F61: NMR–Spectroscopy

T. Gierlich and A. Impertro

May 26th, 2017

Outline

Introduction

NMR-Spectroscopy

Nuclear **M**agnetic **R**esonance

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NMR-Spectroscopy

Nuclear **M**agnetic **R**esonance

Detection of substances

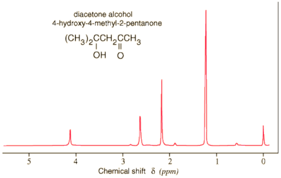

Figure: Carl Nave, Hyperphysics, hyperphysics.phy-astr.gsu.edu

Multidimensional imaging

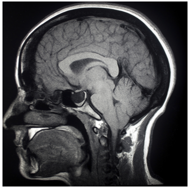

Figure: Sierra Vista Diagnostics, svdrads.com

Theoretical Concepts - Working Principle

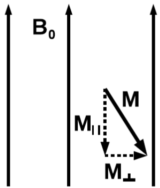

Figure: Magnetization

- Nuclei with spin I have a magnetic moment μ
- Ensemble of many nuclei: Measurable magnetization $\vec{M}$
- Minimal energy $\rightarrow$ Dipole aligned parallel to B-field
- Ground state $\rightarrow M_\perp = 0$

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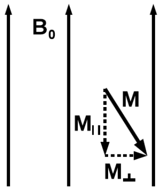

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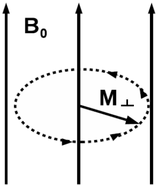

Figure: Larmor-Precession of $M_\perp$

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- Excited states have a component $M_\perp \neq 0$
- $M_\perp$ precesses around the field lines with the Larmor frequency

$$\omega_L = \gamma B_0 \tag{1}$$

- ω_L can be measured!

Theoretical Concepts - Working Principle

How can we create an excited state ?

- An oscillating B-Field $\vec{B}_1$ rotates the magnetization $\vec{M}$ by an angle

$$\alpha = \gamma B_1 \Delta t \qquad (2)$$

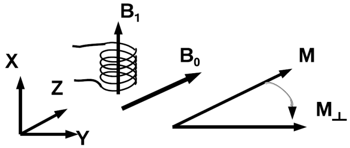

Figure: Rotation of M due to an HF-Pulse

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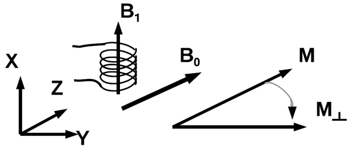


Figure: Rotation of M due to an HF-Pulse

- By choosing Δt, we can create:
  - A perpendicular magnetization (90°-Pulse)
  - An anti-parallel magnetization (180°-Pulse)

Setup and Measurement Principle

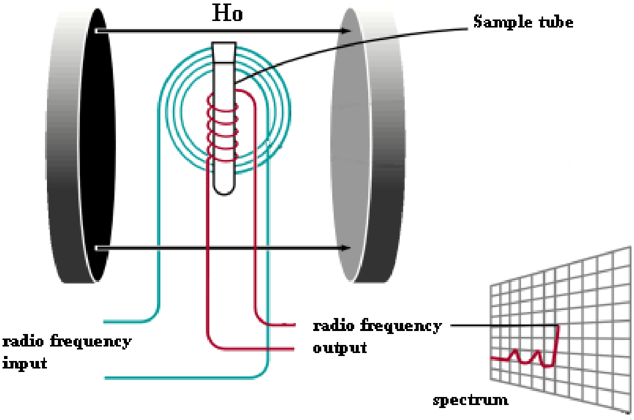


Figure: McGraw Hill Higher Education, mhhe.com

Theory of Relaxation

Excited states decay into the Ground State on a characteristic timescale.
The decay is of exponential nature and described in the *Bloch equations:*

$$\frac{dM_\perp(t)}{dt} = -\frac{M_\perp(t)}{T_2} \tag{3}$$

$$\frac{dM_\parallel(t)}{dt} = -\frac{M_\parallel(t) - M_0}{T_1} \tag{4}$$

- T_2: Spin-Lattice Relaxation
- T_1: Spin-Spin Relaxation

T_2-Measurement: Spin Echo

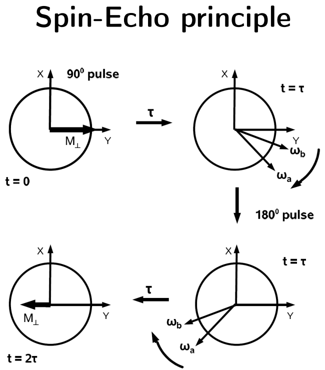


Figure: Principle of the spin-echo method

T_2-Measurement: Spin Echo

Spin-Echo principle

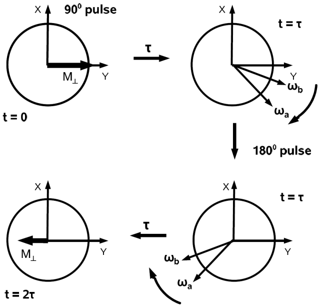


Figure: Principle of the spin-echo method

Pulse sequence

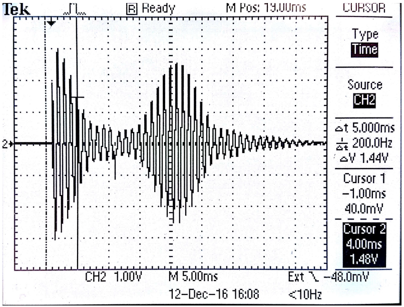
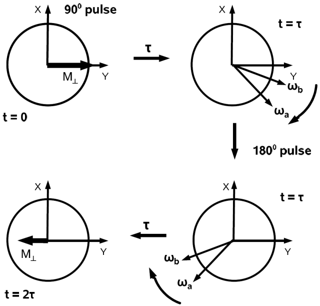


Figure: Spin-Echo measurement with $\tau = 10ms$

T_2-Measurement: Spin Echo

Spin-Echo principle



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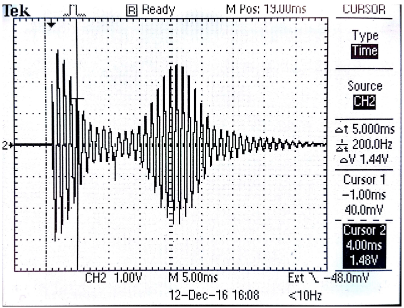

Figure: Spin-Echo measurement with $\tau = 10ms$

- **Disadvantage**: Dephasing for long measurement times!

T_2-Measurement: Spin Echo

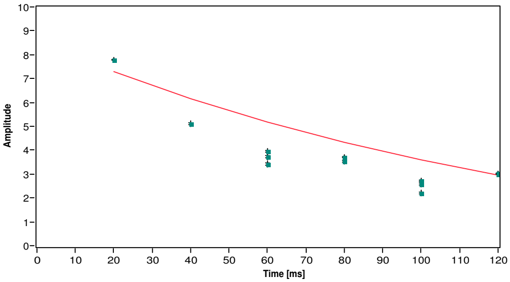

Figure: T2-Measurement Sample 1 with fit.

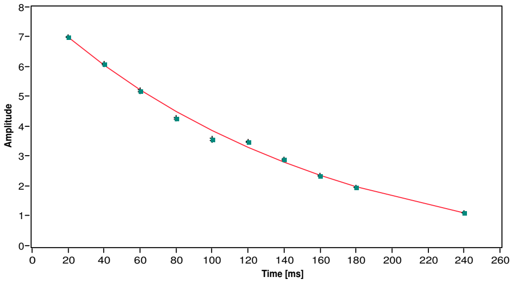

Figure: T2-Measurement Sample 3 with fit.

T_2-Measurement: Carr-Purcell Sequence

Improve dephasing problem of spin-echo method:

- Inject a 180°-Pulse on odd multiples of a time τ.
- The system is phase coherent on even multiples of a time τ.

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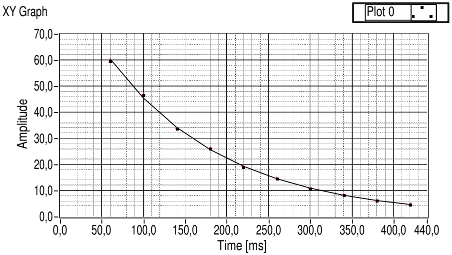

Figure: T2-Measurement using Carr-Purcell, Sample 1, with fit.

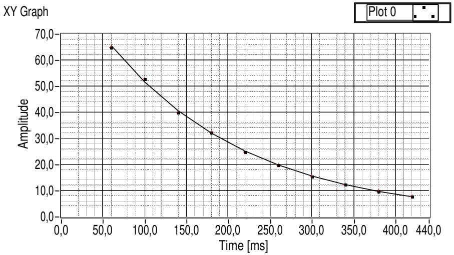

Figure: T2-Measurement using Carr-Purcell, Sample 3, with fit.

T_1-Measurement

Start with a 180°-Pulse (Anti-parallel Magnetization) and probe the magnetization after time τ with a 90°-Pulse

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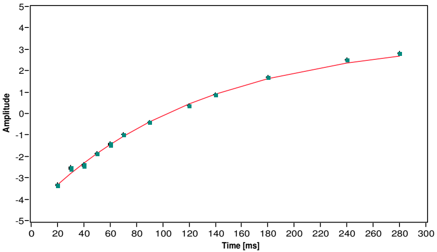

Figure: T1-Measurement Sample 1 with fit.

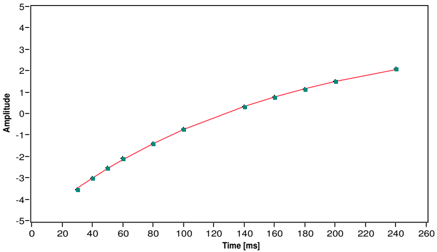

Figure: T1-Measurement Sample 3 with fit.

Relaxation Times: Evaluation

Table: Relaxation times – Measured values

Time Method	T_1 [ms] 180°-90°	T_2 [ms] Spin-Echo	T_2 [ms] Carr-Purcell
Sample 1 (Gd 1:500)	$(125,5 \pm 0,6)$	$(119,5 \pm 0,5)$	$(140,1 \pm 0,4)$
Sample 3 (Gd 1:600)	$(150,5 \pm 1,2)$	$(139,3 \pm 0,8)$	$(166,9 \pm 0,4)$