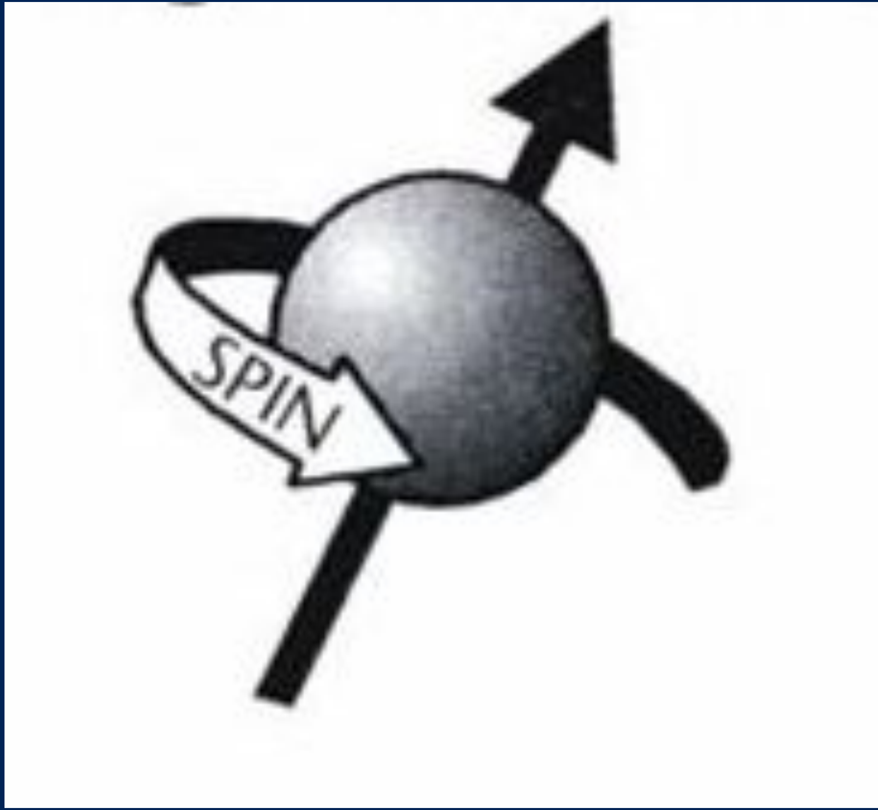

A model for T_1 Extraction

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UVA Polarized Target Group

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Outline

- Our goals.
- What is spin-lattice relaxation?
- First principles derivation.
- T_1 from experimental data.
- The calibration constant.
- Future plans.

Goals

Make predictions about the calibration constant from limited depolarization curve.

→

Minimize pause time taking data during the experiment.

→

More efficient experiment.

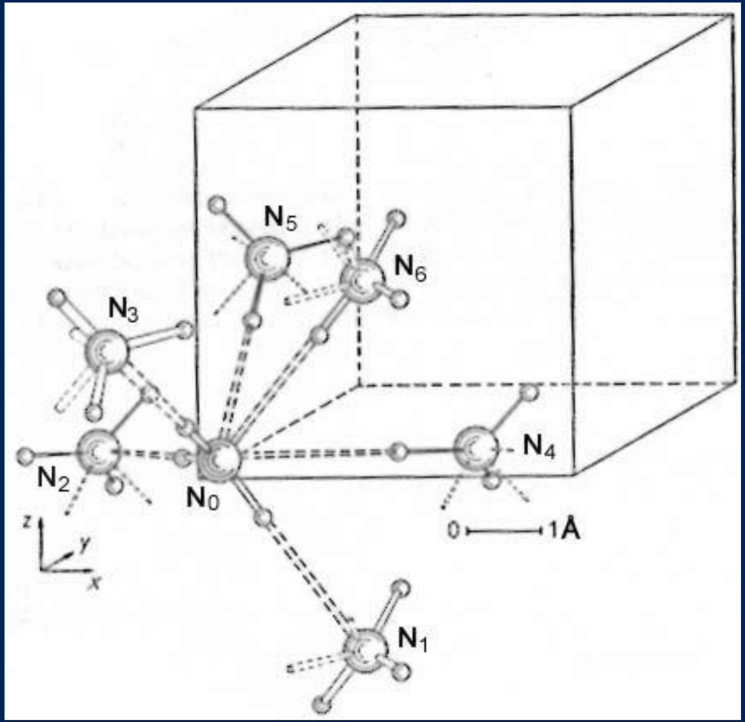
By using lots of experimental data at various temps, target life cycles, and radiation damage to build simulations and produce training data to construct a model to accurately determine a mapping between polarization and area under the signal curve prior to full relaxation.

What is Spin-Lattice Relaxation?

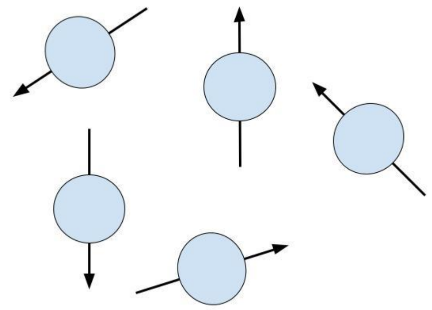
It is the energy diffusion from excited spins across the lattice, returning the spins to thermal equilibrium.

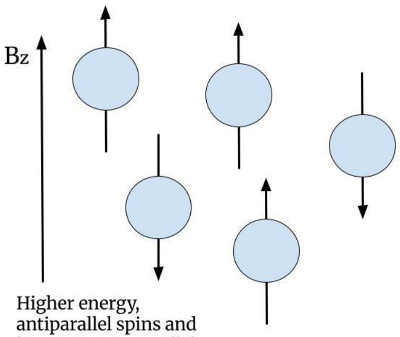
Why Do We Care?

We need to extract the Spin-Lattice Relaxation time which characterizes the time interval of the relaxation process.

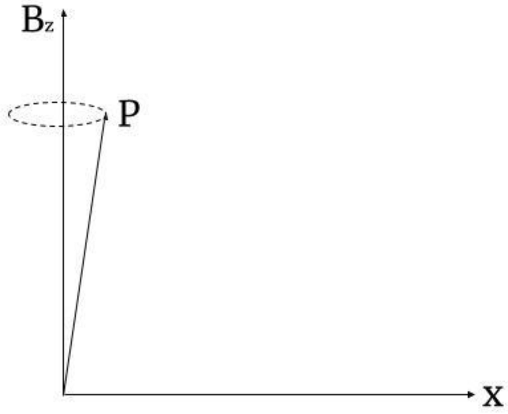


Unit Cell of NH_3 at 171 K.
https://www.researchgate.net/figure/The-crystal-structure-of-ammonia-at-171-K_fig11_30072616

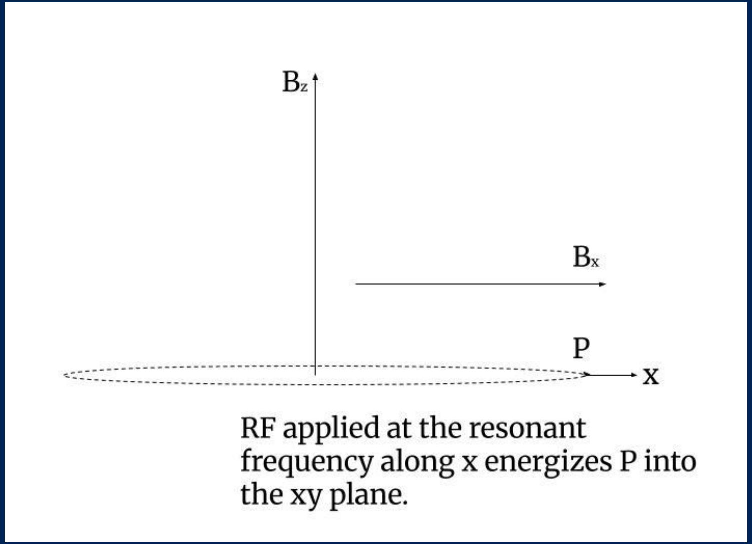


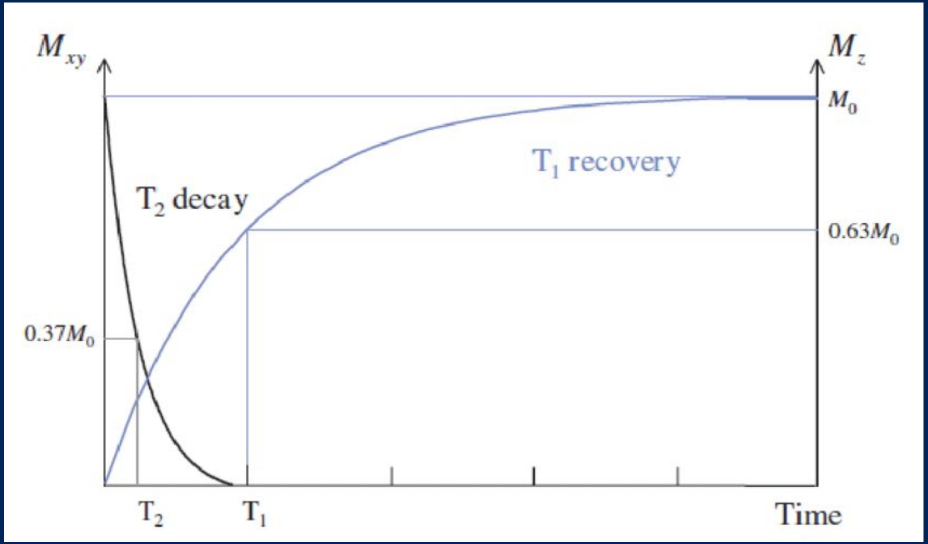


Higher energy, antiparallel spins and lower energy, parallel spins (relative to B_z).



Net polarization of hadron spins precess about the axis parallel to B_z.





https://www.researchgate.net/figure/Relaxation-rates-T1-recovery-is-the-longitudinal-relaxation-and-T2-decay-is-the_fig6_340225510

T_1 from First Principles

Computes constants for a combined prefactor.

Forms array based off NH_3 geometry (fractional positions to Cartesian).

Loops over all NN pairs to compute transition rates.

Diagonalize array of transition rate sums, and the inverse of the smallest nonzero diagonal element is T_1.

Idealized model: did not consider doping and paramagnetic centers, impurities, radiation damage, time since annealing.

The Computation

$$D_{ij} = \frac{\mu_0 \gamma^2 \hbar^2}{4\pi} \left(\mathbf{I} - 3\hat{r}_{ij} \otimes \hat{r}_{ij} \right)$$

$$W_{ij} \propto \frac{1}{r_{ij}^6} \left(1 - 3\cos^2\theta_{ij}\right)^2$$

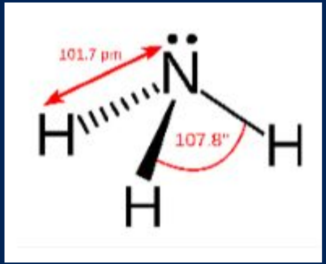
$$T_1 = \frac{1}{\lambda_{min}} \qquad R = \sum_{ij} W_{ij}$$

Single Spin

$$\begin{aligned} 0 &= \begin{vmatrix} -R-\lambda & R \\ R & -R-\lambda \end{vmatrix} \\ &= (R+\lambda)^2 - R^2. \end{aligned}$$

$$\lambda = 0, -2R$$

$$T_1 = -\frac{1}{2R}$$



More Computation

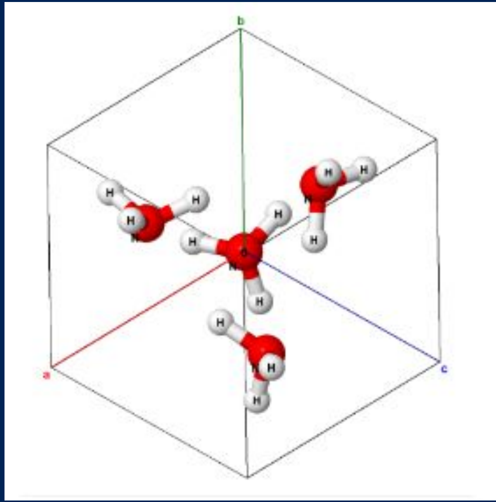
$$\Xi = \frac{3}{20}\left(\frac{\mu_0 \gamma_H^2 \hbar}{4\pi}\right)^2$$

$$\omega_0 = \gamma_H B_z$$

Hydrogen positions : $H = \begin{array}{l}\left[\left(\sin\left(\frac{\theta}{2}\right), 0, \cos\left(\frac{\theta}{2}\right)\right),\right. \\ \left(-\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\pi}{3}\right), \sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\pi}{3}\right), \cos\left(\frac{\theta}{2}\right)\right), \\ \left.\left(-\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\pi}{3}\right), -\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\pi}{3}\right), \cos\left(\frac{\theta}{2}\right)\right)\right]\end{array}$

(relative to N)

$$\text{Bond length}: \ a = 5.1035\text{E} - 10\,\text{m}$$
$$\text{Bond angle}: \ \theta = 107.5^\circ$$
$$\text{Cut off} = 9\text{E} - 10\,\text{m}$$
$$\text{Fractional position of N}: \ (u = 0.215, u, u)$$



N positions in unit cell: $Q = \Big[(u,u,u),\ (0.5+u, 0.5-u, -u)\ (-u, 0.5+u, 0.5-u)\ (0.5-u, -u, 0.5+u)\Big]$

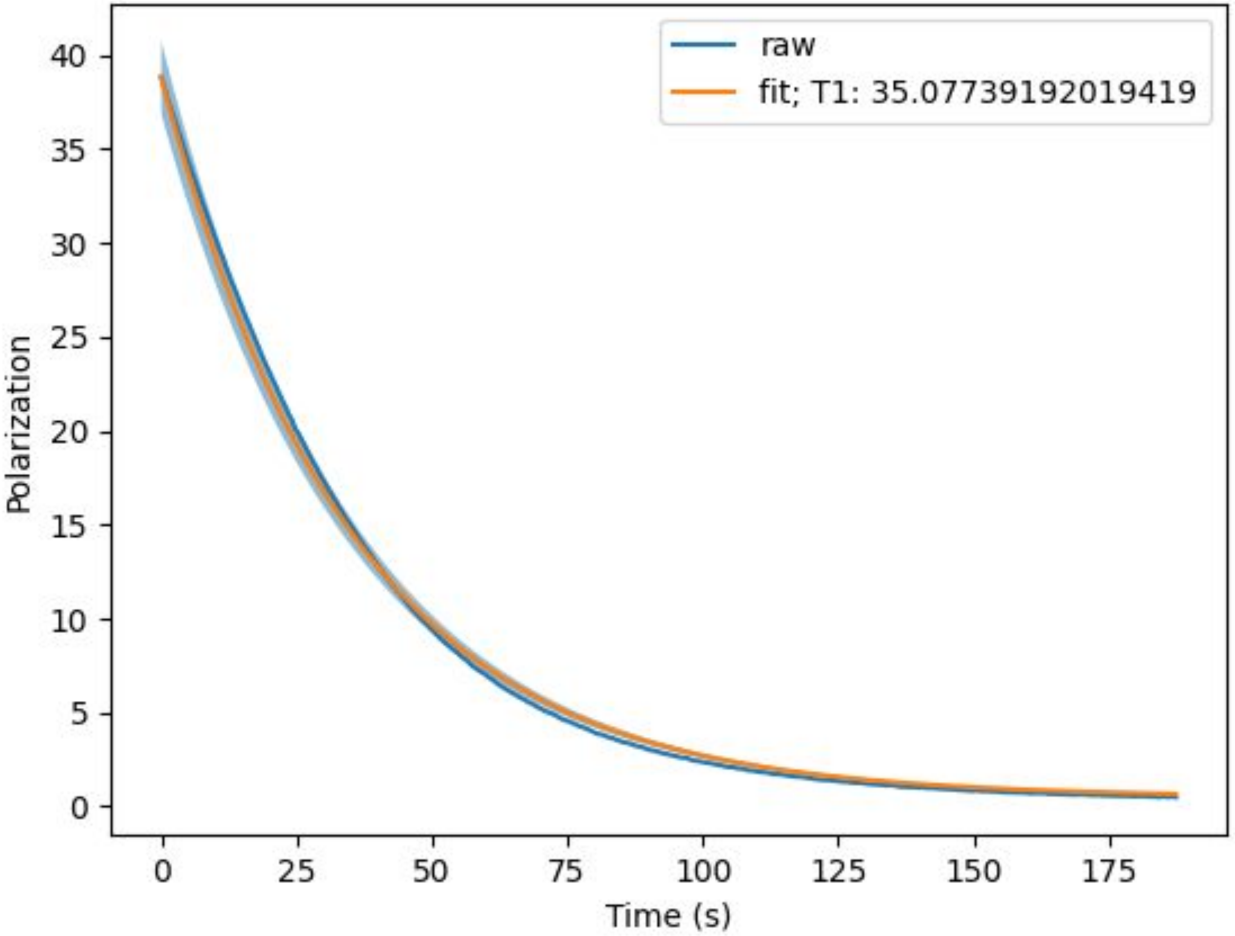
Loop over and add all elements of aQ and H to form the unit cell with 4 NH_3.

Loop over dx, dy, dz shifts times a, then loop over the unit cell protons to add the shifts to each.

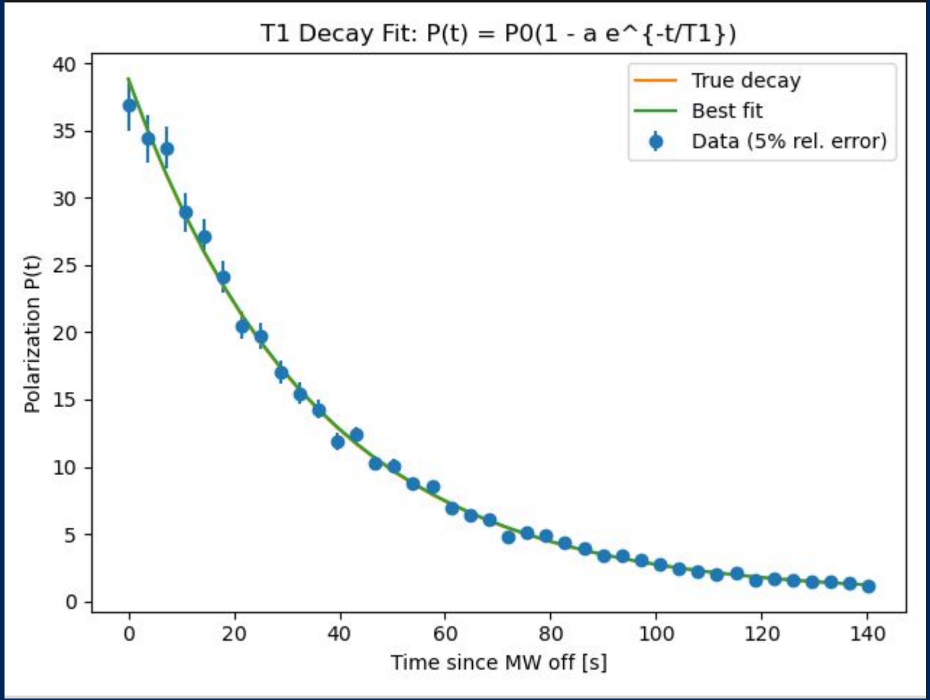
Forms the supercell.

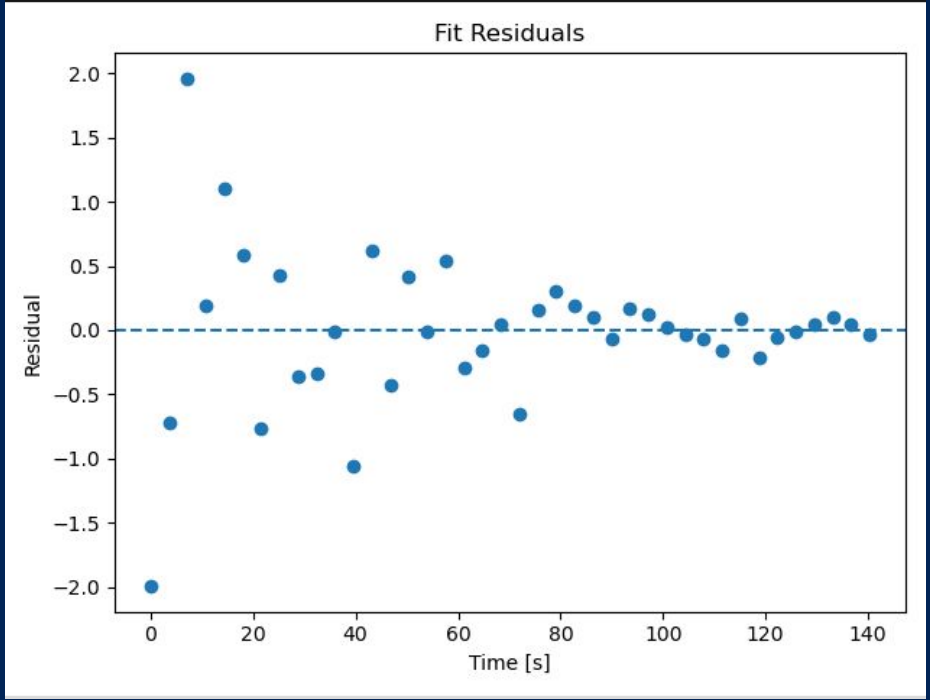
Loop to sum all transition rates between unit cell hydrogens and supercell hydrogens.

Diagonalize relaxation matrix and use transition rate sum to get numerical T_1.



5% relative error.


T1 Decay Fit: P(t) = P0(1 - a e^{-t/T1})
True decay
Best fit
Data (5% rel. error)
Polarization P(t)
Time since MW off [s]
0
5
10
15
20
25
30
35
40
0
20
40
60
80
100
120
140


Fit Residuals
Residual
Time [s]
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
20
40
60
80
100
120
140

The Decay Curve

$P(t)$: Polarization vs time

$P(0) = P_0(1 - a)$: Initial polarization

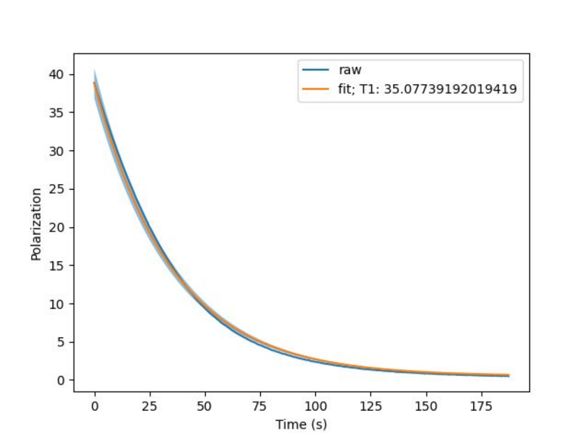
P_0 : Saturation polarization

a : Initial fractional deviation

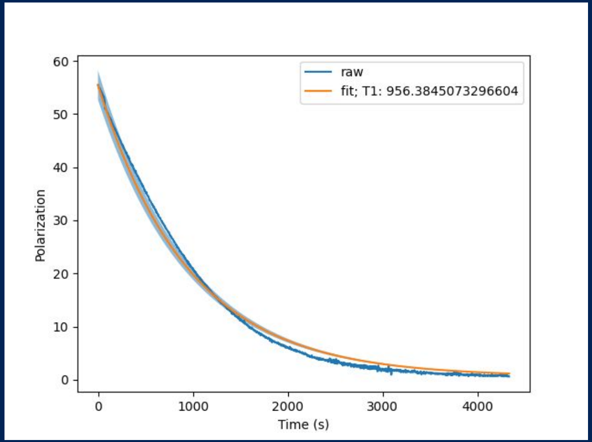
$$P(t) = P_0\left(1 - ae^{-t/T_1}\right)$$

$$a = 1 - \frac{P(0)}{P_0}$$

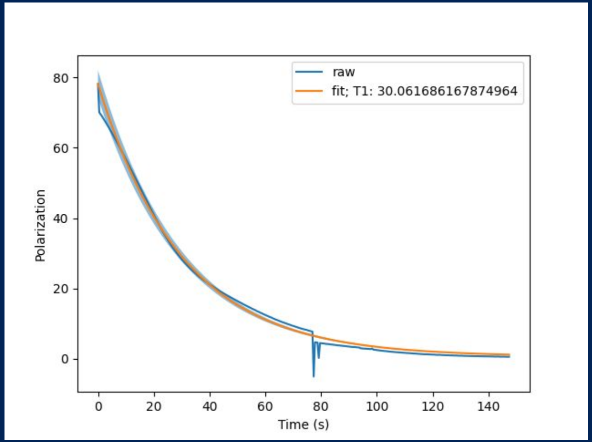
$$\lim_{t\to\infty} P(t) \to P_0$$


raw
fit; T1: 35.07739192019419
Polarization
Time (s)

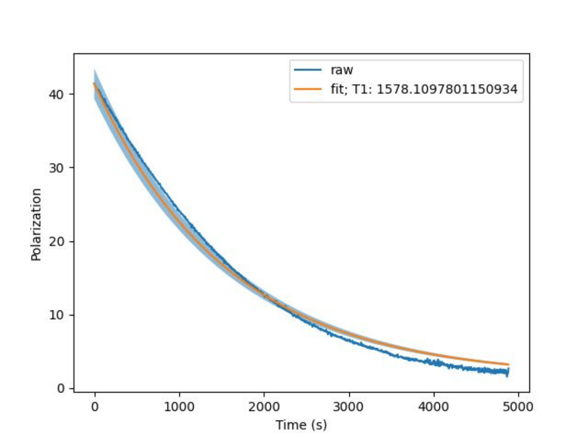
0


raw
fit; T1: 956.3845073296604
Polarization
Time (s)

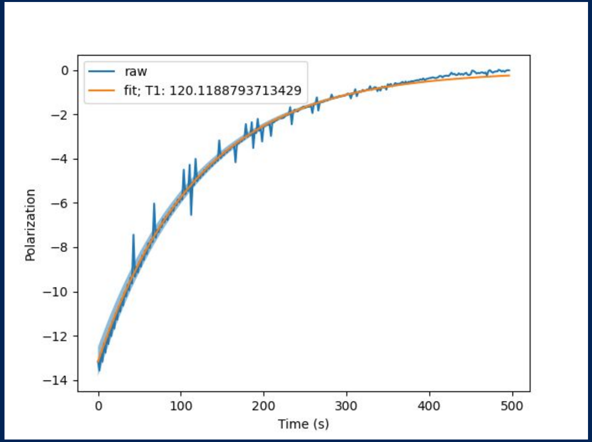
1


raw
fit; T1: 30.061686167874964
Polarization
Time (s)

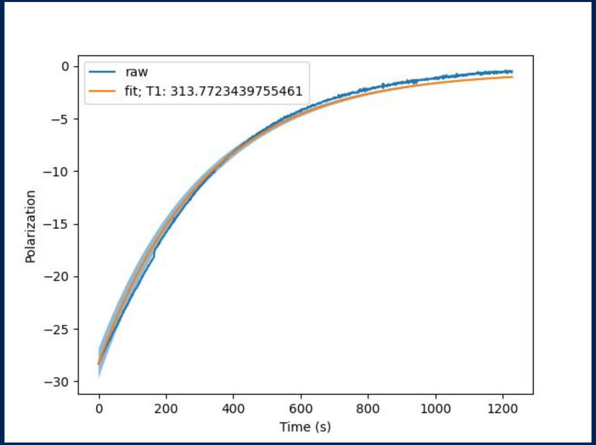
2


raw
fit; T1: 1578.1097801150934
Polarization
Time (s)

3


raw
fit; T1: 120.1188793713429
Polarization
Time (s)

4


raw
fit; T1: 313.7723439755461
Polarization
Time (s)

5

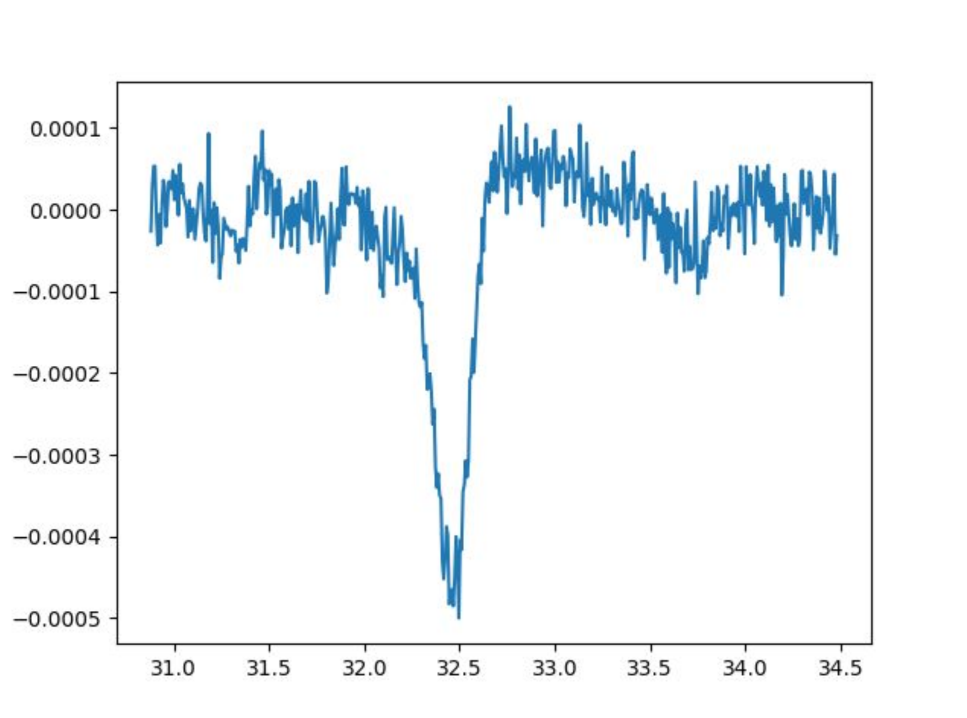
	P0	Pi	T0 (h)	T1 (m)	T1 error (m)	Average Temperature (K)	Average Pressure (Torr)	Chi Square
0	0.4878513	-78.5458985145679	0.584623198669903	35.0773919201942	0.0995557103758684	2.64108954740061	100.010559633028	11.1697564327282
1	0.6123087	-126.577119188409	0.501028102797916	30.061686167875	0.137486228692703	2.60878966461538	98.8166830769231	214.119516712304
2	1.386726	-28.8498694046264	26.3018296702175	1578.10978021305	4.5821513615792	1.46357588363636	3.06569363636364	202.015963828746
3	0.5684835	-96.5427958771011	15.9397417899368	956.384507396208	2.06048948624835	1.46475579405286	3.15081112334802	508.886540615913
4	-1.652316	-18.2648500649997	48.0617289148988	2883.70373489393	11.9638522882166	1.45810657942857	2.87196114285714	196.40639280561
5	-0.03652216	-359.451298608845	2.00198132283043	120.118879369826	0.610995150903476	1.46681159856631	3.00026164874552	49.001505270015
6	-0.4832373	-57.6176812096252	5.22953906651319	313.772343990791	0.688619936605752	1.4760897225	3.37505833333333	137.735547058873

Results

Systematic error.

Event	T1 (m)	P_0	P_i	$T_{\text{avg}}(K)$
1	35.07∓0.0995	0.4878513	-78.545	2.64
2	30.06∓0.1374	0.6123087	-126.577	2.60
3	1578.10∓4.582	1.386726	-28.849	1.46
4	956.38∓2.060	0.5684835	-96.542	1.46

The Calibration Constant



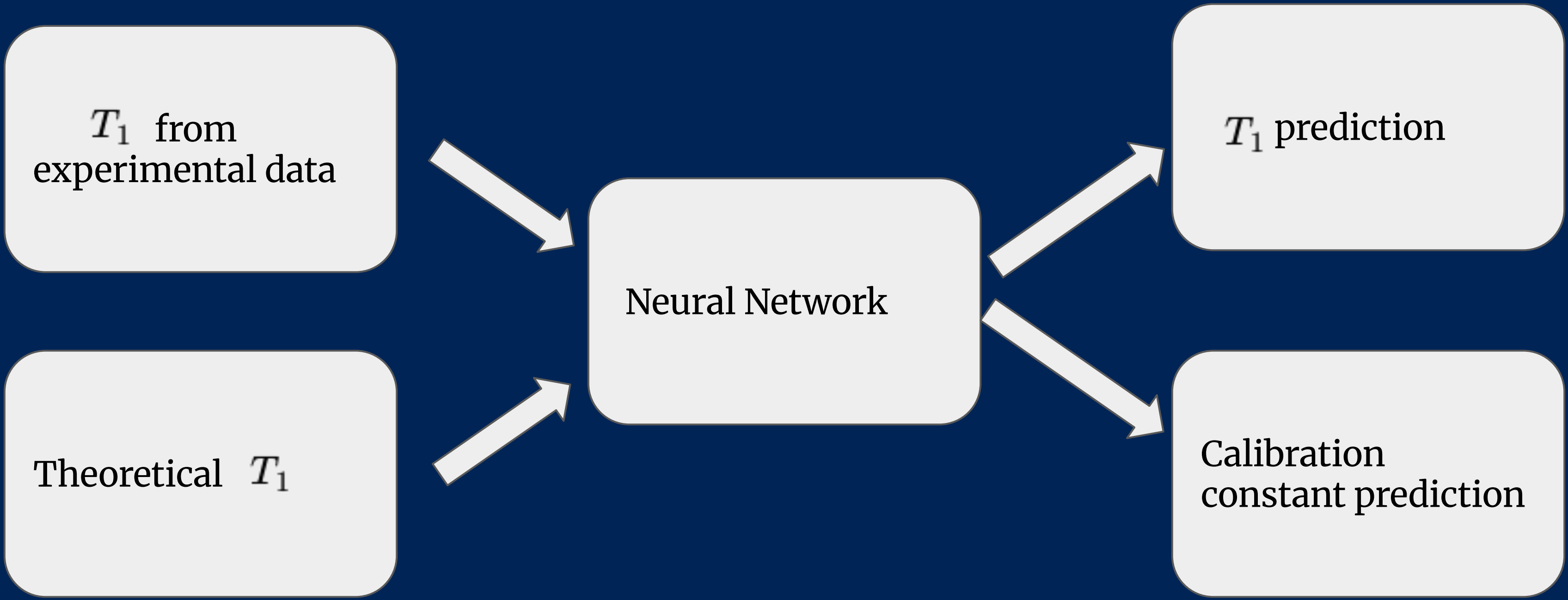
A map between the area under the signal and the polarization.

$$P = CA$$

We would rather not have to stop the experiment to calculate this.

$$P(0) = \tanh\left(\frac{\hbar\omega}{2kT}\right)$$

Future Plans



Thank you.