NMR

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Abstract

Using a TeachSpin Pulsed NMR PS1-D device we determined the spin relaxation constants T_1 and T_2 for a sample of mineral oil using standard techniques. The values were determined to be $T_1 = 21.69$ ms and $T_2 = 6.25$ ms. The theory and usage of NMR are discussed.

1 Introduction

1. NMR is for chemistry
2. allows to determine local magnetic field env

2 Background and Theory

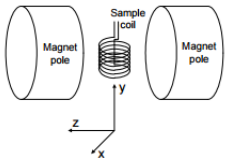

Figure 1: The permanent magnetic field is directed along the $+z$ direction while the sample coil (pickup coil) detects magnetization of the sample in along the transverse (y) axis. Not shown are the RF coils used to tip the spins from alignment with the permanent field. For a diagram of the sample environment Figure taken from A Conceptual Tour of NMR Ref. [1]

2.1 T1

The differential equation describing the Z axis magnetization under the influence of an external magnetic field applied along the axis is:

$$\frac{dM_z}{dt} = \frac{M_0 - M_Z}{T_1}. \tag{1}$$

Solving for $M_Z(t)$ results in:

$$M_Z(t) = M_0 - Ce^{\frac{-t}{T_1}}, \tag{2}$$

In the two pulse technique the first pulse, a π pulse, sets the initial conditions allowing us to solve for C

$$M_z(t=0) = -M_0,$$

$$M_Z(t) = M_0(1 - 2e^{\frac{-t}{T_1}}), \tag{3}$$

A $\frac{\pi}{2}$ pulse at time τ after the π pulse allows us the measure $|M_Z(t)|$ so by varying the delay time τ we can collect data to fit with Eq. 2 in order to determine T_1. However M_Z is not always positive so the value $|M_Z(t)|$ which is measured cannot be fit immediately.

Note that M_Z(t) is monotonically increasing so we know that we cannot directly measure M_Z,

2.2 T2

Field inhomogeneities cause spins to precess at different rates leading to a loss of signal in the pickup coil due to the spins decohering. If this rate of decoherence, T_2*, is short compared to the quantity T_2 a measurement of the FID will be a measurement of T_2* as the T_2 processes will not have had time to become significant.

This issue can be avoided through a two-pulse technique known as spin echo, which forces the precessing spins to recohere allowing measurement of T_2. The application of a $\frac{\pi}{2}$ pulse tips the spins into the x-y plane where they begin to precess. Some time τ later the application of a π pulse will reverse the direction of precession of the spins so that at $t = 2\tau$ the spins will be coherent resulting in a peak in the signal detected. However this signal will be reduced compared to the amplitude of the FID resulting from the first pulse. The difference in amplitude of the first and second FID is the result of spins decaying via T_2 processes. From Ref. [2] we have that spins tipped into the x-y plane by a $\frac{\pi}{2}$ pulse will decay to the Z axis with the following dependence:

$$M_{x,y}(t) = M_0 e^{\frac{-t}{T_2}} \tag{4}$$

At $t = 0$ we have:

$$M_{x,y}(t=0) = M_0 \tag{5}$$

Resulting in:

$$\Delta V = M_0(1 - e^{\frac{-t}{T_2}}) \tag{6}$$

3 Experimental Procedures

A TeachSpin Pulsed NMR PS1-D device was used to produce magnetic pulse and amplify the output of the pickup coil. The outputs were monitored with a Tektronix 200 MHz digital storage oscilloscope connected to a computer via labview.

Prior to determination of the time constants T_1 and T_2 the frequency of the rf field was adjusted to the resonant frequency of the system. This was accomplished by minimizing the amplitude of the beat frequency signal of from the rf coil and the excitation applied.

The length of a $\frac{\pi}{2}$ pulse was determined by finding the minimum pulse width that resulted in a maximum of FID amplitude. After this the pulse width of a π pulse was determined as the first pulse width value greater than the $\frac{\pi}{2}$ pulse width that caused no signal to be detected by the pickup coil.

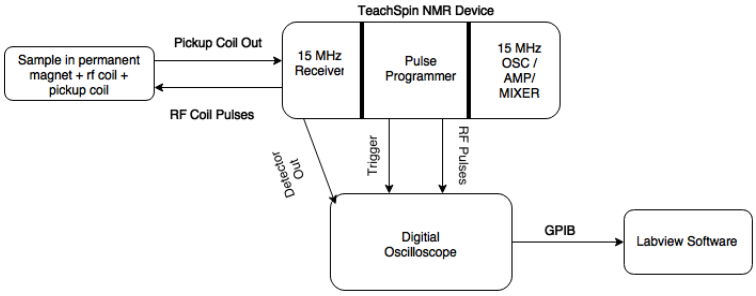

Figure 2: Block Diagram For the experiment. The TeachSpin device would provide RF pulses to flip the spins and output a clean signal to the oscilloscope from which measurement were made. For a diagram of the sample environment see Figure 1

3.1 T1

Following the theory developed in Section 2.1 a π pulse followed by a $\frac{\pi}{2}$ pulse was applied to the sample and the maximum voltage of the resulting peak was recorded along the delay time between peaks. As discussed above data points from the concave up portion of the data curve were taken as the negative values of M_Z.

This Voltage was fit to Eq. 2 with a least squares method in order to determine T_1.

3.2 T2

1. how did

4 Results

Data analysis was performed in Igor Pro the data was fit to functions via a least-squares method. Error was propagated using the Python Uncertainties package Ref. [5].

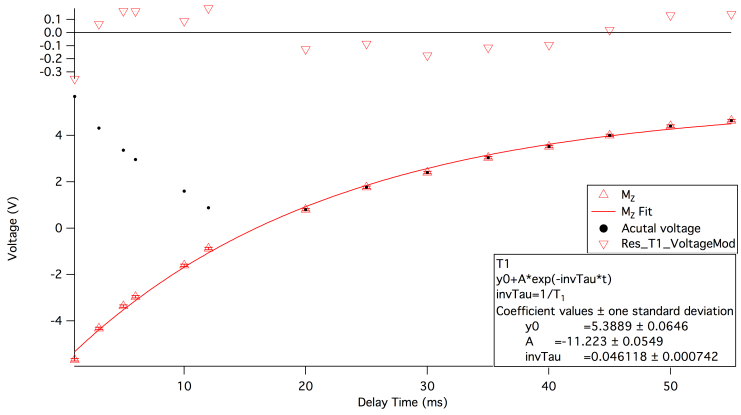

Figure 3: Determining T_1, Black dots are recorded ΔV, red triangles are M_Z as described in Theory Section

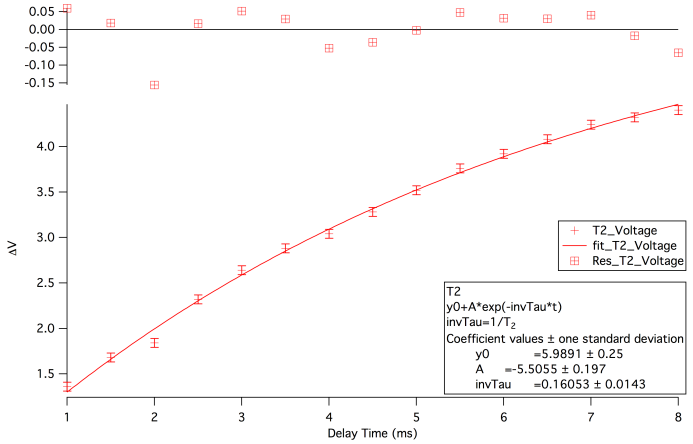

Figure 4: Determining T_2

Values the time constants were determined from these fits and are presented in Table 4

Quantity	Value	Bianchini et. al
T_2^*	.47 ms	N/A
T_2	6.23 ± .55 ms	15.7 ± .01 ms
T_1	21.68 ± .34 ms	25.4 ± .07 ms

Table 1: Values from this work and from Ref. [4]

As expected T_2^* is significantly smaller than T_2. Also note that T_1 is ∼3x more than T_2. This is sensible as T_1 is associated with the realignment of the spins anti-aligned to the external field while T_2 corresponds to the realignment of spins which are perpendicular to the field. So T_1 corresponds to a much more dramatic realignment and also involves transfer of energy to the lattice.

Our values T_1 and T_2 are on the same order of magnitude as as those found by Bianchini and Coffey, that they are several standard deviations apart is not significant as Mineral Oil is not a standard substance. We note that our uncertainties are much larger than those found by Bianchini and Coffey

4.1 Uncertainty Budget

Source	Quantity	Error in Quantity	Propagated Error
Statistical Error	T_1	.35 (ms)	.35 (ms)
Statistical Error	T_2	.6 (ms)	.6 (ms)
Pulse Width	τ	5%	Negligible

Due to the use of oscilloscope cursors to determine the voltages for determining T_1 and T_2 we estimate the error in the voltage values as ±.05V. This combined with statistical errors in fitting is

the dominant source of uncertainty. However as noted in Section 4.2 the error on the voltage may have been underestimated.

The other source of the uncertainty was the the inability of to produce an exact $\frac{\pi}{2}$ pulse. However this is ultimately a negligible effect as the probability of excitation is described by a sin curve and a $\frac{\pi}{2}$ pulse is located at an anti-node of this curve and so a small deviation in pulse width will not have a dramatic effect.

I would like to try to calculate T_1 and T_2 with a few pulse widths in order to get a better sense of the error that this introduces.

4.2 χ^2 analysis

Igor produces χ^2 values when performing a least squares fit, $\tilde{\chi}^2$ values were determined using:

$$\tilde{\chi}^2 = \frac{\chi^2}{d} \tag{7}$$

$$d = N - c \tag{8}$$

Where c is the number of constraints, three for the equations fit to, and N is number of points.

Quantity	χ^2	Deg Freedom	$\tilde{\chi}^2$	Probability
T_1	133.9	11	12.17	≈ 0 %
T_2	18.55	12	1.54	12 %

Probabilities were determined from Ref. [3]

From the residuals of the fits we can see that our fits are not bad. However our χ^2 analysis would seem to indicate a flawed model. A possible reconciliation of this is that we underestimated our uncertainty or did not account for a systematic error. Though the latter seems unlikely due to our residuals.

5 Conclusions

6 Acknowledgements

Pete Sinn was invaluable as a Lab Partner when performing this experiment.

References Cited

[1] Barbara Wolff-Reichert, Conceptual Tour of PNMR, 2008

[2] Teachspin Instructional Pulsed NMR Apparatus Manual, Department of Physics and Astronomy, Knoxville, TN

[3] J.R. Taylor, *Introduction to Error Analysis*, (University Science Books, Sausalito, 1997)

[4] L. Bianchini, L. Coffey, Physics Department, Brandeis University, NMR Techniques Applied to Mineral Oil, Water, and Ethanol (2010)

[5] *Uncertainties*: a Python package for calculations with uncertainties, Eric O. LEBIGOT, http://pythonhosted.org/uncertainties/