change to rotating frame
- Adding 2nd H-field now

$$H = (H_0 - \frac{\omega}{\gamma})e_z + H_1e'_x$$



pictures: 'NMR-MRI, uSR and Mössbauer Spectroscopies in Molecular Magnets' by Carretta, Lascialfari

NMR pulsed: signal

- Same coil for sending pulse and receiving signal
- Signal is proportional to:
 - resonance frequency
 - and to the x-y part of M
- This signal transformed into the rotating frame is called FID free induced decay

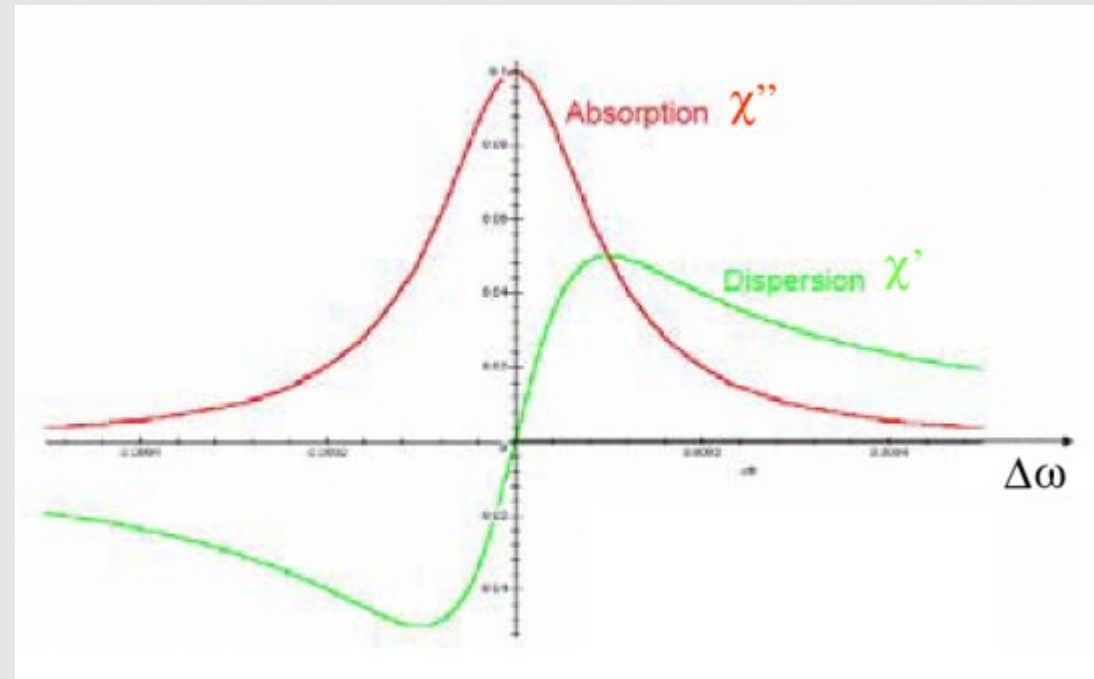
- Bloch equations:

$$\frac{dM_z}{dt} = \gamma(\mathbf{M} \times \mathbf{H}_0)_z + \frac{M_0 - M_z}{T_1}$$
$$\frac{dM_{x,y}}{dt} = \gamma(\mathbf{M} \times \mathbf{H}_0)_{x,y} - \frac{M_{x,y}}{T_2}$$

- Lead to magnetization and susceptibility depending on the frequency

$$\chi = \text{Re}(\chi) + \text{Im}(\chi) = \chi' + \chi''$$

- For a small H_1 :



pictures: 'NMR-MRI, μ SR and Mössbauer Spectroscopies in Molecular Magnets' by Carretta, Lascialfari

NMR spectra

- $f(\omega)d\omega$ Gives the fraction of nuclei with resonance in this frequency area
 - Is proportional to the absorbed power
 - Is proportional to the real part of the susceptibility

$$P(\omega) = \frac{\chi''}{2} \omega \omega_0 H_1^2 f(\omega) 2\pi$$

$$P(\omega) = \frac{1}{2} \omega H_1^2 \chi''(\omega) V$$

CW NMR signal:

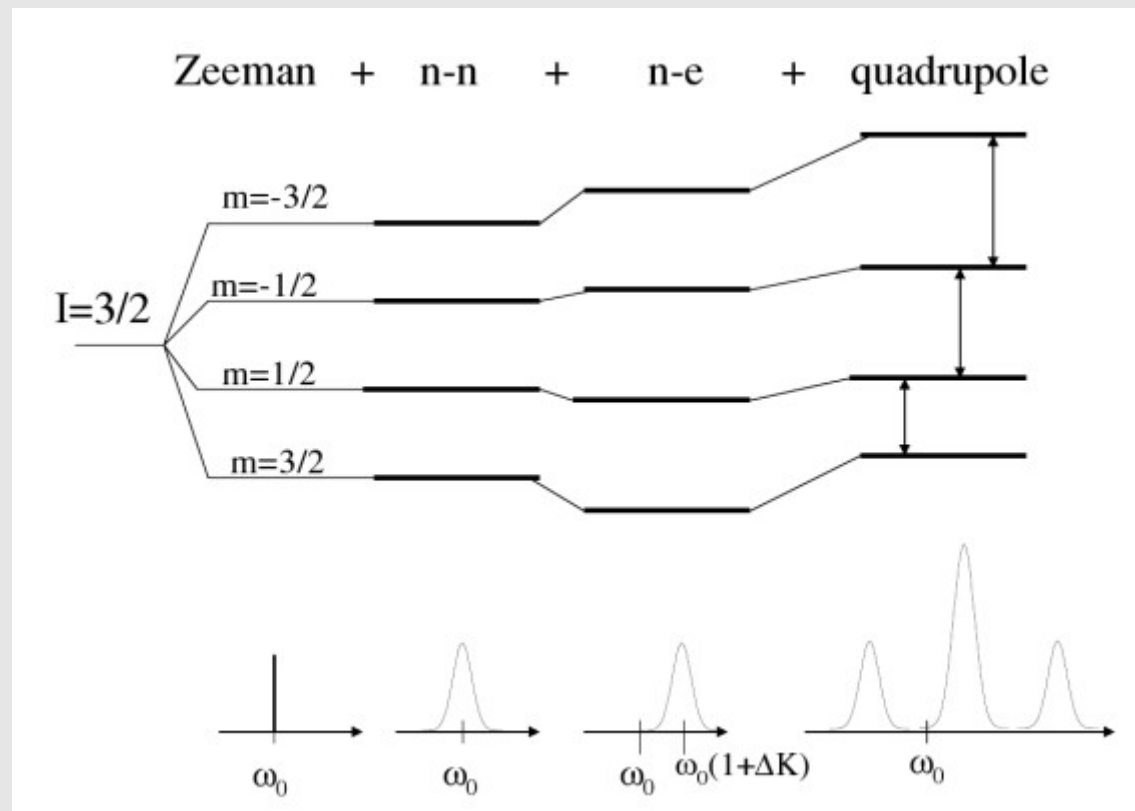
- proportional to absorbed Power

NMR spectra

- pulsed NMR signal: proportional to
 - Resonance frequency
 - Transverse M
- Fourier transform of pulsed NMR signal is the spectrum

NMR hyperfine hamiltonian

$$\mathcal{H} = \mathcal{H}_z + \mathcal{H}_{n-n} + \mathcal{H}_{n-e} + \mathcal{H}_{EFG}$$



pictures: 'NMR-MRI, uSR and Mössbauer Spectroscopies in Molecular Magnets' by Carretta, Lascialfari

references

- 'NMR-MRI, uSR and Mössbauer Spectroscopies in Molecular Magnets' by Carretta, Lascialfari
- Wikipedia
- www.process-nmr.com/
- www.cis.rit.edu/htbooks/nmr/inside.htm