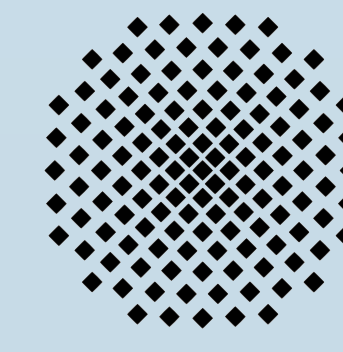


NMR – Nuclear Magnetic Resonance

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Motivation and Application

Nuclear Magnetic Resonance (NMR) describes the interaction of an atomic nucleus in a magnetic field with external, alternating magnetic fields, where the nuclei absorb and emit these alternating fields.

In physics NMR is used to determine properties of various materials, especially fluids. Knowing the properties of certain materials, an NMR-Spectroscopy can be done to reveal the structure of an unknown sample.

The most popular application of NMR is of course the medical method of magnetic resonance imaging as a diagnostic technique.

Theoretical Background

Quantum Mechanical Background

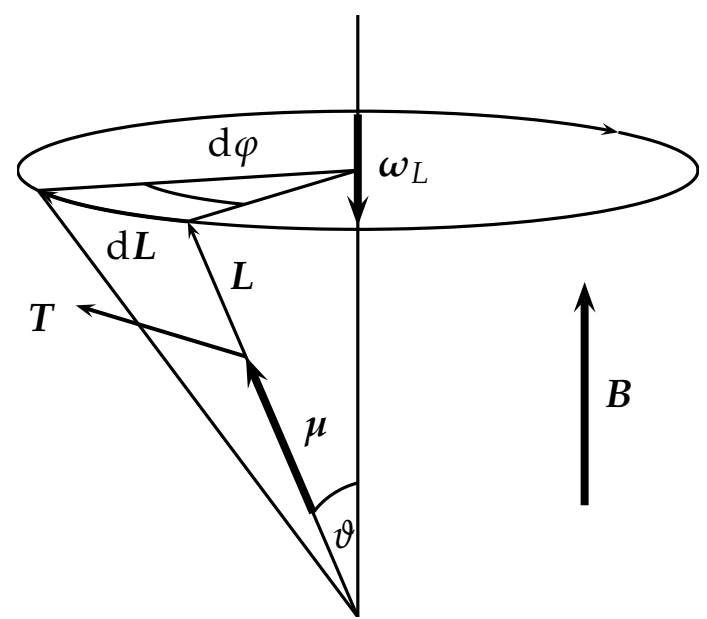
Like electrons, also nuclei have a spin I . The magnetic moment of this spin also interacts with a magnetic field, which is described by

$$\mu_I = -g_I \frac{\mu_N}{\hbar} I = -\gamma I$$

μ_N : nuclear magneton

g_I : Landé factor

γ : gyromagnetic ratio



The torque T towards the magnetic moment leads to the angular momentum I to precess around the axis defined by the magnetic field at the Larmor frequency ω_L .

$$\omega_L = \frac{|\mu_I|}{|I|} B = \gamma B$$

The potential energy of the magnetic moment reads

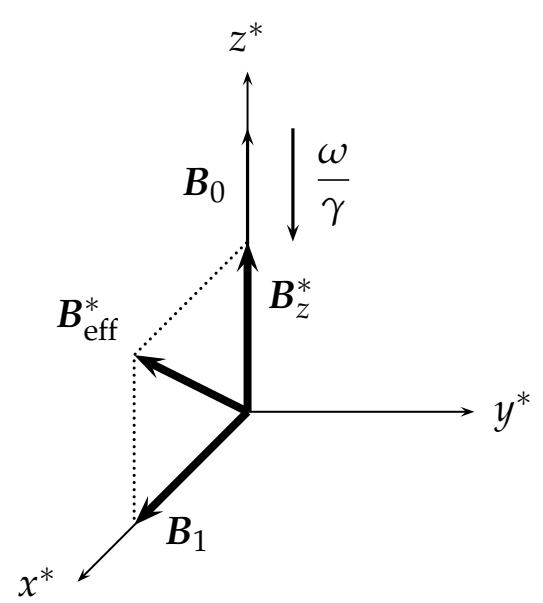
$$E_\mu = -\mu \cdot B = -m_I \hbar \gamma B$$

A static magnetic field coupled to a magnetic moment.

It follows, that the energy difference of two adjacent energy levels is $\Delta E = \hbar \gamma B$.

Magnetization

- When a magnetic field is applied it takes some time for the system to reach the equilibrium state of magnetization M_0 .
- The process of approaching this state can be described by a differential equation with the longitudinal relaxation time T_1 . Because the spin exchanges energy with its surroundings (called lattice), this one is called *spin-lattice-relaxation time*.
- There also exists a transversal magnetization M_x and M_y , which depend on the transversal relaxation time T_2 (spin-spin relaxation time).



The rotating frame.

If now a magnetic field is applied, which operates near the Larmor frequency, we get the so called *Bloch equations* in the rotating frame; for a derivation see [2, p. 14].

$$\frac{d}{dt} M_x^* = (\gamma B_0 - \omega) M_y^* - \frac{M_x^*}{T_2} \quad (1a)$$

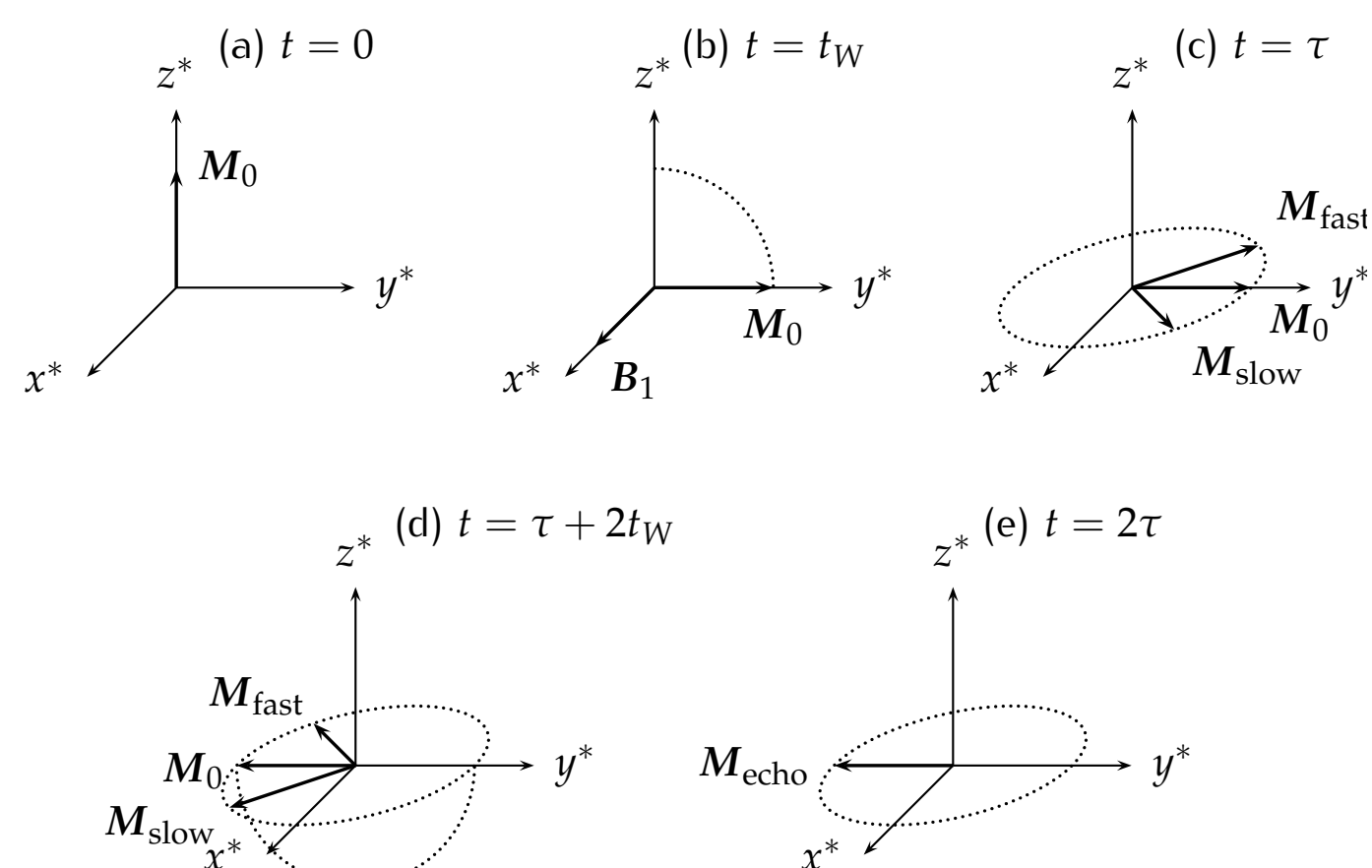
$$\frac{d}{dt} M_y^* = -(\gamma B_0 - \omega) M_x^* - \gamma B_1 M_z^* - \frac{M_y^*}{T_2} \quad (1b)$$

$$\frac{d}{dt} M_z^* = -\gamma B_1 M_y^* - \frac{M_z^* - M_0}{T_1} \quad (1c)$$

The terms containing the times T_1 and T_2 describes the relaxation process, while the terms containing B_0 describe a precession around the magnetization M^* and the terms with B_1 reflect a movement around the x^* -axis, see the adjacent figure for an illustration.

Pulsed NMR

A homogeneous static magnetic field $B_0 = B_0 e_z$ is applied in z direction. The nuclear spin now precesses around this field. Now a high frequency magnetic pulse B_{HF} is put on, perpendicular to B_0 , the magnetization is deflected towards the field resulting from a superposition of B_0 and B_{HF} .



After this pulse the magnetization returns to equilibrium as described by Bloch's equations (1,a-c). In the time, when the spin magnetic moment does not precess around B_0 , an oscillating magnetic field is induced.

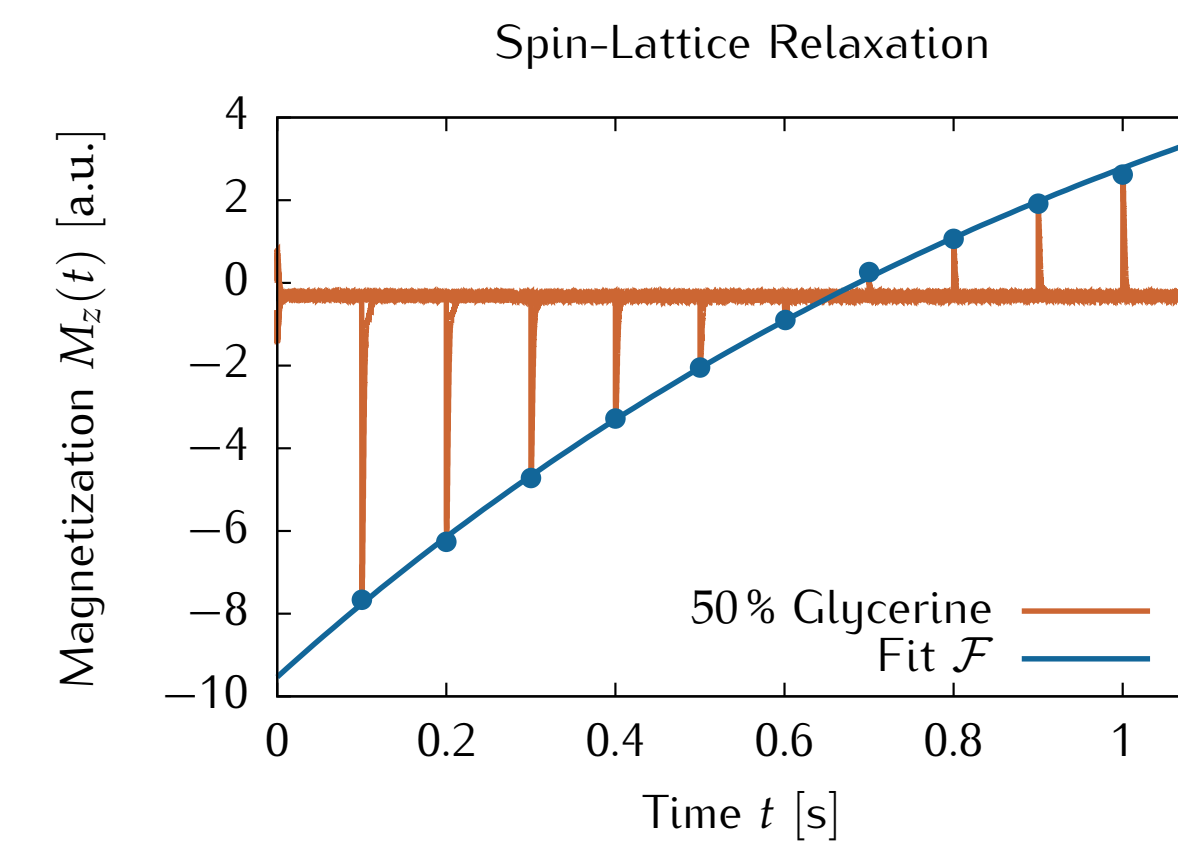
The oscillating field is applied in two modes:

- 90°-pulses last the time t_W , which exactly deflects the spin from its idle state to the x, y -plane.
- 180°-pulses last for $2t_W$ and invert the spins.

The time between two pulses is τ .

After the 90°-pulse is put in some spins precess faster than others due to inhomogeneities in the field B_0 and the various magnetic surrounding in the sample itself. Because of the precessions drifting apart we obtain a decaying signal, called FID-Signal (free induction decay). After 2τ a *spin echo* can be measured because when inverting the spins the precessions start to approach again and when they meet the resonance signal is at a maximum, due to all spins being in phase.

Analysis

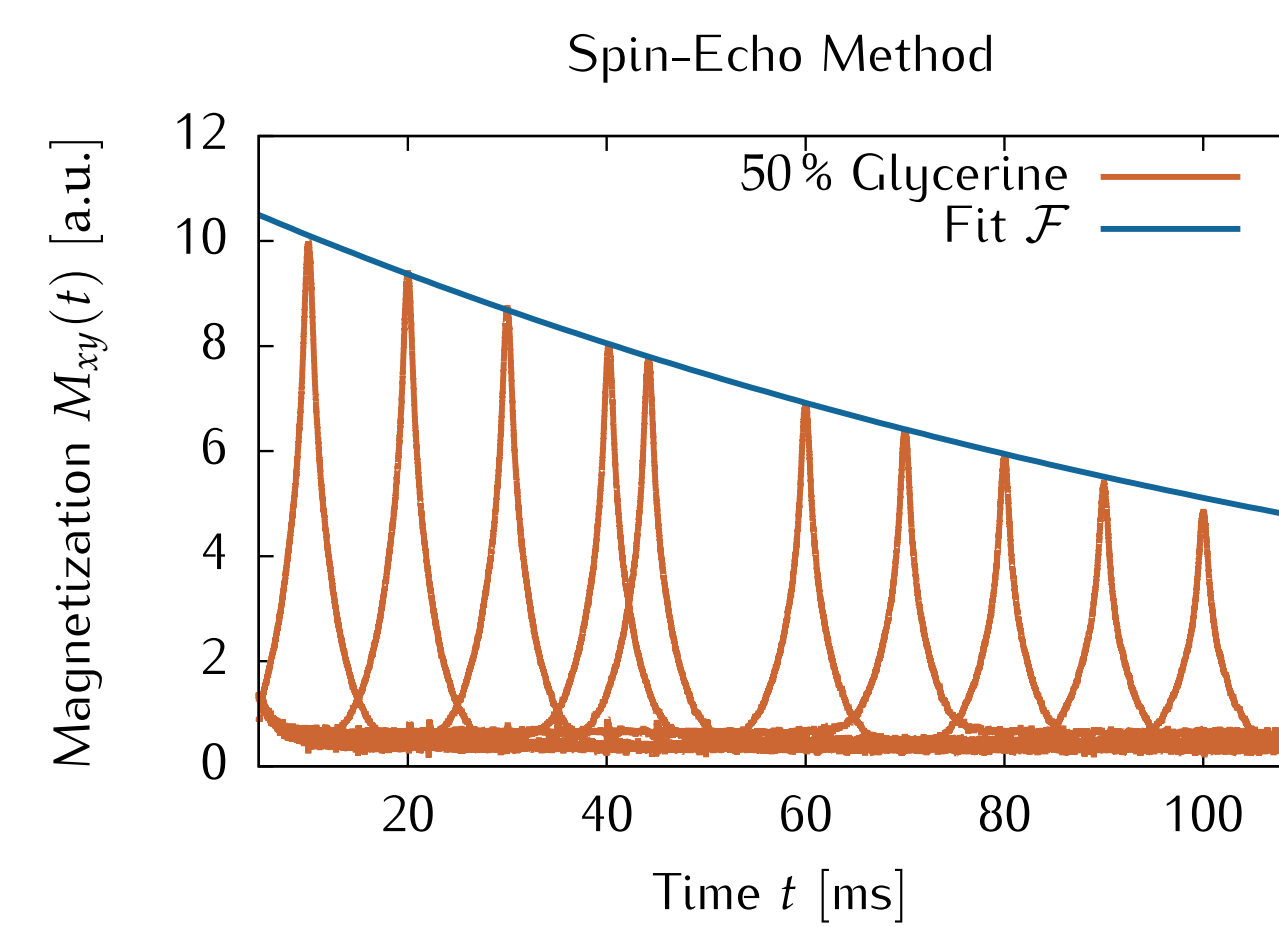


The longitudinal relaxation time T_1 is the time, that the z component of the magnetization needs to return to its idle state. Therefore a 180°-pulse is induced to invert the magnetization followed by a 90°-pulse. Afterwards the FID-Signal can be measured. Through variation of τ , M_z can be recorded at different times and an increase can be observed.

The fitted function has the form

$$\mathcal{F}_{M_0, T_1}(t) = M_0 \left[1 - 2 \exp\left(-\frac{t}{T_1}\right) \right]$$

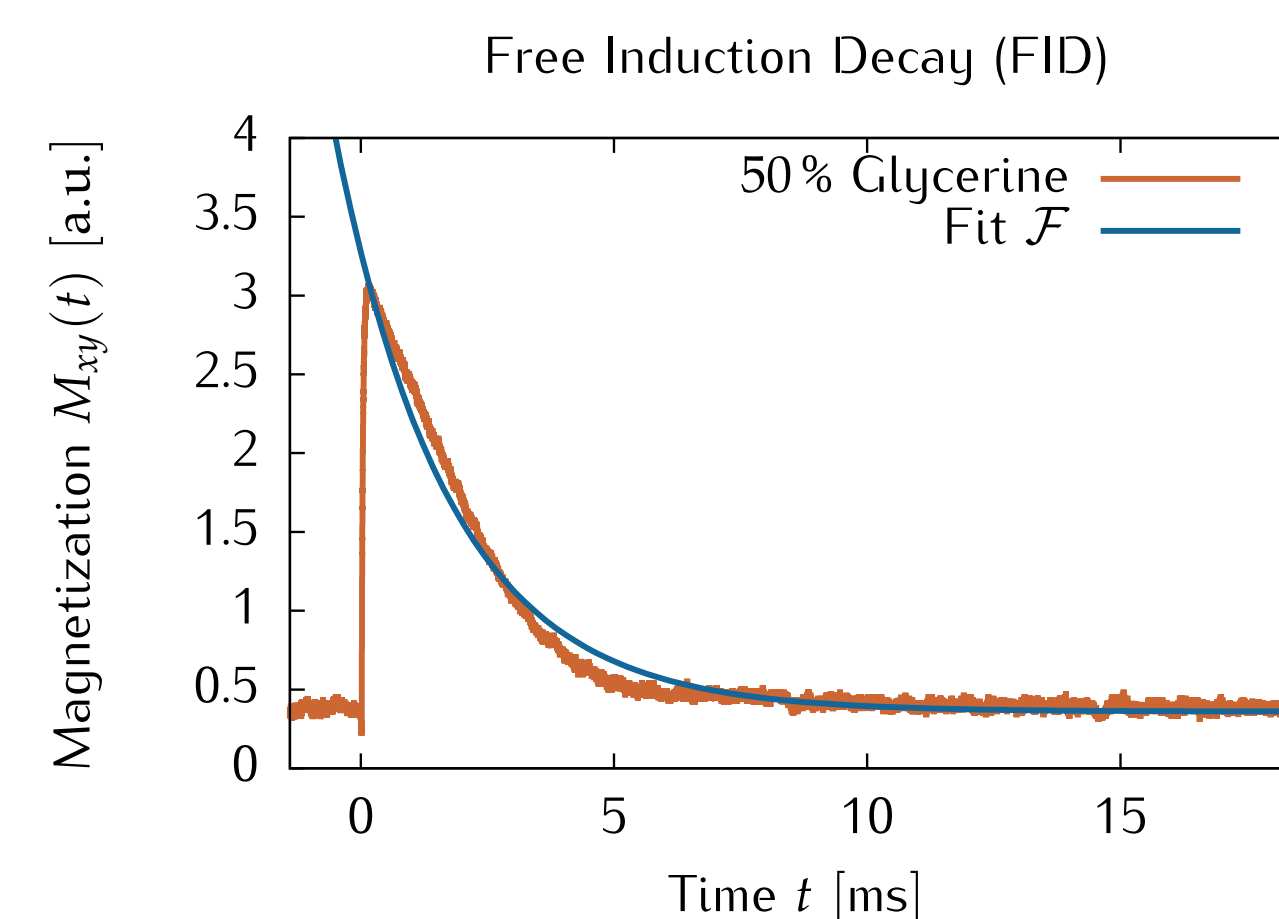
which is derived from (1c) in z direction without a HF-field.



The Spin-Echo method is described in detail in the adjacent block titled *Pulsed NMR*. As proposed and described in detail in [2, p. 29] the fitting function

$$\mathcal{F}_{M_0, T_2}(t) = M_0 \exp\left(-\frac{t}{T_2}\right)$$

can be used to determine the transversal relaxation time T_2 .



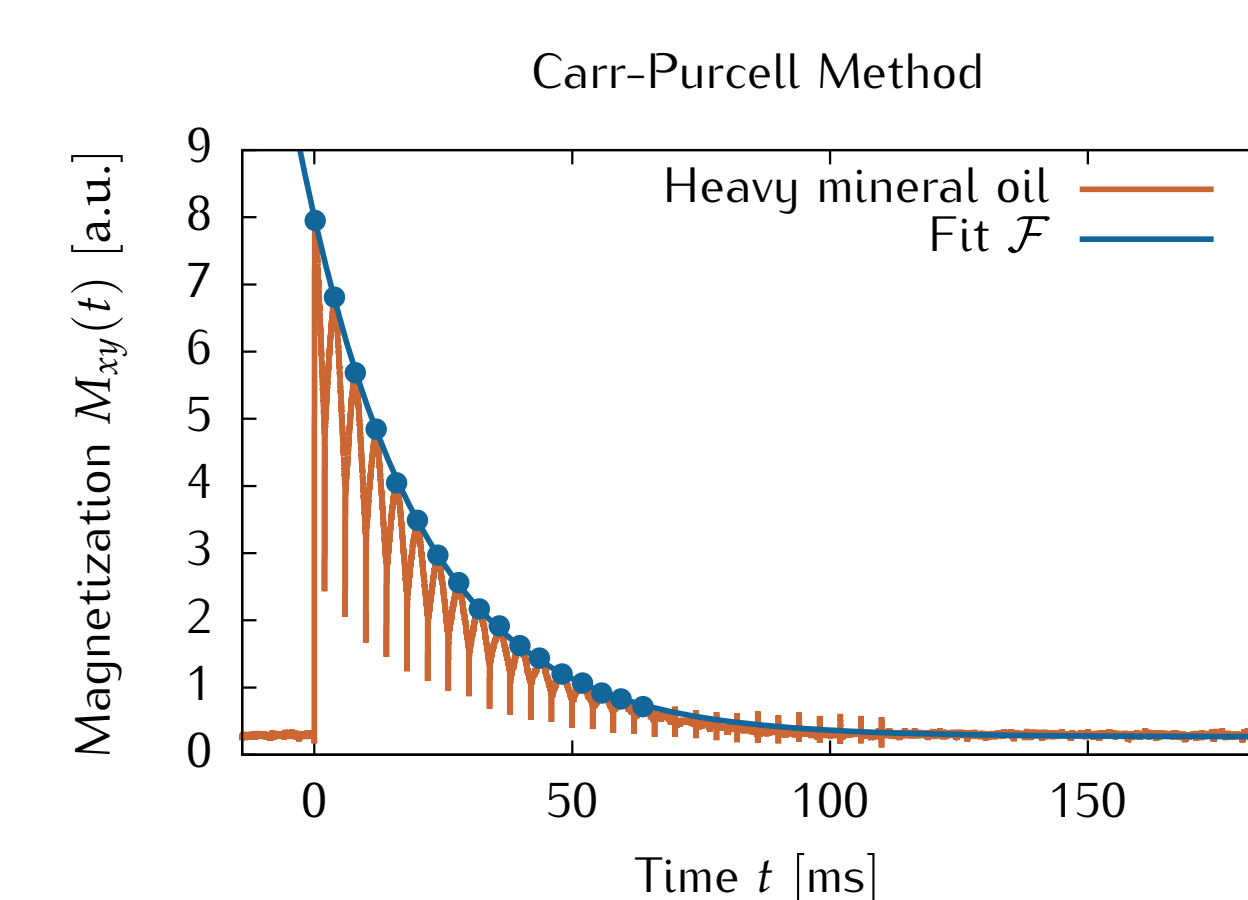
As for the Spin-Echo method, the function

$$\mathcal{F}_{M_0, T_2}(t) = M_0 \exp\left(-\frac{t}{T_2}\right)$$

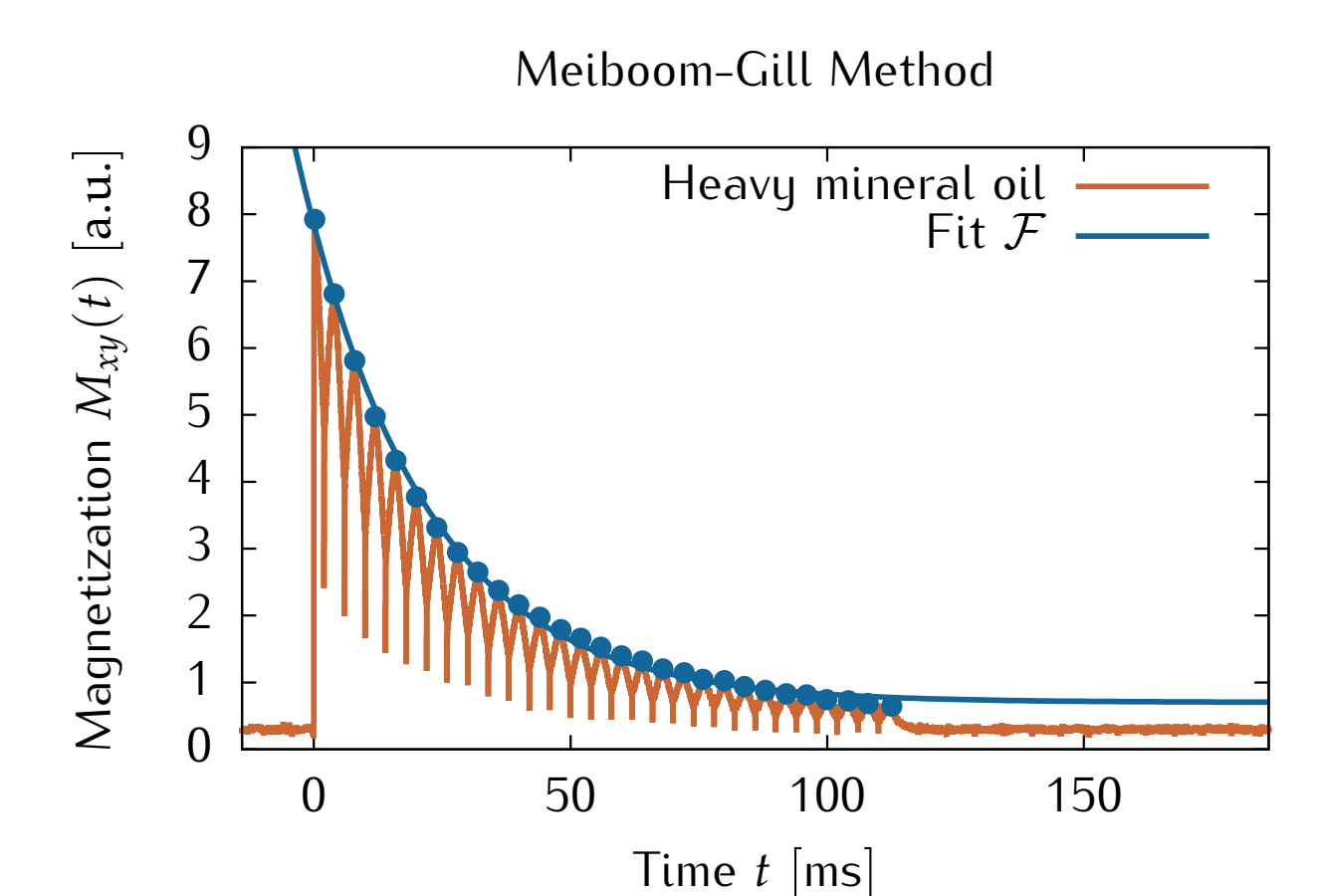
will be used for determining the relaxation time T_2 . The obtained value is called T_2^* , because it will differ from T_2 received by the Spin-Echo method, as inhomogeneities in the magnetic field can't be compensated. All the relaxation times are listed in table ??.

Multipulse methods

The *Carr-Purcell-Method*: After a 90°-pulse a 180°-pulse is used to produce a spin echo. Afterwards several 180° pulses are induced to produce more echoes. These are fitted with the same function as for T_1 .



The *Meiboom-Gill-Method*, fixes the issue of the Carr-Purcell-Method, that errors in the pulses add up. Therefore a phase shift of 90° is introduced, such that the spin inversions are always in opposing directions.



Résumé

The different relaxation times were determined for various samples. These consist of a mixture of glycerine and water at varying ratio (100 %, 50 %, 20 %, 10 % and 0 %) and two different mineral oil (light and heavy).

- T_1 : For the glycerine mixtures the relaxation times span through 18.361 ms to 199.529 ms for the ratio glycerine/water 100 %, 50 %, 20 %, 10 % and 0 %. For the two mineral oil the following times were measured: $T_{1, \text{heavy}} = 34.388$ ms and $T_{1, \text{light}} = 52.216$ ms.
- T_2 : This time the relaxation times for glycerine in water are in the range 129.989 ms to 184.328 ms. Heavy mineral oil needs 31.546 ms while light mineral oil takes 64.027 ms.
- T_2^* : The relaxation times determined from a single FID are for glycerine in water in the domain 1929.478 ms to 1654.289 ms. The times for heavy and light mineral oil are $T_{2, \text{heavy}}^* = 2.382$ ms and $T_{2, \text{light}}^* = 2.536$ ms.

References

- [1] H. Haken and H. C. Wolf. *Atom- und Quantenphysik*. 8., aktual. u. erw. Aufl. Springer Verlag, 2004.
- [2] D. Wiesche. 'Aufbau eines Versuches zur gepulsten und cw-NMR Spektroskopie'. Ruhr-Universität Bochum, Sept. 2009.