Dynamik von Spin-$\frac{1}{2}$-Teilchen mittels kernmagnetischer Resonanz

Lab Report

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Institute for Applied Physics

Jens Erler & Alexander Harder
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1 Prerequisites

1.1 principle of nuclear magnetic resonance

For atomic nuclei, the relation between angular momentum $\vec{J}$ and magnetic moment $\vec{\mu}$ is given by

$$\vec{\mu} = \gamma \vec{J}$$

where γ is the gyromagnetic ratio. The angular momentum is proportional to the spin of the nucleus I as:

$$\vec{J} = \eta I$$

where

$$\eta \in \mathbb{N}$$

In a magnetic field, a particle with angular momentum recieves a torque as follows

$$\vec{M} = \frac{d}{dt}\vec{J} = \mu \times \vec{B} = \gamma \vec{J} \times \vec{B}$$

When brought into an external magnetic field in the direction of z, the magnetic moments start to precess. Its frequency depends on the local atomic magnetic fields and is therefore unique for every type of atom. This frequency is also called *Larmor frequency* and one can write

$$\omega_0 = \gamma B_0$$

Thus, one can write for the magnetic energy of the nucleus:

$$U = -\mu_z B_0 = -\gamma \eta I_Z B_0$$

The possible values of I_Z are given by m_I with $m_I \in \{-I, -I+1, ..., I-1, I\}$
In our experiment we work with hydrogen and fluor. Both have spin $\frac{1}{2}$. Hence:

$$m_I = \pm \frac{1}{2}$$

There are only two possible magnetic energy states for the named nuclei when exposed to a constant magnetic field. The energy separation is given by:

$$\Delta U = \eta \omega_0 = \gamma \eta B_0$$

1.2 Spin-$\frac{1}{2}$-systems

A system, which only supports two possible states $|\downarrow\rangle$ and $|\uparrow\rangle$, as well as superpositions of them, is called a two state system. An example for such a system is the spin state of a spin-$\frac{1}{2}$-systems, which can either be "spin up" or "spin down". In equilibrium, the occupation number of both stats is stable, until the system is disturbed from outside.

1.3 Bloch vector and Bloch sphere

The Bloch sphere can be used to visualize a two-state system of N particles. Every possible vector in this sphere, pointing from its center to a certain point on its surface, represents a possible state. The two poles on the z-axis represent two basis vectors. They can be interpreted as the two pure states, $|\downarrow\rangle$ and $|\uparrow\rangle$. Any other vector in the sphere can be understood as a superposition of the two states. The vectors in the equatorial plane consist of both states in equal parts.

1.4 Spin-Dynamics in an external magnetic field

1.4.1 Rabi-Oscillation

Rabi-Oscillation is observed, when a quantum mechanical system is disturbed form outside, e.G. by an oscillating magnetic field

$$B_1(t) = B_1(\cos(wt)\vec{e_x} + \sin(wt)\vec{e_y})$$

The observed period $\Omega_R = \gamma B_1$ is called the Rabi frequency. In addition, one can define the detuning $\Delta = \omega_{12} - \omega$, where ω_{12} is the frequency of the transition and ω is the frequency of the disturbance. In case of a resonance ($\Delta = 0$) the Bloch-Vector changes its position from θ to $-\theta$ and than the other way around. Without resonance, the Bloch-Vector oscillates between two latitudes.
The most important pulses are the following:

- π-pulse: 180° turn
- $\frac{\pi}{2}$-pulse: 90° turn

1.4.2 inversion

1.4.3 Spin-Echo

In order to eliminate the effect of transversal relaxation, the sample is exposed to an π-Pulse, which turns all spins 180°in the x-y-plane. This causes the spins to stay in the x-y-plane and unite in a signal, called the spin-echo. In graphic terms, this means that the "slower" spins catch up with the "faster" ones.

1.5 Thermal Equilibrium

When a probe of hydrogen with N protons, where $N >> 1$, is placed into a homogeneous magnetic field, the particles will reach a state of thermal equilibrium. Let N_2 and N_1 be the number of spins in the two quantum states, where the energy of $|2>$ is higher. Then we can write $N_1 > N_2$ because there are always mor protons in the lower state. The population ratio, given by the Boltzmann factor is:

$$\frac{N_2}{N_1} = e^{\frac{\Delta U}{k_B T}} = e^{\frac{\eta\omega_0}{k_B T}}$$

The difference of the magnetic energy ΔU is small compared to $k_B T$, what means that $N_2 \approx N_1$. Nevertheless, the difference $N_1 - N_2$ is still large enough to cause a magnetization M_Z in the direction of z:

$$M_Z = (N_1 - N_2)\mu$$

With no external field applied, we have $N_1 = N_2$. This means that, during magnetization, some spins lose energy to its surrounding while some others gain energy. This surrounding is called lattice.
In thermal equilibrium, the magnetization per unit volume for N particles is given by

$$M_0 \approx N\frac{\mu^2 B}{k_B T}$$

where $N = N_1 + N_2$.
The resulting magnetization is only in the direction of z, because the z-components of $\vec{\mu}$ sum up, while the x- and y-components cancel each other out to zero.

1.6 Decoherence Mechanisms

1.6.1 Thermal Relaxation Time (T1)

If a sample is placed in a magnetic field, magnetization does not appear instantaneously. Magnetisation in the z-direction yields the following differential equation:

$$\frac{dM_Z(t)}{dt} = \frac{M_0 - M_Z}{T_1}$$

The time T_1 is also called thermal relaxation time. It depends on the interaction of the spins with the surrounding medium. With the boundary condition $M_{Z(t)} = 0$, e.c. the material is not magnetized at $t = 0$, one will get:

$$M_{Z(t)} = M_0(1 - e^{-\frac{t}{T_1}})$$

1.6.2 Spin-Lattice-Relaxation Time (T2')

Is the system in addition disturbed by an oscillating magnetic field

$$B_1(t) = B_1(\cos(wt)\vec{e_x} + \sin(wt)\vec{e_y})$$

it is possible to turn the magnetization in the x-y-plane and therefore create an temporal x-y-magnetization.
After the pulse, the system goes back into an equilibrium state. The timescale for this relaxation is T_2. For magnetization in the x-y-plane the following differential equation has to be solved:

$$\frac{dM_{x/y}(t)}{dt} = -\frac{M_0}{T_2}$$

The solution is:

$$M_{x/y} = M_0 e^{-\frac{t}{T_2}}$$

unfortunately, this yields a small effective magnetic moment. The cause for this are small of the magnetic field, which causes the spins to separate. The corresponding time constant is called

1.6.3 Spin-Spin-Relaxation Time (T2*)

1.7 Aperture

The central part of the aperture is one big permanent magnet, which creates an homogeneous magnetic field in the z-direction. Between the magnetic poles lies the sample coil, which holds the sample. The sample coil can either measure the magnetization of th sample in the x-y-plane, or create a magnetic field. To execute these tasks, the sample coil can either be connected to a synthesizer, in order to to create an oscillating magnetic field in the x-y-plane, or it can be connected to an oscilloscope, in order to measure the magnetization of the sample. The sample coil is connected to some capacitors to create an RLC circuit. Via the synthesizer it is possible to vary the period of the pules sequence.

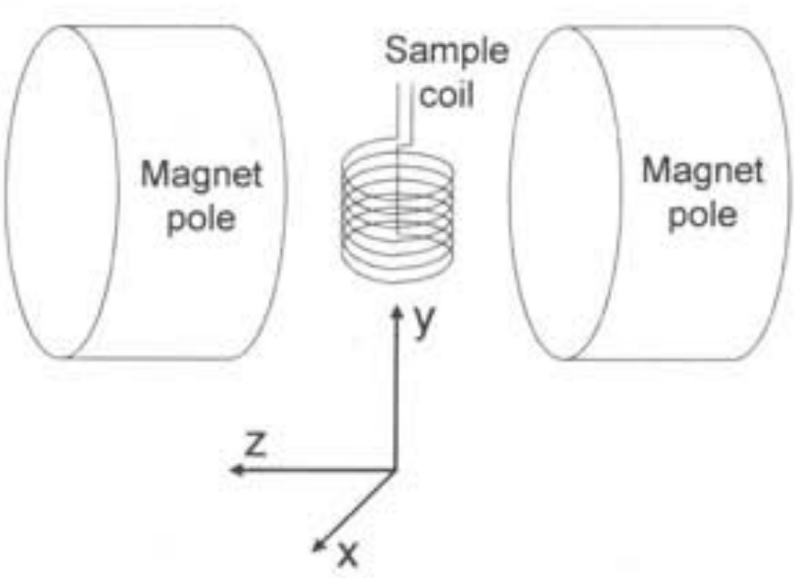

Figure 1: schematic configuration

2 Analysis

2.1 $\frac{\pi}{2}$-pulse condition

Our first task was to find the adjustment for a $\frac{\pi}{2}$-pulse. To create an homogeneous magnetic field, we calibrated the magnetic field gradients in the x-,y-,z- and z^2-direction in order to get a maximum decay time. We used the following adjustments for our measurement:

- frequency: 21,17530 MHz
- pulse length: 3,46 μs
- repetition period: 400ms

The chosen repetition period should be long enough to observe a full relaxation. We observed the following signal:

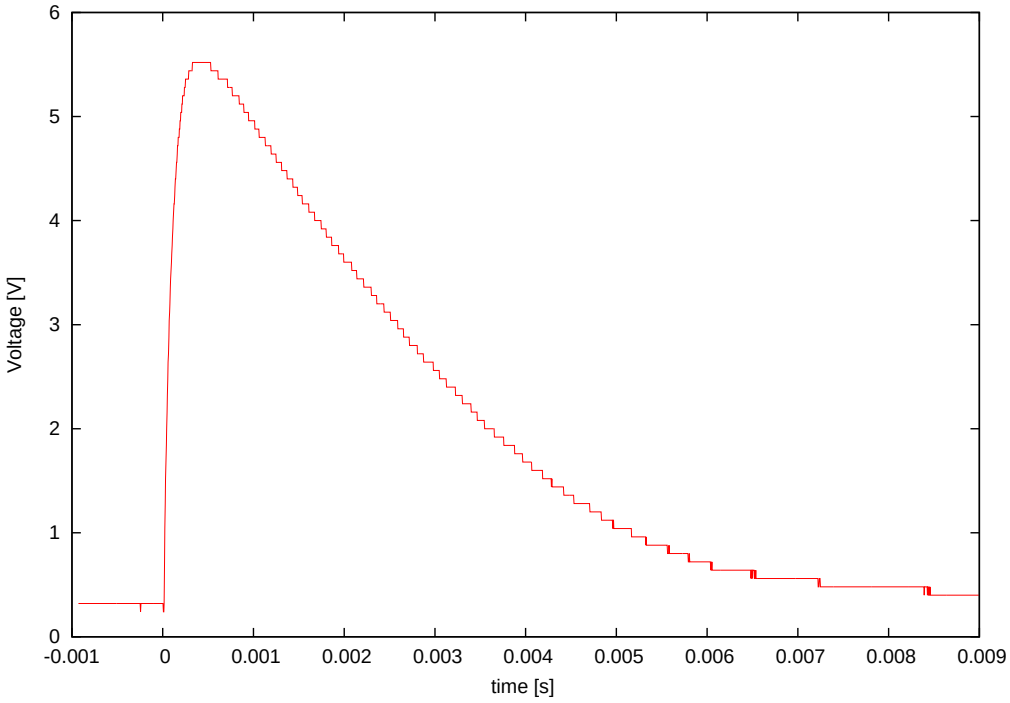

Figure 2: observed signal - $\frac{\pi}{2}$-pulse

A small variation of the frequency yielded a dramatic change in the amplitude of the signal, which is a strong evidence for an resonance.
We double checked our observation by doubling the pulse length. We expected the signal to vanish and this was also observed.
After the double check, we searched for secondary maxima in a large frequency interval of $(21\pm2)\ MHz$. Because a small variation of the frequency triggers a large drop of the amplitude, it was hard to find secondary maxima, but for the following adjustments we could observe one:

- frequency: 21,17530 MHz

- pulse length: 9,86 μs
- repetition period: 400ms

The observed signal is shown here:

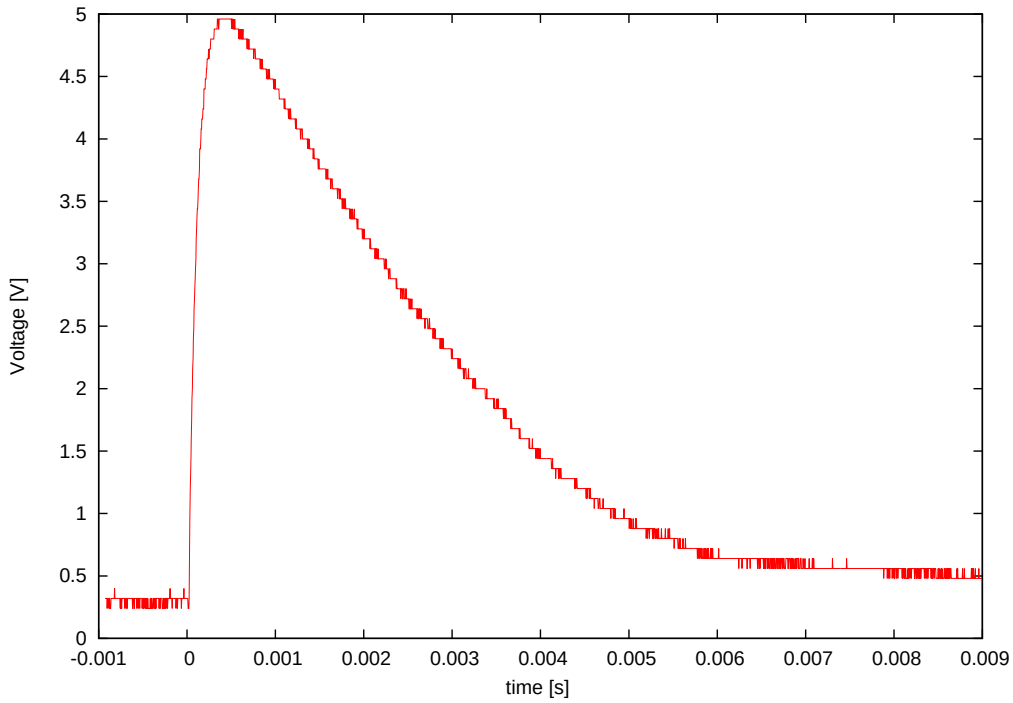

Figure 3: second maximum - $\frac{\pi}{2}$-pulse

2.2 π-condition

To find the right adjustments for a π-pulse, we first doubled the $\frac{\pi}{2}$-pulse length. The resulting signal had a strongly suppressed peak, but the envelope was still to high. By a fine adjustment of the magnetic field gradients, the frequency and the pulse length, we were able to suppress almost the entire signal. Unfortonatly, one small peak remained. This peak is due to the capacitors used in the aperture. The following adjustments are our final set:

- frequency: 21,17526 MHz
- pulse length: 7,30 μs
- repetition period: 400ms

The observed signal is shown in the following graph:

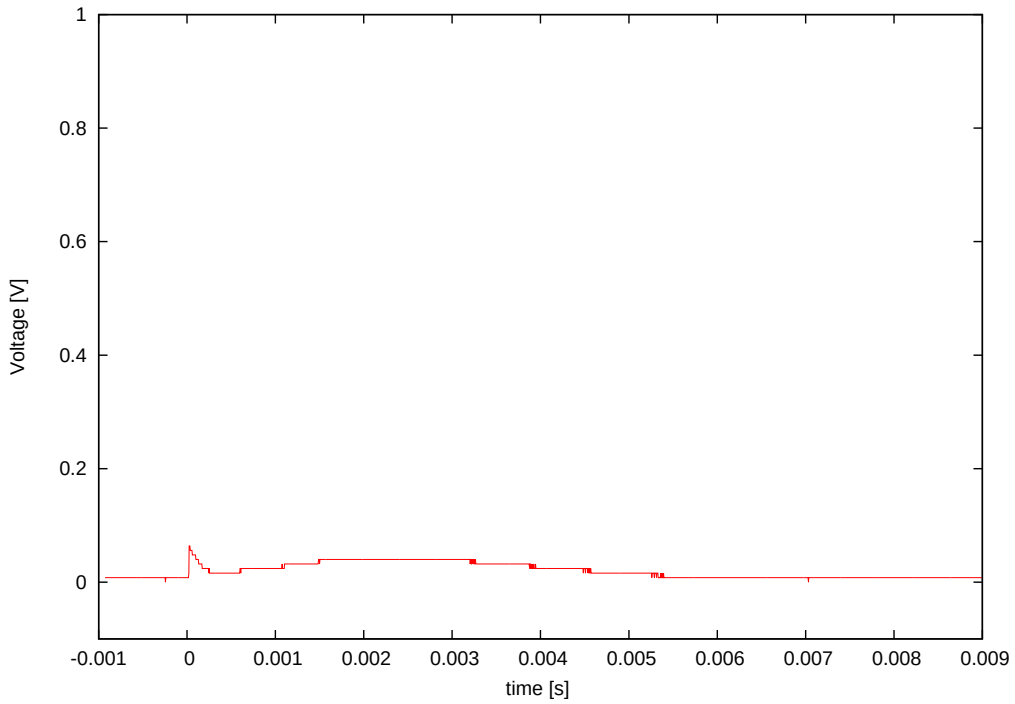

Figure 4: π-condition

After we found acceptable settings for a π-pulse, we checked our adjustments for the $\frac{\pi}{2}$-pulse. Due to the optimized magnetic field gradients, the resonance frequency was shifted towards the same frequency used for the π-pulse.
With these settings, we were able to determine the inhomogeneous T_2^*. We fitted the following function via Gnuplot:

$$U(t) = U_0 \exp\left(-\frac{t}{T_2^*}\right)$$

The fitted curve is shown in this digram:

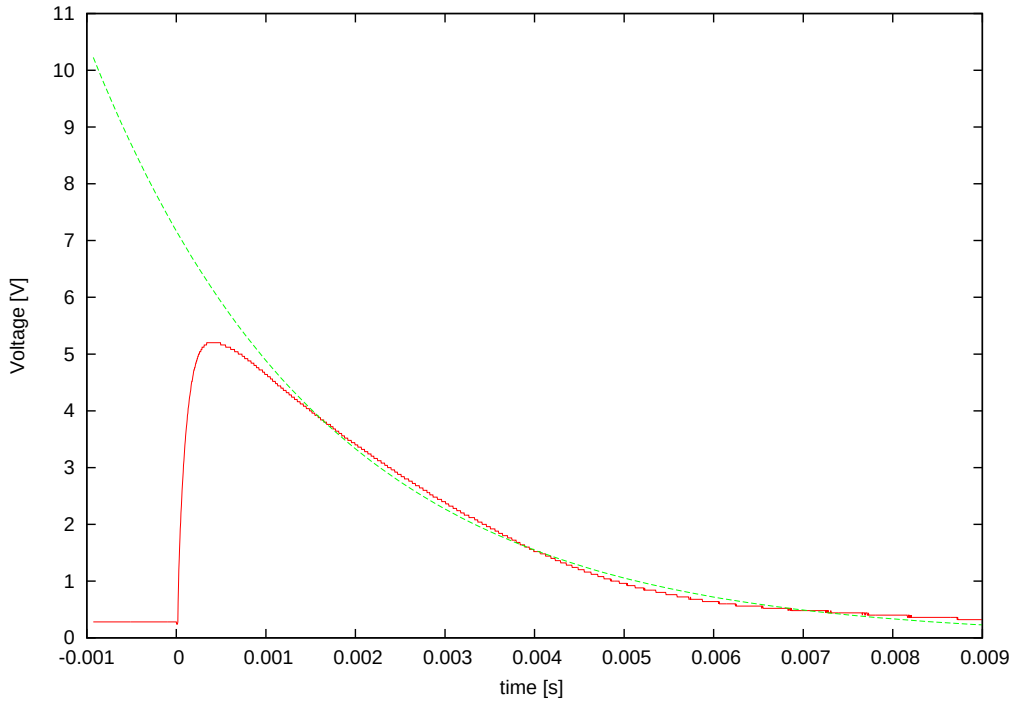

Figure 5: $\frac{\pi}{2}$-condition with fit

The fit yields the following values:

- $U_0 = (7,167 \pm 0,015)$ V
- $T_2^* = (0,002610 \pm 0,000005)$ s

2.3 Homogeneous transverse decoherence time T2

To determine the homogeneous transverse decoherence time T2, we use two different methods.

2.3.1 Carr-Purcell-method

In this method, the probe is exposed to a $\frac{\pi}{2}$-pulse. Then, after a time τ a row of N π-pulses is applied with a delay of 2τ between each pulse. The repeated application of N π-pulses result in N echoes which can be observed. The maxima of these echoes show an exponential decrease. A fit with Gnuplot to the maxima yields the homogeneous transverse decoherence time T2, using the formula

$$U_{max}(t) = U_0 \exp\left(-\frac{t}{T_2}\right)$$

The following graph shows the plot of the observed voltage, including the fit:
The fit yields the following values:

- $U_0 = (5,19 \pm 0,13)$ V
- $T_2 = (0,0119 \pm 0,0005)$ s

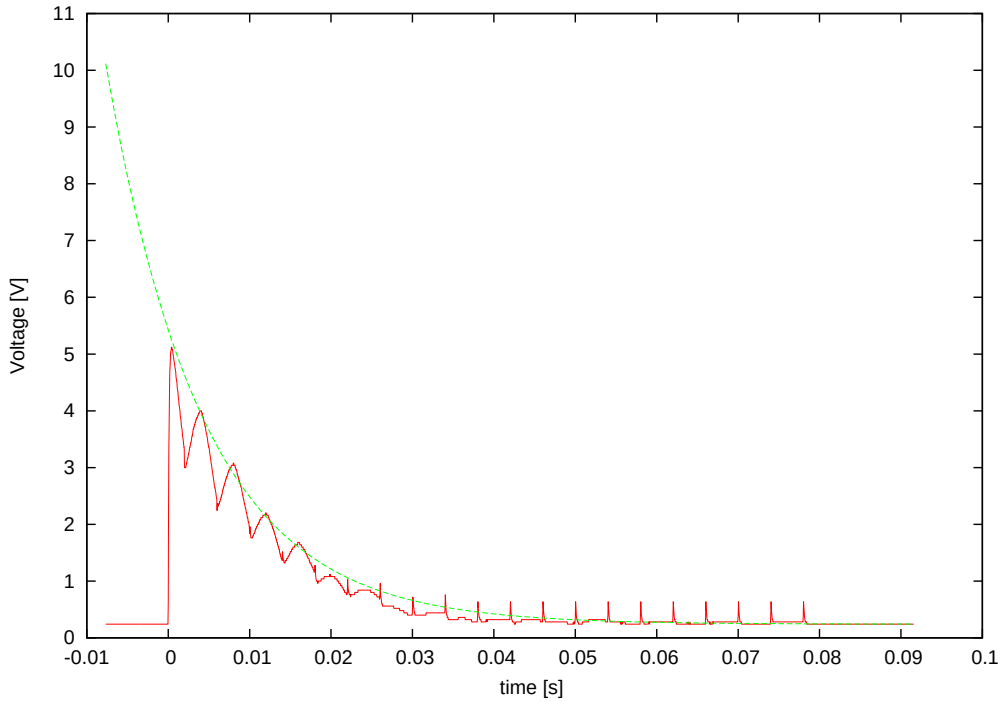

Figure 6: measurement of T_2 with Carr-Purcell-method

To improve the quality of the fit, we extracted the maxima of the graph into another file. Then we used this file as input for the fit.

2.3.2 Meiboom Gill Method

A problem of the Carr-Purcell-methods is that the errors in pulse length add up with each new pulse. The Meiboom-Gill-method reduces this systematical error by shifting the phase between the pulses about 90^0. This means that the errors of the pulse lengths point in different directions, canceling each other out when they are added. By fitting the same function as before, we get a better value for T_2. The observed signal with active Meiboom-Gill is plotted in the next diagramm:

Compared to the last method, we observed a longer decay time, thanks to the smaller errors. The fit of the decay function yields the following values:

- $U_0 = (4,44 \pm 0,06)$ V
- $T_2 = (0,0157 \pm 0,0005)$ s
- offset: $(0,725 \pm 0,042)$ V

2.4 comparison of the results for T_2

- $T_2^* = (0,002610 \pm 0,000005)$ s
- $T_2^{CP} = (0,0119 \pm 0,0005)$ s

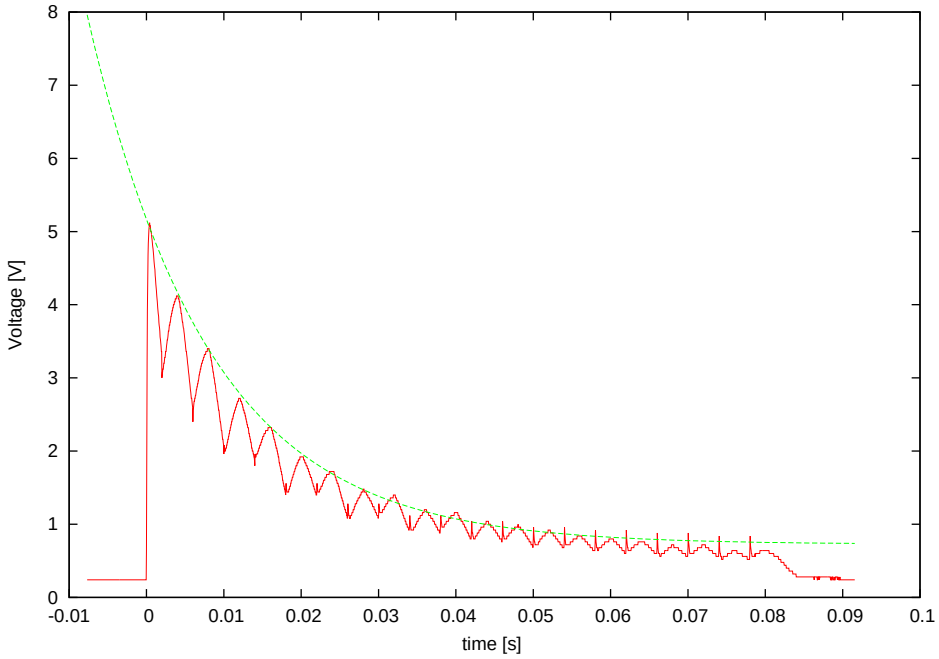

Figure 7: measurement of T_2 with Meiboom-Gill-method

- $T_2^{MG} = (0,0157 \pm 0,0005)$ s

As predicted, the inhomogeneous time T_2^* is smaller than the the determined homogeneous times T_2^{CP} and T_2^{MG} about a factor of $\approx \frac{1}{5}$. The homogeneous times are about the same with a difference of about 30% where the time determined with the Meiboom Gill method can be considered a more accurate value.

3 Longitudinal Decoherence Time T1

for determining the longitudinal decoherence Time T1 we again use two methods.

3.1 Saturation Recovery Method

In this method we apply a pair of $\frac{\pi}{2}$-pulses an vary the time τ between the pulses. During this time the spin begins to recover to thermal equilibrium, while the second pulse forces the spin to fall back into the x-y-plane. The now observed peak reaches its maximum if τ equals T_1 and then goes into saturation. For our measurement we started with $\tau = 0,02$ s. τ was raised until we reached $\tau = 2$ We noted the height of the peaks and plotted the results. We used the following function for a data fit:

$$U(t) = U_0 \left(1 - \exp\left(-\frac{t}{T_1}\right)\right)$$

The fit yields the longitudinal decoherence time T_1.

The fit was done with Gnuplot. We got the following results:

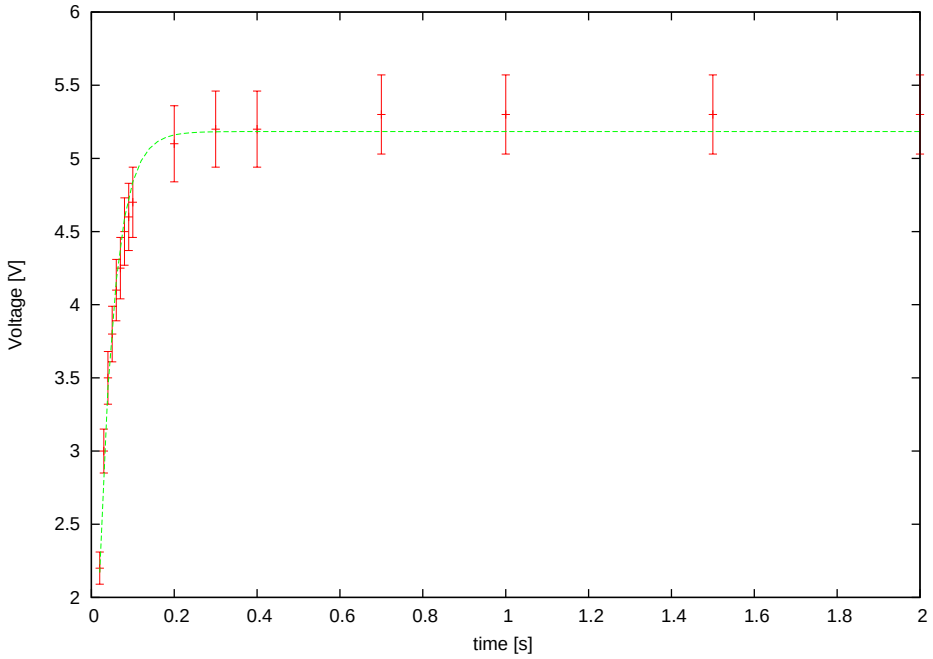

Figure 8: plotted data for the saturation recovery method

- $U_0 = (5,18321 \pm 0,04362)$ V
- $T_1 = (0,0368638 \pm 0,0008909)$ s

3.2 Polarization Recovery Method

Here we used a π-pulse followed by a $\frac{\pi}{2}$-pulse. The first one changes the orientation of the spin from z to -z in the Bloch sphere. The measured value in the x-y-plane is zero. The second pulse forces the spin to go back halfway into the z direction. In the time between the two pulses the spin starts to moves back to thermal equilibrium. While the spin is in the lower half of the Bloch sphere, the value measured after the second pulse decreases and reaches its minimum if it is in the x-y-plane at the beginning of pulse two. When the spin is in the upper half, the measured value increases again until it reaches saturation.
The time T_1 can then be determined by finding the minimum of the resulting graph. In this graph, the peak height is plotted against the delay time. This was accomplished by fitting a Gaussian curve via Gnuplot:

$$U(t) = U_0 - \frac{A}{W\sqrt{\frac{\pi}{2}}} \exp\left(-2\left(\frac{t-T_1}{W}\right)^2\right)$$

The resulting graph and fit curve are:
The results are:

- $A = (229,30 \pm 39,88)$ V
- $W = (39,517 \pm 7,381)$ s
- $T_1 = (16,148 \pm 2,136)$ s

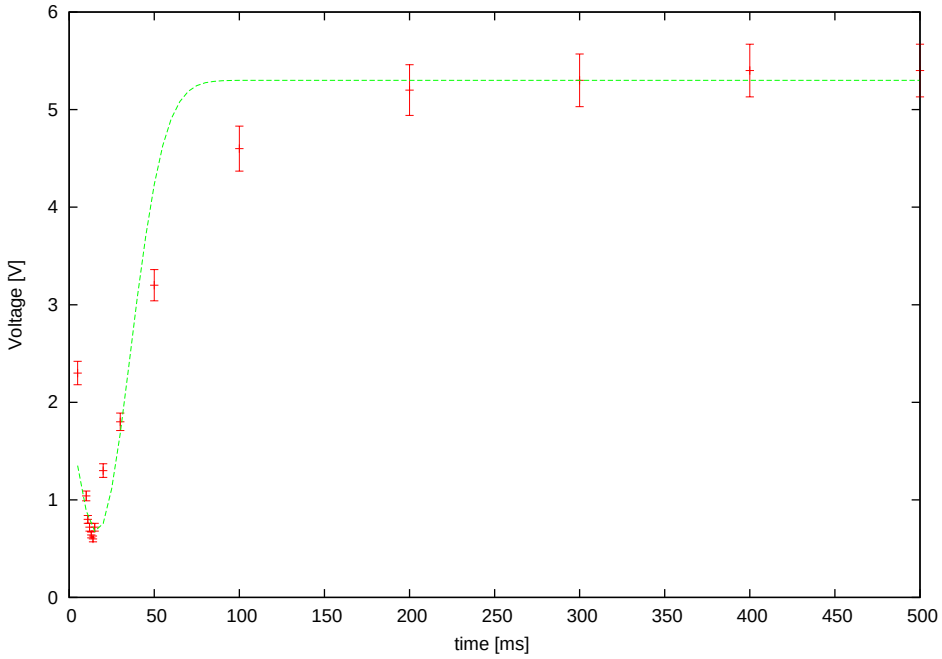

Figure 9: plotted data for the polarization recovery method

3.3 comparison of the results for T_1

The two applied methods yielded the following results for the longitudinal decoherence time T_1:

- $T_1^{sat} = (0,037 \pm 0,001)$ s
- $T_1^{pol} = (0,016 \pm 0,002)$ s

The two values are not compatible in their error boundaries. The value, determined with the saturation recovery method, is roughly twice as big as the value determined with the polarization recovery method. A reason for this circumstance might be the fact, that we had a high offset voltage in our signal, which made it pretty hard to determine the minimum condition. We also observed a non-vanishing peak in the spectrum that might be due to the used capacitors. Therefore the value measured with the second method is much less accurate than the other value.