PHYSICS
UNIVERSITY OF
TORONTO

Book #2 2025-02

Subject ADVANCED PHYSICS LAB

Name ADITYA K. RAO

Address ADI.RAO@MAIL.UTORONTO.CA

Computation Notebook
4 x 4 Quad., 11 3/4" x 9 1/4"

ADITYA KANURU RAO
1008307761
ADI.RAO@MAIL.UTORONTO.CA
+1(416) 802-5648

SUMMARY ABSTRACT

Nuclear Magnetic Resonance is a spectroscopic technique used to determine the structure, composition, and dynamics of nuclei. It is based on the principle that the magnetic constituents of such nuclei are driven by a magnetic moment and an angular momentum component (the latter of which is quantized). In this experiment a TeachSpin NMR spectroscope to measure various properties of Heavy Mineral Oil, Light Mineral Oil, and Distilled Water.

Namely, investigations focused on tuning the machine, measuring the T_1 spin-lattice relaxation time, the FID signal, and attempting to measure the spin-spin relaxation time known as T_2. Additional ~~e~~exploration into the applications of NMR in other fields was also conducted, namely Quantum Computing where NMR ~~is used~~ esque techniques can be used to implement single and two qbit unitary gates in Trapped Ion systems

Experimental findings yielded $T_2 \approx 447.8 \pm 0.8\ \mu s$, though this may be flawed as a proper resonance condition was not achieved. Note that this measurement was for mineral oil (heavy).

T_2 and T_1 (accurate) measurements were made, but errors in data collection meant ~~adequate~~ insufficient data was obtained to properly calculate.

Additions to the experiment include a Foray into Quantum Computing, Measurements on Spin-spin diffussion (T_2) for H_2O (distilled) and a non-inverting operational amplifier circuit being made to boost low signals.

Future endevours would primarily be guided by better time management and more complete data collection.

Aknowledgements:

I would like to thank Professor Pinsavard and Teaching Assistant Kyle Tompson for their guidence when conducting the lab. Additionally I would like to thank Professor Ania Hardt and Professor Tobir Shaman for their ideas on extensions for the lab. Finally, I would like to thank the lab technician for helping me remove the distilled H_2O sample when it almost got stuck in the machine.

TABLE OF CONTENTS

QUICK REFERENCE MATERIAL

Procedures

Pg #	Code	Purpose
14	P02.11A	Experiment Apparatus ~~Connection~~ Setup Verification
16	P02.11B	Experiment Apparatus Cable Connections
18	P02.11G	Single Pulsed NMR Experiment Procedure

Key Contacts

~~Name~~

Name: Prof. Pierre Savard
Email: SAVARD@PHYSICS.UTORONTO.CA
} Supervising Professor

Name: TA. Kyle Thompson
Email: KTHOMPSON@PHYSICS.UTORONTO.CA
} Supervising Teaching Assistant

Name: Prof. Ania Harlick
Email: ANJA.HARLICK@UTORONTO.CA
} Course Coordinator (PHY426)

Personal Contact Info

← should this book be found, please contact me at one of the following methods.

Name: Aditya Kanuri Rao (Adi Rao)
Email: ADI.RAO@MAIL.UTORONTO.CA   ADITYAKRAO.PROJECTS@GMAIL.COM
Phone: +1 (416) 802-5648
Github: @ADIRAO-PROJECTS

REFERENCES

1 D. Baily, J. Harlow, J. Vise, and J. Pitre, NMR Nuclear Magnetic Resonance, edited by J. Shepard (University of Toronto, 2013)

2 TeachSpin Inc., TeachSpin Inc. Pulsed/CW NMR Spectrometer Instructors Manual

3 A. Trabesinger, "Long live the spin," Nature Physics 8, 781-782 (2012)

4 T. Wogan, "NMR Spectroscopy without the "m" - physics world" (2011)

5 L. Yarris, "Researchers increase NMR/MRI sensitivity through hyperpolarization of nuclei in diamond," (2012)

6 L. Zyga, "143 is the largest number yet to be factored by a Quantum Algorithm" (2012

7. M.A. Nielson and I.L. Chuang, Quantum Computing and Quantum Information (Cambridge University Press, 2010)

25-02-09 BACKGROUND THEORY

~~Nuclear~~

3.47 Nuclear Magnetic Resonance, or NMR, is a phenomena primarily observed in systems where the ~~magnetism~~ constituents has both a magnetic moment and angular momentum. Almost all stable nuclei have this property.

51 Classically, we may consider a spinning dipole to emulate such nuclei:

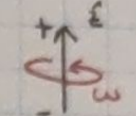


Fig 02.09 A.1

59 which induces this magnetism. Then, we may link the angular momentum $\bar{J}$ with the gyromagnetic ratio γ to obtain the resultant magnetic moment $\bar{\mu}$

unique for each nucleus

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

406 From Quantum Mechanics, we also know that are angular momentum is indeed quantized leading to a direct relation b/w angular momentum and the spin of the particle

$$\bar{J} = \hbar \hat{S}$$

spin

$\frac{h}{2\pi}$ ← plank's constant

508 We may then calculate the total magnetic energy in an external field as

$$\bar{\mathcal{E}}_M = -\bar{\mu} \cdot \bar{B}$$

522 In our experiment, we will primarily only be applying this in the $\hat{z}$ direction leading to a simplification of the equation to

$$\mathcal{E}_M = -\mu_z B = -\gamma \hbar S_z B_0$$

→ Quantized w/

$M = \cancel{S, \ldots}$, $S \pm n$

527 For fermionic spin-$\frac{1}{2}$ systems, ~~this leads~~ (or spinors) this leads to the ~~magnetic~~ allowed values of S to be $\pm\frac{1}{2}$ or spin down and spin up respectively (I may use $|0\rangle$ and $|1\rangle$ to denote these in the computational basis).

→

1532 Then our allowed energies become

$$\mathcal{E}_{m_0} = -\gamma\hbar(-1/2)B_0 = \frac{\gamma\hbar}{2}B_0$$

and $$\mathcal{E}_{m_1} = -\gamma(\hbar)(1/2)B_0 = -\frac{\gamma\hbar}{2}B_0$$

1539 which may be visualized as follows

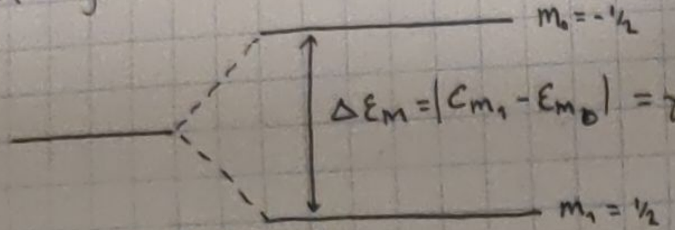


Fig 02.09B.1

From [2]

So $$\Delta\mathcal{E}_m = \left|-\frac{\gamma\hbar}{2}B_0 - \frac{\gamma\hbar}{2}B_0\right| = \gamma\hbar B_0$$

1611 which implies our energy can be written in terms of some angular frequency $\omega_0 = \gamma B_0$

$$\Rightarrow \quad \Delta\mathcal{E}_m = \hbar\omega_0$$

1613 Note that this only is in a constant magnetic field (B_0) in the z direction.

From [2], we note for a proton:

$$\gamma_{pro} = 2.675 \cdot 10^8 \text{ rad } (sT)^{-1}$$

1616 and $f_{pro} = 42.58 B_0 T$ resonant frequency.
Then, say we have N_0 spins in the down state and N_1 in the up state, in Thermal Equillibrium, then the population ratio of the spins is given by the Boltzmann factor

$$\frac{N_1}{N_0} = \exp\left\{\frac{\Delta\mathcal{E}_m}{KT}\right\} = \exp\left\{\frac{\hbar\omega_0}{KT}\right\}$$

with magnetization

$$M_z = (N_0 - N_1)\mu$$

1627 However, in our NMR experiment, this will not appear instantly. Instead the spin relaxation time (Spin-Lattice Relaxation time) known as T_1 is given from solving the ODE

$$\partial_t M_z = \frac{M_0 - M_z}{T_1} \qquad M_0 = (N_0 + N_1)\tanh\left(\frac{\mu B}{kT}\right) \approx N\frac{\mu^2 B}{kT}$$

1637 Placing an unmagnetized sample implies that at $t=0$, $M_z=0$,

$$M_z(t) = M_0\left(1 - \exp\left\{-\frac{t}{T_1}\right\}\right)$$

which can be used to find our T_1 time later on.

1643 Pulsed NMR (what this experiment deals with) is especially suited to measuring such relaxation times as it can make "direct unambiguous measurements" [6]

1645 However, our machine may only measure in the xy plane. This can be understood classically

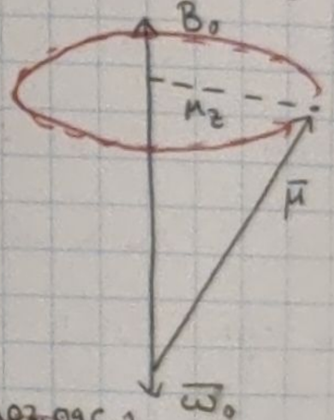


Fig02.09C.1

$$\bar{\tau} = \partial_t \bar{J} \Rightarrow \underbrace{\bar{\mu}\times\bar{B}}_{\text{Torque}} = \partial_t \bar{J} \longmapsto \underbrace{\bar{\mu}\times\bar{B} = \frac{1}{\gamma}\partial_t \bar{\mu}}_{\text{in xy plane}}$$

1658 Then, through some manipulation, we may get the net magnetization in the xy plane as

For non-constant magnetic field.

$$\partial_t \bar{M} = \gamma \bar{M}\times\bar{B} \quad \text{and} \quad \bar{B}(t) = B_1\cos\omega t\,\hat{x} + B_1\sin\omega t\,\hat{y} + B_0\hat{z}$$

1720 We may manipulate these fields to manipulate the magnetisation. If we create a rotating field at our resonant frequency

$$\omega_0 = \gamma B_0$$ ~~we~~

→

1725 The result is that the magnetization begins to precess about the driving field at $\Omega = \gamma B_1$, as can be seen below

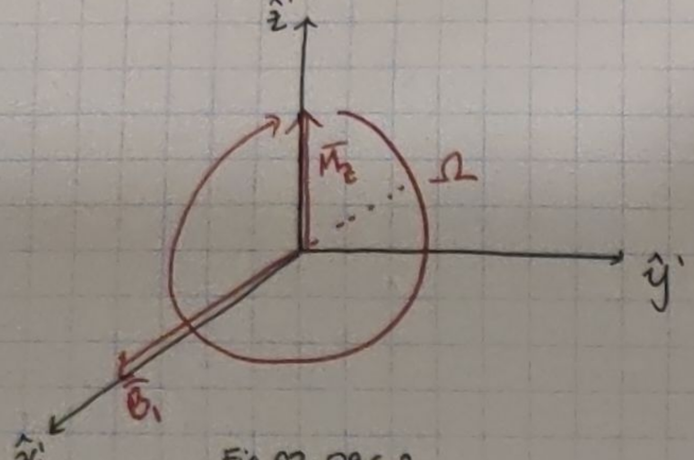


Fig 02.09C.2

1735 Depending on the duration of this magnetic pulse, the following transformations will be observed.

$\pi/2 \longmapsto M_z \longrightarrow M_y$ (Quarter Rotation)

$\pi \longmapsto M_z \longrightarrow -M_z$ (Half Rotation)

$2\pi \longmapsto M_z \longrightarrow M_z$ (Full Rotation)

1743 Signing out ~~Appr~~

2025-02-12 Note this bit of background was written 2025-02-11 so I have omit some graphs of the spin echo

1609 Given that our aforementioned spectrometer only measures in the xy plane, we may see only some of the magnetization comps as it passes in the xy plane.

1615 We may solve for this as

$$\partial_t M_{x'} = \frac{-M_{x'}}{T_2} \quad \text{AND} \quad \partial_t M_{y'} = \frac{-M_{y'}}{T_2}$$

w/ solutions given by

$$M_{x'} = M_0 \exp\{-t/T_2\} \qquad M_{y'} = M_0 \exp\{-t/T_2\}$$

where T_2 is known as the spin-spin relaxation time.

1626 which we may record by seeing how long it takes a spin to return to its equilibrium state. which may look as the following:

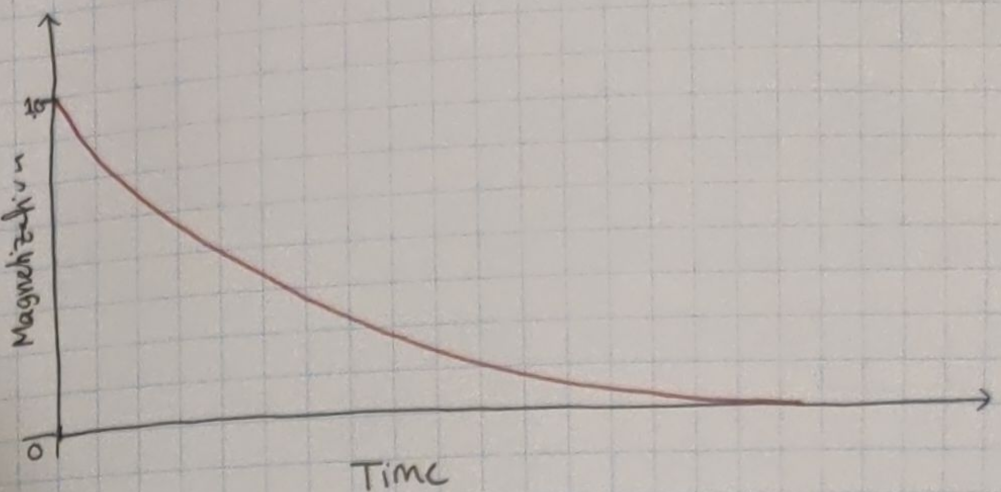


Fig 02.09D.1 : sketch of FID (Free Induction Decay) signal expected for spin-spin relaxation w/ influence from machine.

1901 ~~Lat~~ In the figure, this may look like the T_2 relaxation time, but is actually the Free Induction Decay (FID) which is actually due to the non-uniformity of the magnetic field. For the PS2 controller [2] if the $T_2 < 5ms$, then the FID $\approx T_2$ time since it is accurate enough to produce a magnetic field of uniformity of 0.3 ms decay time which can be improved using shim coils to improve the T_2^* time (decay time due to magnet).

1911 Even without these methods, we may use E. Hahn's discovery of a spin-echo to still accurately measure T_2 [2]. ~~that~~ Comparing the maximum height of the Echo and FID signal, one would notice a distinct difference.

1932 This loss occurs due to "fluctuations at the nuclear sites" [2] which are a measure of T_2. Then, varying the delay b/w signals, T_2 may be obtained from the equation

$$M_{xy}(2\tau) = M_0 \exp\left\{-\frac{2\tau}{T_2}\right\}$$

1947 Signing out A[signature]

2025-02-04

1029 Signing into lab

1030 Setting up lab book

1101 Discussions w/ Prof PS and TA KT
- Make sure to use o-rings before putting sample into magnet
- Document figures well

1200 Figure setups done, reading lab manual & literature.
+ setting up filestructure and code base

1320 Setup preliminaries & examining setup.

1358 Not much completed today other than clearing station and getting set up.
likely will review manual & background today a~~nd attempt~~ and
plan out friday session (+ roadmap for full ~~course~~ experiment).

1400 Signing out of lab

-02-07

32 Signing into lab

32 Completing some grading work for 11:00, did some light review for ~~WBM~~ NMR last night.

119 Schematic of spectrometer

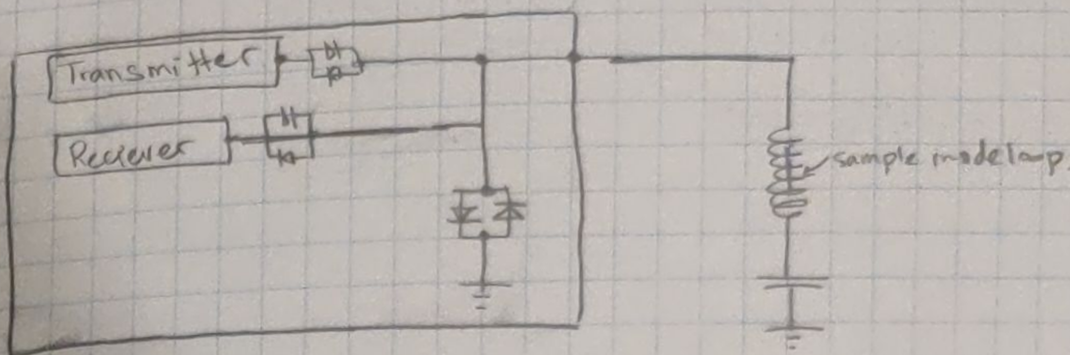


Figure 02.07 A.1 : Schematic of Spectrometer

1132 As in Fig 02.07A.1, we place the sample w/i the pickup coils

1133 Inspecting apparatus

1142 Setup below

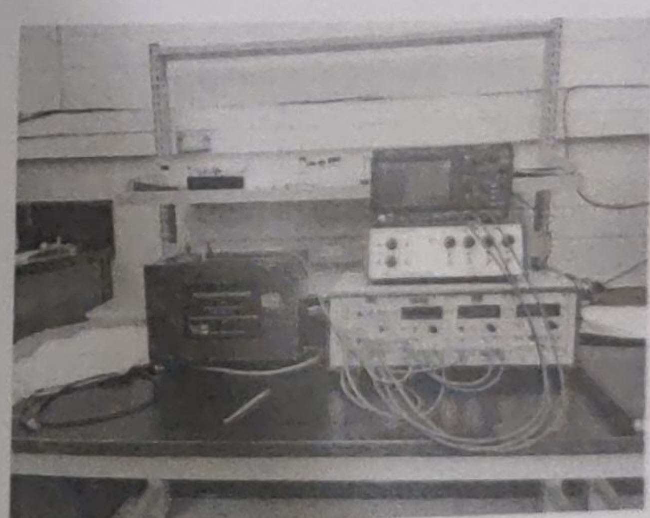


FIGURE 02.07A.2: Initial experimental setup for NMR.

→

1202 Experiment Plan & Reading Literature

1. Initial Measurements
2. Fundamental Literature Review
3. Advanced Measurements
4. ~~Ex~~ Data Analysis
5. Extension
6. Literature Review in Quantum computing or other field.
7. Literature Review in Frustrated ~~states~~ Magnetic States.

1329 Signing out of lab AR

5-02-11

910 Signing into lab

0916 Objectives

1. Write in Procedures

2. Some data collection

0920 From the F02.07A.2, the sample sits w/i the coil. B/w the transmitter and receiver, which a pair of crossed diodes. These restrict the minimum ~~maximum~~ voltage flow to ~0.6V from the sample (reduction of noise).

The crossed diodes to ground protect input from overvolt from transmitter

⇒ NMR output in of millivolts

when far from Resonance, we expect to see Fig 02.11A.1 at the Probe Head and Fig 02.11A.2 at LF-HF Output w/ the RC Filter at HF.

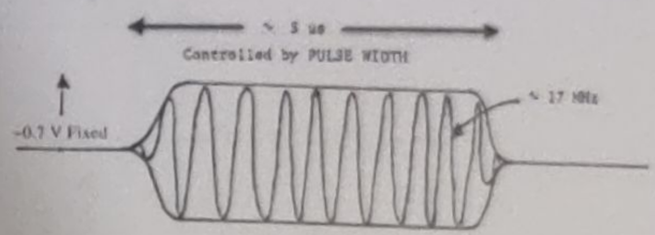


FIGURE 02.11A.1: Conceptual sketch of r.f. pulses at the PROBE HEAD from the lab manual [1].

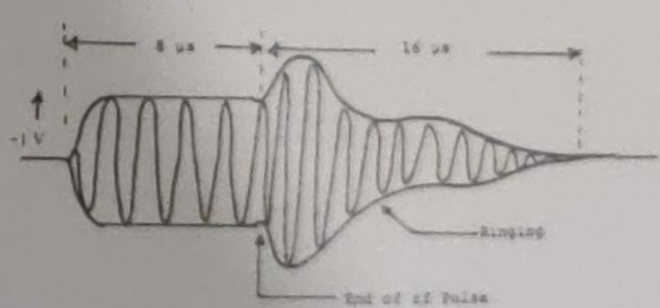


FIGURE 02.11A.2: r.f. pulses at the LF-HF Output for RC Filter set to HF from the lab manual [1].

0935 One experiment we will conduct as a preliminary is finding the resonance of $FeCl_3$.

0936 Procedure (P02.11A)

1. Set RC filter to 0.5
2. Connect LF-~~RF~~ out to oscope
3. Verify settings correspond w/ obs. output.

4. Verify Magnet coolant is ON
5. Verify Magnet Current ^ Voltage controls set at ZERO

6. Set Magnet PSupply to voltage limiting mode } As temp ↑ voltage may drift
6.1 L Set Current to Max (Voltage ZERO)
6.2 L Turn up voltage until induction coil observed
DO NOT EXCEED 7A
6.3 L To Turnoff Reverse step 6
7. To Turn of magnet, reverse step 7 → 1

~~0942 Performing Proc. P02.11A~~

0942 Reading literature from TeachSpin manual
0954 ~~Summary of key points~~ Full Background will be evaluated later

Resonance freq $\omega_0 = \gamma B_0$

$\gamma_{proton} = 2.675 \cdot 10^8$ rad s^{-1} T^{-1}

$f_{proton} = 42.58$ MHz T^{-1}

$f_{fluorine} = 40.055$ MHz T^{-1}

Thermal equilibrium // $\vec{H}$ field, approaches eq following exp rise w/ T_1 spin-relaxation time.

Classically $\frac{d}{dt}\vec{\mu} = \gamma(\vec{\mu} \times \vec{B})$ May be time dependent

→

57 Pulsed NMR employs rotating RF described by

$$\vec{B}(t) = B_1 \cos \omega t\, \hat{x} + B_1 \sin \omega t\, \hat{y} + B_0 \hat{z}$$

$$\vec{H} = B_1 \hat{x}' + (B_0 - \omega/k)\hat{y}'$$ ← Effective field

when on resonance $\omega = \omega_0 = \gamma B_0$ and $H = B_1 \hat{x}'$ and precesses around $\vec{H}_1$

$\pi/2$ Pulse : left on long enough for M_0 to rotate about $\hat{x}$-$\hat{y}$ plane.

$$t_w = \frac{\pi}{2\omega_1} \quad w/\ \omega_1 = \gamma B_1$$

$$\Rightarrow t_w(\pi/2) = \frac{\pi}{2\gamma B_1}$$

T_2 is spin relaxation time

Spin echo allow measurement of T_2 from below in Fig 02.11B.1

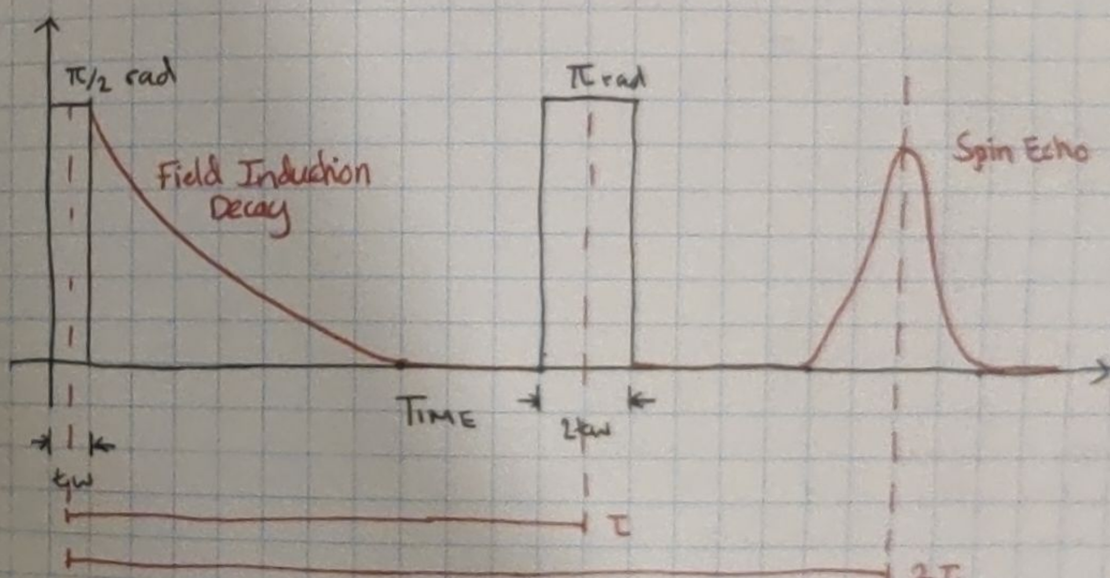


Figure 02.11B.1: Spin Echo Generation using $\frac{\pi}{2}$-Pulse and π-pulse to measure spin relaxation time T_2 of sample. Figure sketch from [2]

1011 Notes ~~on Instrument~~ from "Getting Started" in [2]

→

→

1014 Procedre P02.11B

1 Connect the Blue 18in cable from $\underbrace{\text{Pulsed RF out}}_{}$ to Pulsed RF In
(Synth over "Pulsed RF out"; Rec over "Pulsed RF In")

2 Connect the following BNC Connections

Q(PP) w/ Q(Synth)
I(PP) w/ I(Synth)
Blanking out (PP) w/ Blanking out (Synth)
~~RF~~ out (Synth) w/ ~~RF~~ In (Rec)

3 Connect the following to oscope.
Sync Out (PP) w/ Trigger
Env. out (Rec) w/ ch1
Q/I out (Rec) w/ ch2.

4 Perform/Verify the following

CW out (Synth), B Pulse(PP), MG (PP) OFF
Sync to A (PP) Toggle
Pulse to A (PP) Toggle
Rct out (Synth) ON
Filter TC to 0.1 (Rec)
Gain 75%
Band to 8 (Rec)
Blanking on (Rec)
width 75% (Rec)

Do NOT CONNECT
Rec (Rec) CW IN RF OUT
Synth (Synth) ~~RF out~~ SWEEP IN, CW OUT
PulseProg (PP) Ext start
Lock in All CONNECTORS

1023 Verifying Proc. P02.11B

1023 Verifying Do Not Connect

CW IN ✓ SWEEP IN ✓ Ext Start ✓
RF OUT ✓ CW OUT ✓ Lock In (all) ✓

→

verifying {1} (P02.11B-1) ✓

verifying {2} (P02.11B-2)

Q (PP) - Q (Synth) ✓ Blanking (PP) - (Synth) ✓
I (PP) - I (Synth) ✓ Ref out (Synth) - Ref In (Rec)) ✓

~~verifying (P02.11B-3)~~
Sync Out (PP) w/ Trigger

Digital oscope - DSOX1204G has no trigger input, will perform manual / auto trigger

1030 Env out w/ Ch1 ✓ ~~Q/I Out (Rec) w/ Ch2~~

Q/I out on Reciever { Switched Q to Ch2
Switched ~~Q~~ I to Ch3

1031 verifying (P02.11B-3)

CW out, OFF ✓	B Pulse, OFF ✓	MG OFF ✓	Ref out ON	FILTER TC Adj to 0.1
~~Sync A~~	Sync A ✓	Pulse toggled to A ✓	Gain 75%	Band P
			Blanking ON	Width

{No gradations on width, roughly set to 75%.

1037 No gradations on width knob, ~~eyeb~~ Roughly read, set to 75%. Used masking tape and sharpie to mark gradation.

1041 Setting computer hw connections

1045 Discussion w/ Prof DS
1. Need to calibrate.
2. Needed to explain NMR and roughly the physics of the experiment
3. Will go back at end of session.

→

~~1046 Procedure (P02.11C)~~

1046 Module Paramaters adjusted w/ Push to select rotary encoder.

Synth Default Settings		
F	Frequency	18.00000 MHz
P	Refer Phase	-180°
A	CW Power	-10 dBm
S	Sweep	0 kHz V^{-1}

Pulse Programmer Default		
A	A length	0.02 μs
B	B length	0.02 μs
τ	Tau	0.00015
N	Number B	0
P	Period	0.2 ms

Lock-In Default

G	Gain	80V
P	Reference Phase	-180°
T	Time Const.	0.5s
M	Modifier Amp.	OFF
H	Field off	0.00G
S	Sweep Mode	OFF
A	Sweep Amp.	0.031G
D	Sweep Duration	10s

1052 Procedure (P02.11C) : Single Pulse Experiment for Mineral oil

1. Ensure sample only fills 5mm of tube — will take lower miniscus
2. Ensure O-Ring Stop at 39mm
3. Utilize Pickup Probe to measure RF fields during pulse — voltage maximized at 0.5 cm
4. Utilize Pickup Probe to tune to Larmor Frequency at Proton
5. Place Probe into sample solenoid
6. Set Synth Freq to [illegible]
7. Set A length to 2.5 μs
8. Set P to 100 ms
9. Set Oscope [illegible]
10. [illegible]

57 Discussion w/ TA KT
→ Turned on machine
→ Explained how to Tune capacitors of Magnet

102 Inserted Pickup Probe into sample area, plugged probe into Ch4. Adjusting capacitors until maximum obtained.

103 Turning off equipment. Noticing error signals on PS2 controller

1106 Tuning capacitor schematic Fig 02.11C.1

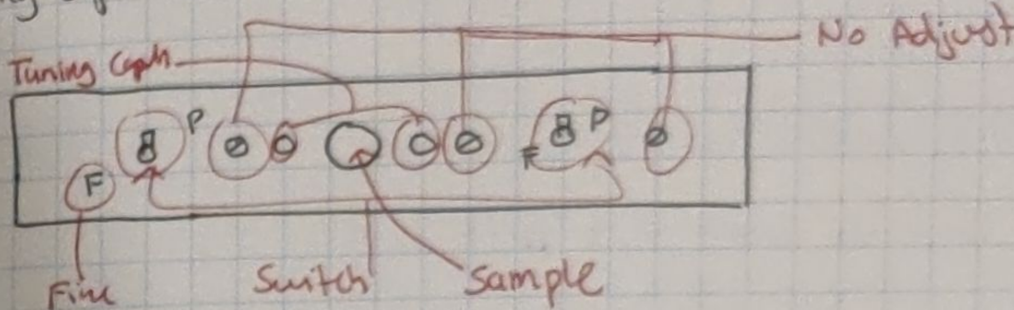


Figure 02.11C.1

1109 Turning on equipment and adjusting to default parameters.

1112 Verified Default settings. Changing relevant settings to those in Proc. (P02.11C-6-8)

Synth to 20.90000 MHz
A_len to 2.5 µs
P to 100 ms

1114 Opting to change oscope on the fly.

1115 Pickup probe placed in sample.

1117 Scope image in Fig 02.11 D.1

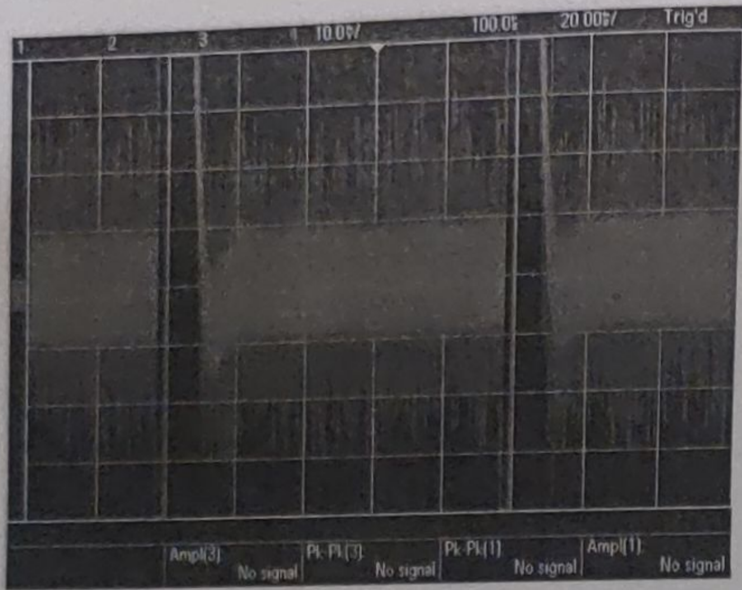


FIGURE 02.11D.1: Initial Reading from Osciilloscope. Notice Peaks

1118 Adjusting capacitors until 40 V_{pp} observed.

1122 only observing maximum ~~pk~~ V_{pp} of 32 V

1133 Discussion w/ TA. KT and LT. LA

~33 V_{pp} should be okay despite what the manual says.

Going to continue at current timing. Images then

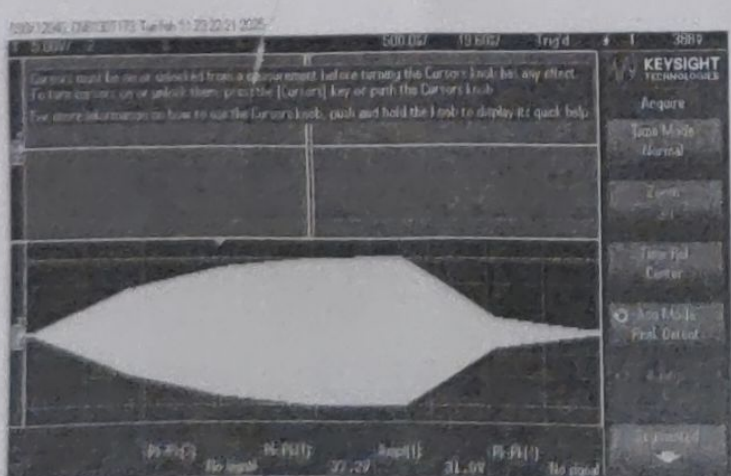


FIGURE 02.11D.2 Scope readings using zoom mode. Clearly we can see the packet.

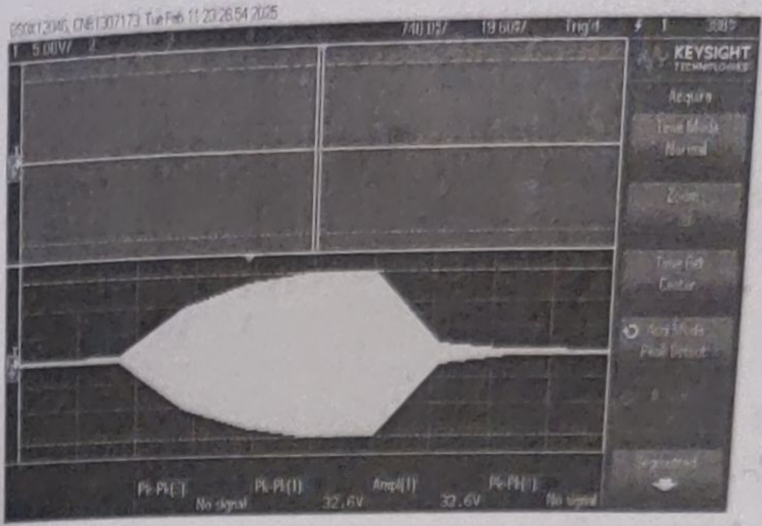


FIGURE 02.11D.3: Another scope reading using zoom mode. Maximum voltage observed $V_{pp} = 31.5 \pm 0.5$ V

1204 Preparing mineral oil samples for Free Induction Decay Measurement

Seeing as this is just a test, will use prepreppared sample.

1210 Connect Ch1 to ENV out, disconnected & removed pickup probe

I and Q outputs are the product of the signal from precessing spins with the the reference signal from the oscillator

$$\sin(\omega_{ref} t)\sin(\omega_{spin} t) = \frac{1}{2}\cos\underbrace{(\omega_{ref} - \omega_{spins})}_{\text{Present at output (Beat / Difference Frequency)}} t - \frac{1}{2}\cos(\boxed{\omega_{ref} + \omega_{spin}}) t$$

should be filtered out ~ 40MHz

We want the Beat freq to be at 0 so the oscillator has nearly the same freq as precession freq.

1216 Setting X, Y, Z, Z^2 to zero. Placing mineral oil in RF sample probe

1223 observing something similar to a FID packet (Ch1) and Difference signal. See figure 02.11E1

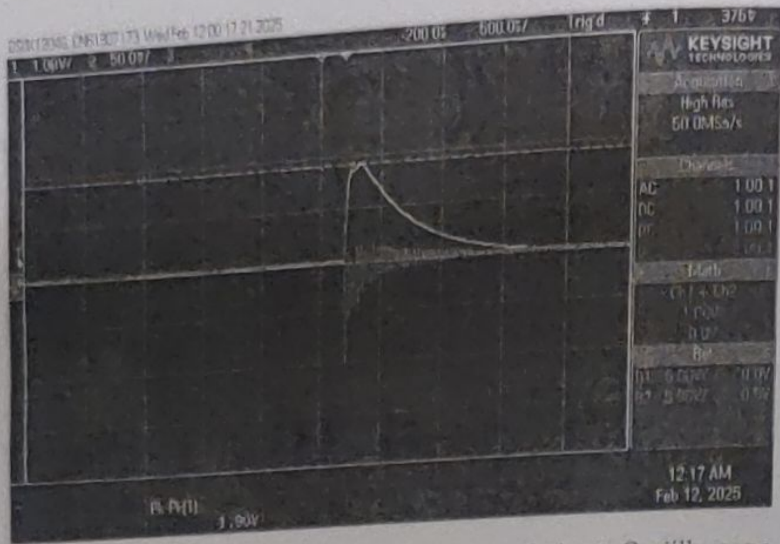


FIGURE 02.11E.1: FID Signal (Channel One) from Osciilloscope with Difference Signal From Q Output (Channgel Two)

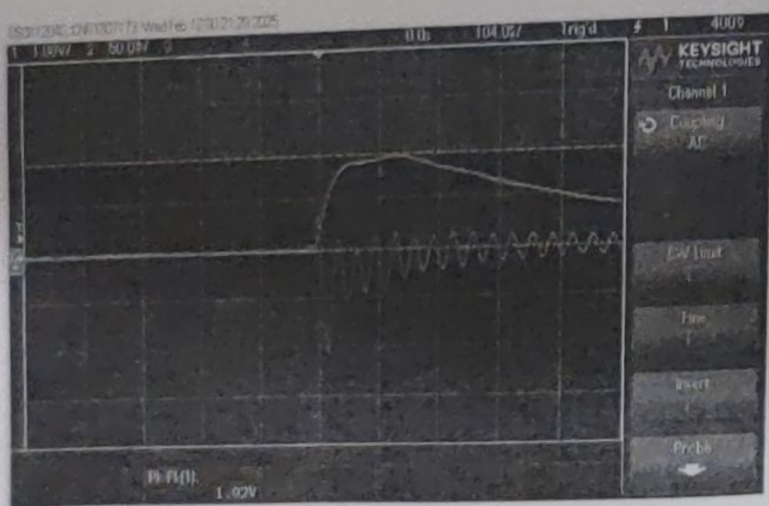


FIGURE 02.11E.2: Zoomed in version of the previous figure.

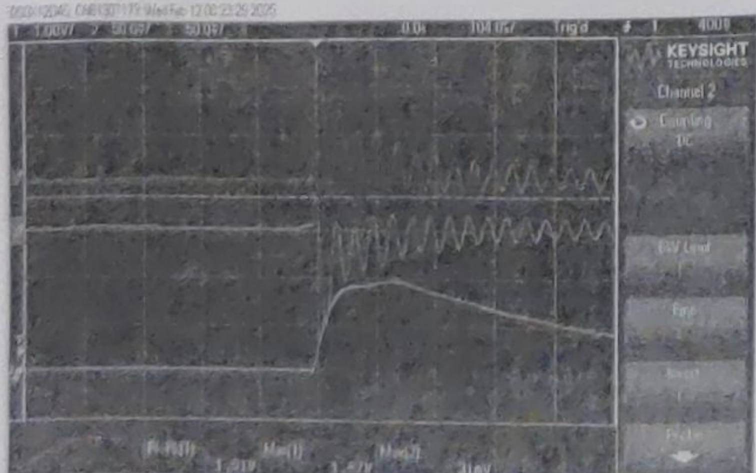


FIGURE 02.11E.3: FID Signal (Channel One) from Osciilloscope with Difference Signal From Q Output (Channgel Two) and Difference Signal [illegible] (Channel Three)

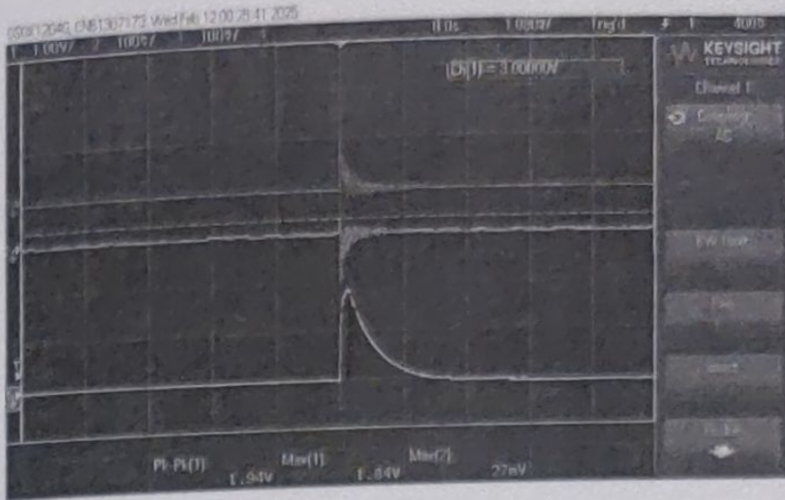


FIGURE 02.11E.4: Zoomed in version of the previous figure.

248 Finished pushing images. Taking break. Turning off equipment.

311 Returned, going to do mini commentary on data and then signout / plan experiment for tomorrow

1333 Clearly seeing what seems to be a FID signal on Channel 1 in Fig 02.11E.1, however, it is not a sharp peak as expected from the lab manual ~~[illegible]~~. [2, pp III-7]. Instead we see a more rounded peak evident in Fig 2.11E.3. However, Fig 02.11E.4 looks more similar to what is expected. Expected signal in Fig 02.11F.1.

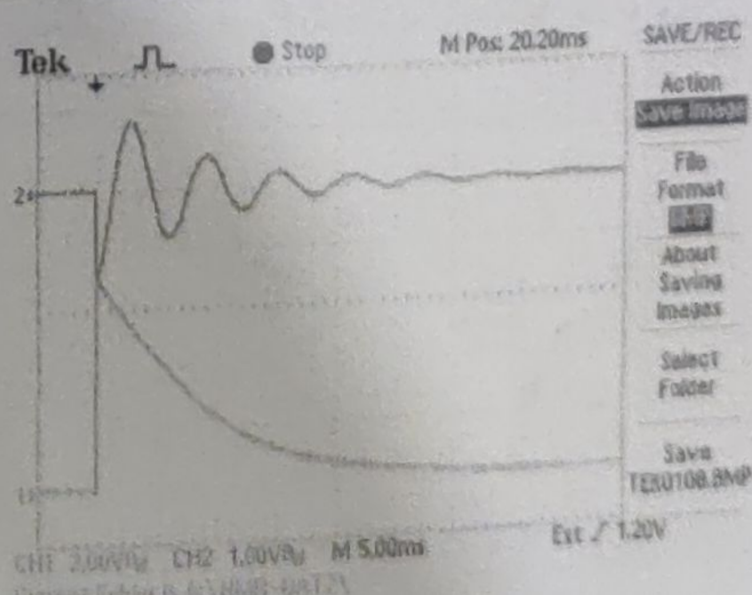


FIGURE 02.11F.1: Expected FID and Difference signals from the Teach Spin Cw Laboratory Manual [2] (p. III-7)

⟶

~~[illegible]~~

1353 Further investigation and analysis to be conducted

1354 Objectives for next session :

1. Analyze Data From Today
2. Characterize and understand theory

1359 Objectives for lab book :

1. Read and write background theory
2. Read some extentions
3. Plan remaining lab sessions + proposal for Part PS for overall experiment.

1400 Signing out of lab [signature]

02-14

05 Signing in lab

08 Objectives:
- Discuss Findings w/ P.PS
- Collect data for one more sample*
- Organize (Theory should be studied over Reading week).

35 Discussion w/ T.KT
- Data looks good
- lab manual has interesting extensions
- Lower Vmax just means pulses will be longer

40 Turning on equipment and trying to obtain same results

045 Parameters changed from last time. Tuning to Proc (P0211C)

050 Better data obtained!

055 Discussion w/ P.PS
- Overall objectives should be derived
- After Reading week, discuss w/ P.PS about Theory & Ideas.

1058 Adjusted oscope save settings. .

1124 ~~setting~~ Putting in light mineral oil.

1127 After cycling oscope, Light mineral oil data observed. looks qualitatively different.

1324 Will post images later today. For now signing out of lab

2025-02-15

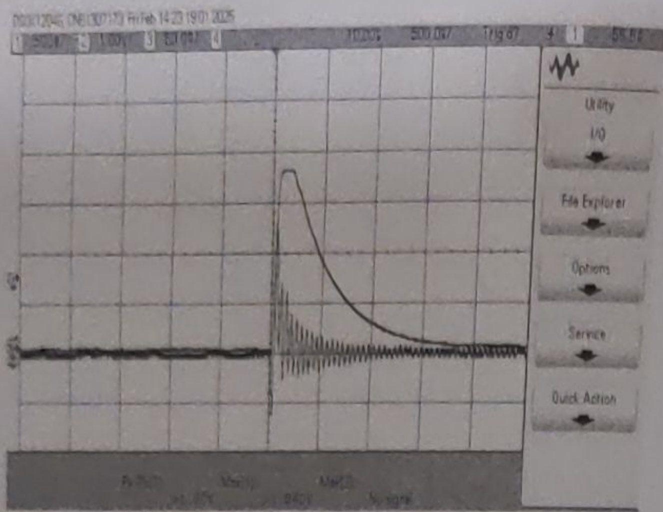


FIGURE 02.14A.1: New Data Obtained from scope for heavy mineral oil. We can clearly see a more distinct pulse width forming as is expected from Fig. 02.11F.1 and from the 'spin echo' section of the lab manual [1].

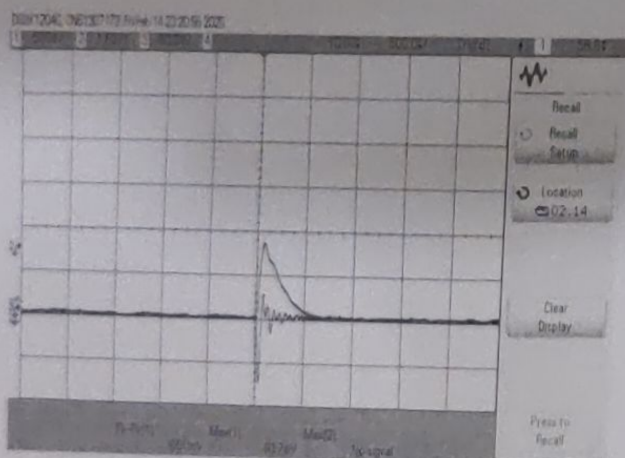


FIGURE 02.14B.1: Peak obtained when measuring light mineral oil. Clearly, as compared to Fig. 02.14A.1, there peak is signifianly smaller.

Time not Recorded

Signing out (just pasting images from yesterday)

02-20

Signing in, conducting some light analysis on data collected on 2025-02-20 (pg 26). Mainly just going to write code and verify that things make sense.

.20 Writing Analysis code

125 Using normal pd.~~load~~read_csv(...) for dataframe values.

558 Plots fits very non-ideal, significant issues w/ finding good guess.

701 After significant debugging, there are still issues. Going to discuss w/ Prof. PS and/or TA. KT ~~[illegible]~~ on 2025-02-25 (next supervised lab session).

727 Signing out ~~AR~~

2025-02-23

2157 Signing in

2159 Plan for measuring T_1 and T_2.

22 00 T_2 Plan:
Fit FID signal, this should correspond w/ crude estimates from fitting FID signal

22 10 From [1] T_1 can accurately be measured using a 2 pulse sequence as

$$\partial_t M_z(t) = (M_0 - M_z(t)) \cdot \frac{1}{T_1}$$

$$\Rightarrow M_z(t) = M_0\left(1 - \exp\left\{\frac{-t}{T_1}\right\}\right)$$ as in the background theory.

$$\pi \xrightarrow[\tau]{} \pi/2 \rightarrow$$

↳ initial amplitude of FID post $\pi/2$ pulse & M_z pre $\pi/2$ pulse

22 19 So taking a few τ values will give us T_1.

2220 T_2 can be measured using a reverse sequence $\pi/2 \xrightarrow[\tau]{} \pi \xrightarrow[\tau]{}$ Echo

using $M_m(2\tau) = M_0\left(\exp\left\{-2\tau/T_2\right\}\right)$ to ~~[illegible]~~

2228 echo amplitude as a function of τ yields the T_2 time

~~[illegible]~~ ~~[illegible]~~

2231 Signing out.

25 Signing into lab

Discussion w/ KT, about future experim.

Data Analysis

9 After debugging, decent initial plot found to tail of pulse.

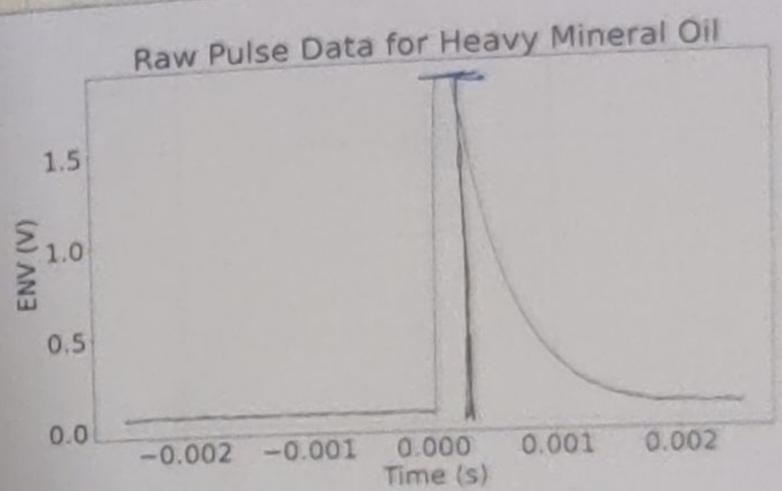


FIGURE 02.25B.2: Raw Pulse data obtained from the Oscilloscope. We will casterate this dataset to fit the tail of the exponential.

To fit to this data, castrate $-0.002 \rightarrow 0.000$ and $0.00015 \rightarrow \infty$. This was found through trial and error.

Using this, the values on ~~following page~~ Page 30 were found

For initial estimation of uncertainties the min and max of the noise from $-0.002 \leftrightarrow 0.000$ was recorded. This was used as the uncertainty in the y data. No uncertainty was assumed for x data.

This will be finetuned and analyzed later

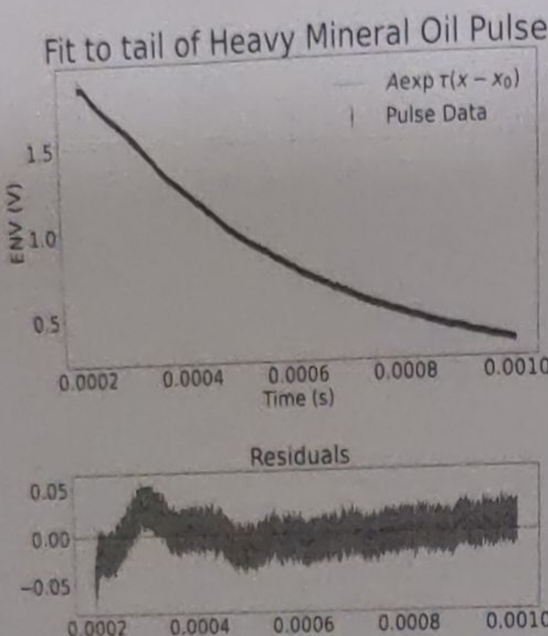


FIGURE 02.25B.3: Obtained fit using the equation in the graph. Obtained parameters are as follows, $A = 2.0 \pm 70000$ $\tau = -2233 \pm 4$, and $x_0 = 0.0002 \pm 16$ with a $\chi^2_{red} = 0.2$.

1212 Clearly, we have a decent fit, $\chi^2_{red} < 1 \Rightarrow$ some overfitting to noise, however, I believe this is more likely an overestimation of uncertainties as the pattern in the residuals is quite insignificant (apart from the ~~beginning~~ end of the pulse width).

1216 It follows then that T_1 for Heavy Mineral Oil is given by

$$T_1 = \frac{1}{\tau} = 0.0004478 \pm 0.0000008$$

$$\cancel{4478}$$

$$\cancel{4478 \pm 8}$$

$$= 447.8 \pm 0.8 \ \mu s$$

1221 Same procedure will be followed for Light Mineral Oil.

1222 Signing out of lab

2-28

Signing into lab

0 Discussion w/ LT-Larry about old NMR machine
- Issue probably due to sheilding on Copper tip of probe becoming desoldered

25 (Premium) Discussion w/ Arnish (prior student doing NMR).
- Observed problem w/ old NMR machine is that no Spin Echo was observed.

35 Discussion w/ TA-KT:
- Should try and observe spin echo
- No expected result if we blast sample w/ laser
- Fixing old machine would be interesting.

46 Helped another setup briefly.

053 Lab Objectives:
- Measure T2,
- Try and observe Spin Echo
- Setup Spin Diffusion in Distilled water.

055 T_2 Measurement Procedure (P02.28A)
^ π pulse

1. Tune Spectrometer to Resonance and ~~observe~~ obtain best π pulse possible.

2. Adjust Fine Tuning Capacitor, if FID tail smaller => keep adjusting in that direction.

3. Adjust till no tail (or nearly no tail) observed in FID signal.

1105 oscope settings loaded from 2025-02-14, no signal observed, checking apparatus parameters from P02.11C

1126 New Signal observed, hmm different from before.

⟶

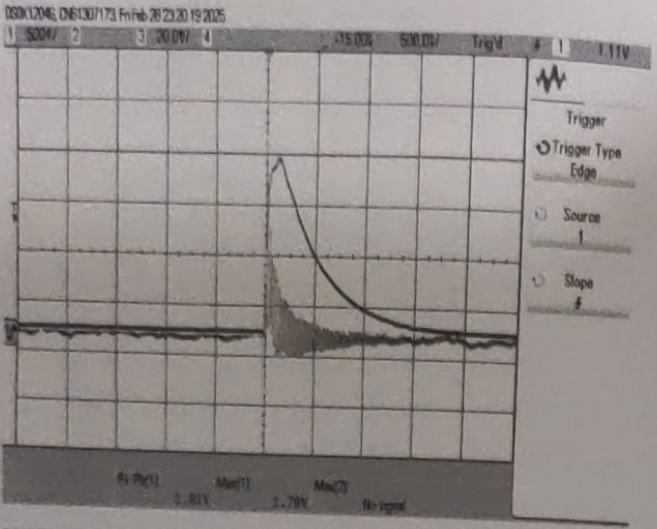


FIGURE 02.28A.1: Differerent signal than previous measurements observed. Need to retune and adjust parameters.

1130 Break

1146 Returned.

Adjusting to obtain π-pulse parameters for Heavy Mineral Oil as per {P02.28A}.

1148 Discussion w/ Prof. Tahir Shaaran

Slope 95% of gradient (plot $\ln(I/I_0)$ against G^2) and use Stejskal-Tanner Equation to obtain spin diffusion coefficient)

For measuring Spin diffusion in Distilled Water.

1152 Returning to π-pulse parameters [11:48 · 2025-02-28]
1157 Reading TeachSpin Manual.

1210 B pulse not working, Procedure outlined in manual not working.

1217 Adjusting ~~[illegible]~~ w/o manual

1238 Spin echo Observed?

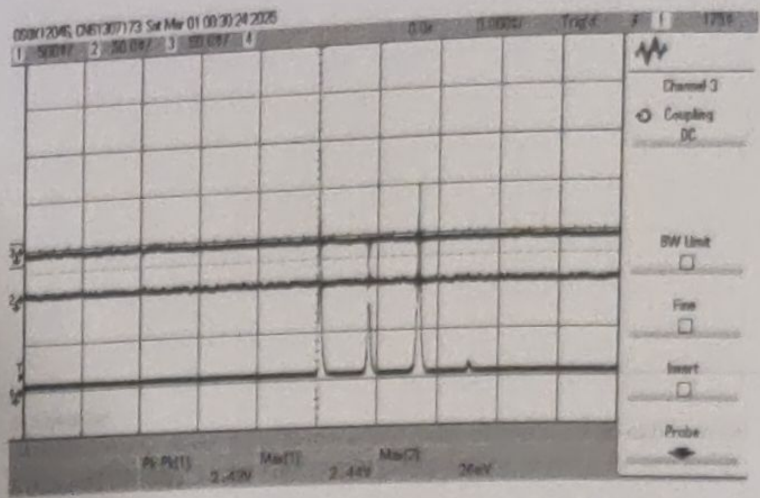


FIGURE 02.28B.1: Possible Spin Echo observed. First peak is from a $\frac{\pi}{2}$-pulse, second peak is a π-pulse. The third peak may be the observation of a spin echo.

1240 Parameters (PP):

A len : 3.90
B_len : 7.80
τ : 0.0042
Num_B : 1
Period : 100.0 ms

Sync : A
A : ON
B : ON
Mk : OFF

Rest all same as before.

1241 Having a headache. Going to take a break and do reading + Analysis over weekend.

304 signing out for lab. AK

2025-03-03

15 14 Signing into lab

Measure T_2^*

1520 Discussion w/ Shravan K. Shridar (SKS)

Testing π then π/2 pulse.

st

1528 Scope use is hist image for today

→ SCROFULOUS PULSES
to third order invariant

1538 SKS suggested FFT give you beat frequency allowing us to find resonance.

1547 Fixing FFT code.

1604 Need to fill in f: 20.86200 MHz

1605 Sentinel ...

-03-03

Signing in

Explination of work conducted today @ 1520 :

→ Discussion w/ SKS about data

→ SKS noticed pulse seemed to be off Resonance and suggested a method to find Resonance

B:23 Take Q or I data and get Fourier Transform. Out put should be similar to Fig 03.03A.1

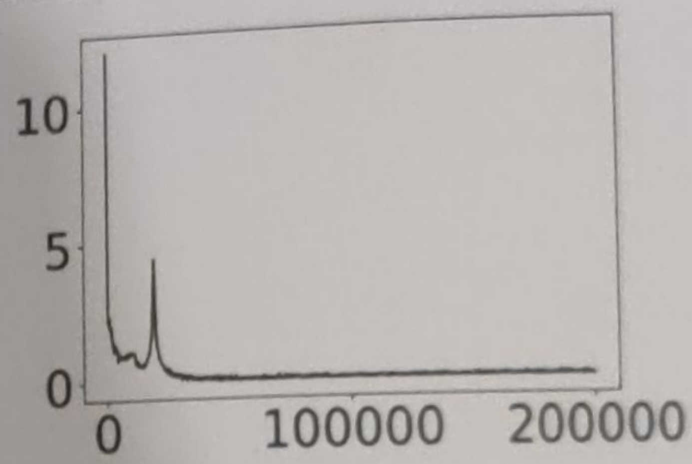


FIGURE 03.03A.1: Data obtained from taking the fourier transform of the I signal data. Notice the existance of two distinct peaks. One being the mean and the other being the resonance frequency.

837 Now take ~~Maximu~~ mean and remove it from the signal. The next highest peak should be near the resonance frequency. This can be seen in Fig 03.03A.2. ~~The~~

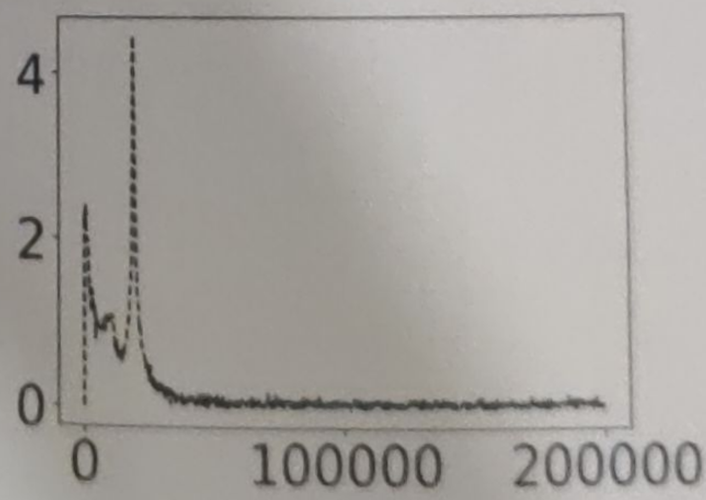


FIGURE 03.03A.2: Mean removed fourier transform.

18:42 Finding this resonance frequency ~~has the~~ full and applying it ~~to~~ as an edit ± f to the ~~[illegible]~~ machine has the following effect on the I pulse (Fig 03.03B.1)

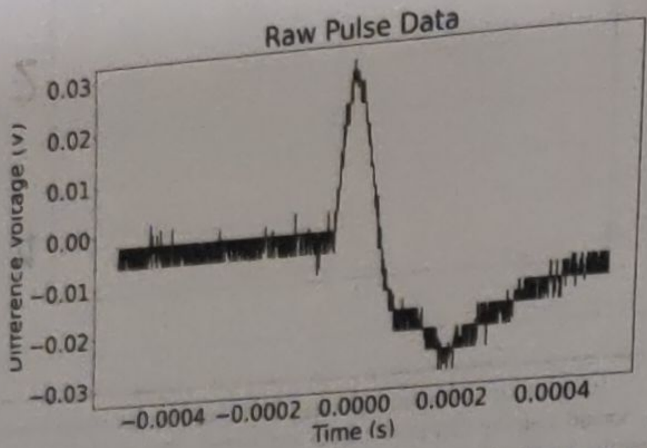


FIGURE 03.03B.1: Resultant I-signal observed after tuning using fourier transofmr method suggested by SKS.

18:52 Further edits/fine adjustments yielded Fig 03.03B.2. From here, f_R = 20.8620 MHz was found as the Resonance frequency of heavy mineral oil.

1900 Lab Objectives for 2025-03-04

1. Retake HMO and LMO data.
2. Record T_1 and T_2 times using π then $\pi/2$ pulse
   Spin Relaxation
3. Look into spin relaxation for unifying equations?

~~[illegible]~~

Note, these notes were filled in later. Images were posted the following ~~week~~ day

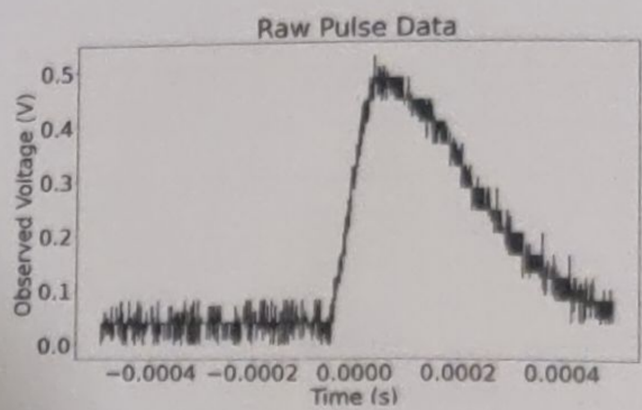


FIGURE 03.03B.2: Corresponding signal.

1905 Signing out AR

5-03-04

30 Signing into lab

931 Turning on equipment, reviewing notes from ~~??~~ 2025-03-03

948 ~~Turning up~~ Tuning Equipment

952 Tuned to $f_R = 20.88620$ MHz, ~~A f_A — f_B~~

Had to perform fine adjustments

$\ell_{\pi/2} = 3.90\ \mu s$, $\ell_{\pi} = 7.80\ \mu s$

0959 Lab Objectives

1. Verify f_R
2. Retake data for HMO and LMO
3. Take data for Distilled H_2O

Difference

1013 Verified $\ell_{\pi/2} = 3.80$

$\Rightarrow \ell_\pi \approx 7.60$

↳ we may verify this now

1014 Output w/ $\ell_\pi = 6.94\ \mu s$ in Fig 03.04A.1

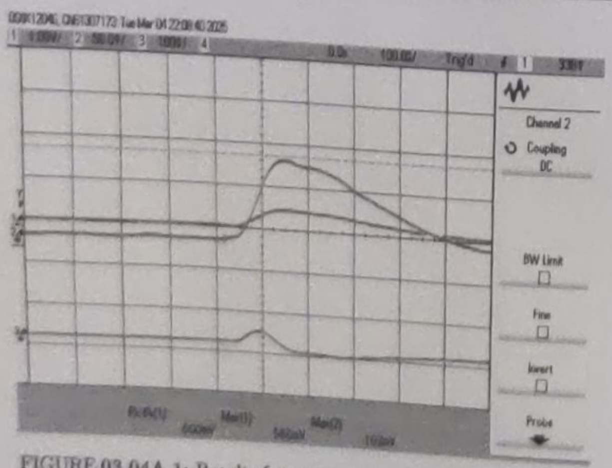


FIGURE 03.04A.1: Result of a π pulse with pulse length $\ell_\pi = 6.94\,\mu s$.

016 Noticing there is still an unexpected FID signal. Consulting lab manual [1] to verify procedure,

027 New parameters (which I hope are correct):

$$l_{\pi/2} = 3.80\ \mu s \pm 10\mu s$$

$$l_{\pi} = 7.40\ \mu s \pm 10\mu s$$

$$f_R = 20.86114\ MHz$$

Relavent output in Fig 03.04B.1

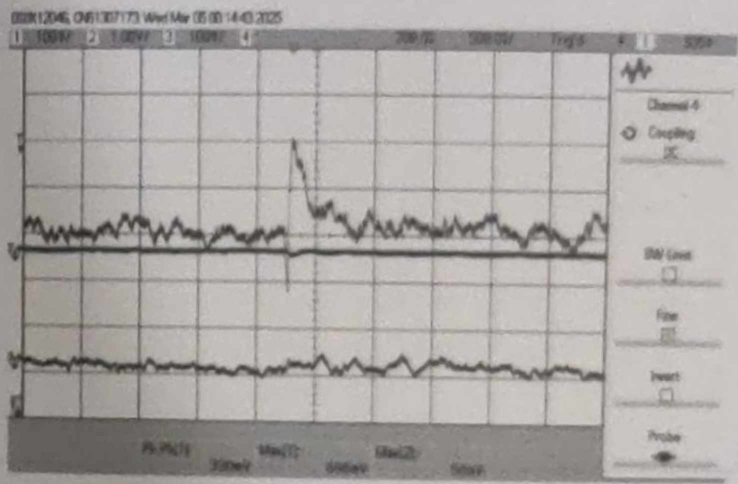


FIGURE 03.04B.1: Relavent output with new pulse length parameters.

1070 Now, we may attempt to observe the spin distillation in water. Relevant theory will be added later. For now, important immediate information follows:

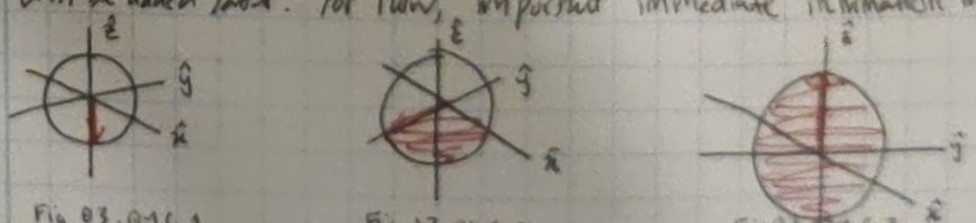


Fig 03.04C.1 Fig 03.04C.2 Fig 03.04C.3

Fig 03.04C: Bloch spheres of Ground State (C.1), $\pi/2$ pulse (C.2) and π pulse (C.3)

1033 In order to measure the spin distillation in ~~sp~~ distilled H_2O, consider the following procedure:

1. ~~To~~ Flip spins from Ground state,

2. Interrogate Spins using $\pi/2$ pulse.

3. Measure Relaxation time.

1050 Sample filled ~~and~~ w/ distilled H_2O. Putting into Machine.

1055 Sample stuck in Machine, asking LT for help

1058 Was able to remove sample. Setting machine up again

1101 Noticing output signal very small. Need to feed in signal into op-amp

1102 Coffee Break (~~15~~5 min max) — Didn't end up taking

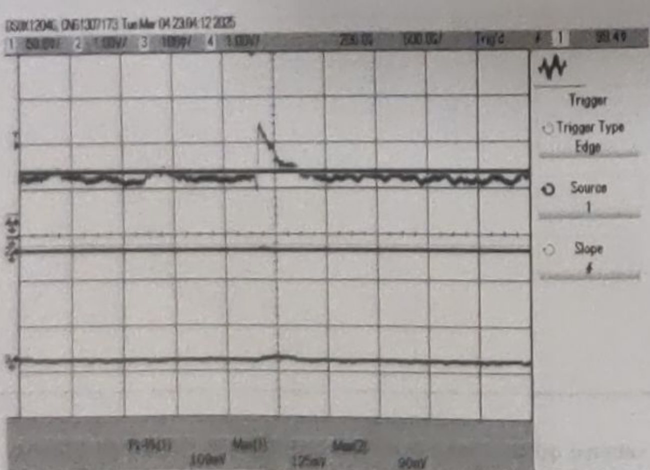


FIGURE 03.04D.1: Output signal from distilled water sample. Notice that the signal strength is quite low and very noisy.

1111 just realized amplification device is a lock in amplifier, not a non-inverting op-amp.

1112 Going to quickly make non-inverting op-amp using LM358

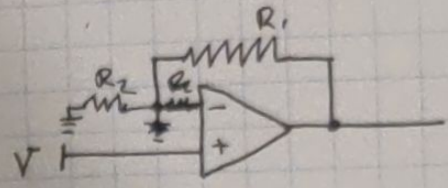


Fig 03.04 E.1

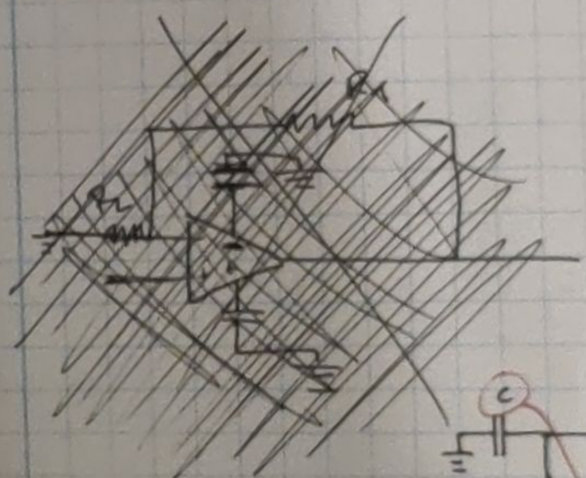
$$\text{Gain} = 1 + \frac{R_1}{R_2}$$

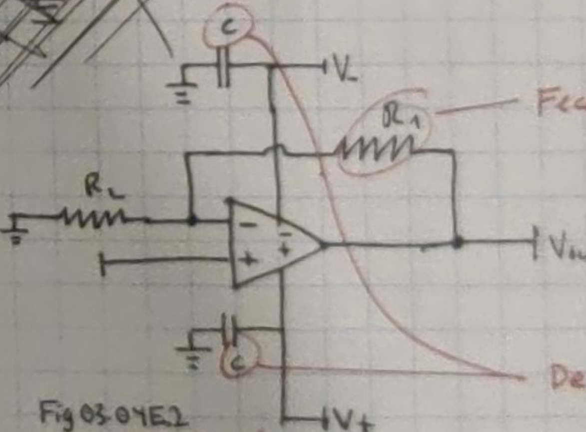
closed loop voltage gain,

we want $\simeq \times 10$ gain

$\Rightarrow R_1 = 1k\Omega$,

$R_2 = 100\Omega$.

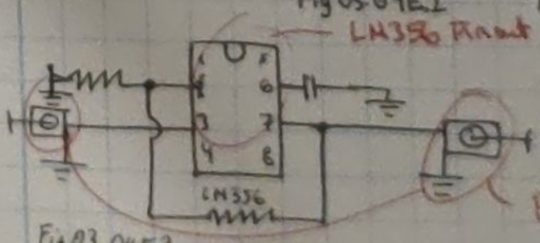




Feedback Resistor

Decoupling Capacitors
~ 1pF is sufficient

Fig 03.04 E.2



LM358 Pinout

- 1 = X
- 2 = V- in
- 3 = V+ in
- 4 = X
- 5 = X
- 6 = Power (+) In
- 7 = Vout
- 8 = X

Fig 03.04 E.3

1447 Designed and finished soldering op-amp. Taking break and showing both to Prof. A.H.

1219 OpAmp Remade

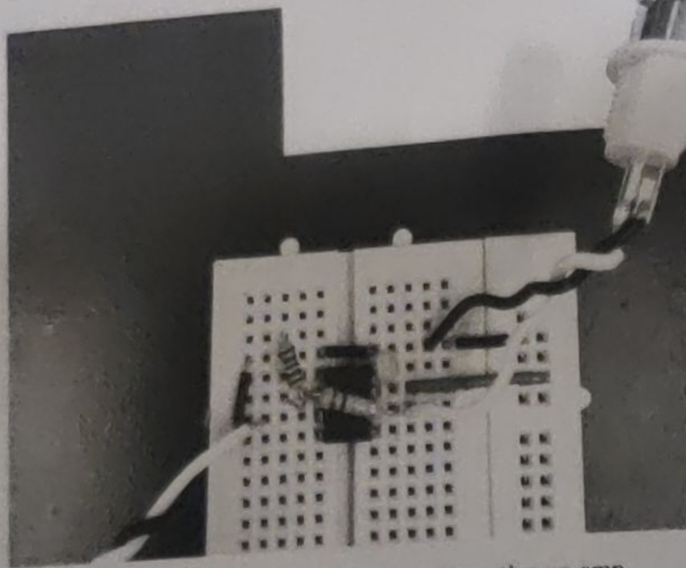


FIGURE 03.04F.1: Breadboard of non-inverting op-amp.

1220 Still not fully working as intended, taking data w/o and going to debug circuit at home.

1220 Setting pulse delay $\tau = 50\mu s$, Running π followed by $\pi/2$ pulse and recording data.

1222 Signal extremely noisy

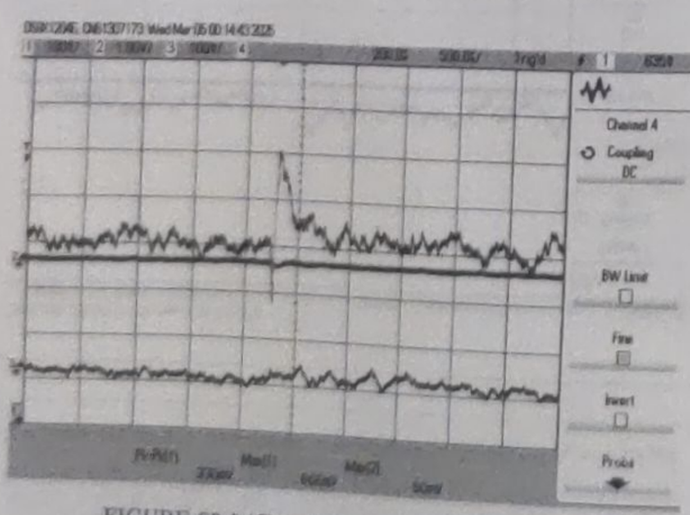


FIGURE 03.04G.1: Noisy small signal observed.

22 Adjusting delay, switch Oscope to time mode averaging.

224 Results not good, switching to High-Res Mode.

1225 Resulting signal observed

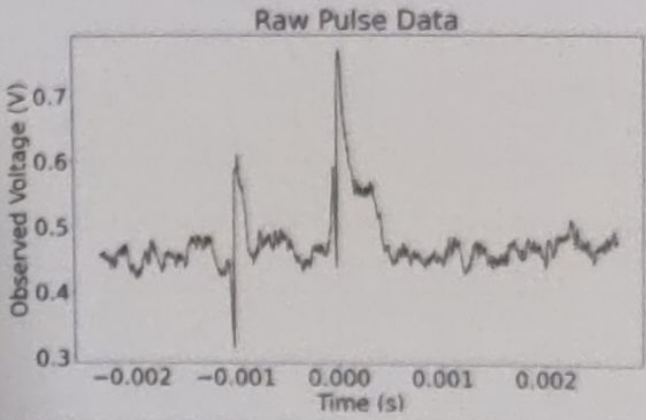


FIGURE 03.04G.2: Observation for Distilled Water.

—

1226 Adjusting ~~t = 5μs, so that π/2 pulse~~ τ = 7.80 μs so ~ 8μs
so that π/2 pulse directly follows π pulse. Resulting signal

—

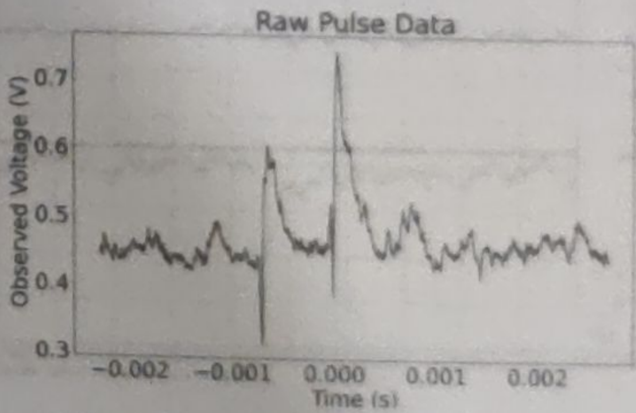


FIGURE 03.04G.3: Observation for Distilled Water.

—

→

1230 Turning Blanking off has the following output

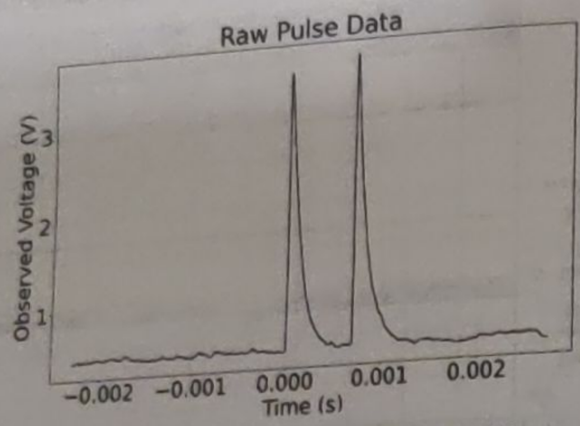


FIGURE 03.04G.4: Observation for Distilled Water.

1231 Not conducting Data Analysis Now/Today. Will now retake some Heavy & Light Mineral Oil Measurements after a break

1232 Taking Break.

1255 Returned from break

Heavy Mineral Oil

1255 Taking Readings for HMO and LMO

Light Mineral Oil

1256 Removed Distilled H_2O, put in LMO

1257 Gain reduced to 0.75 as before.

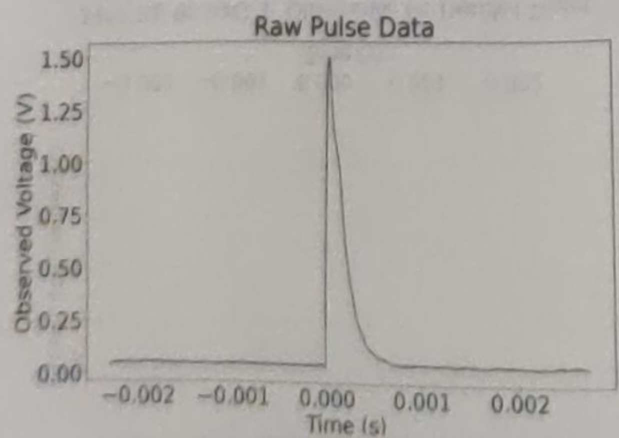


FIGURE 03.04H.1: Observation for Light Mineral Oil.

1258 ~~Re~~ Changing to π pulse

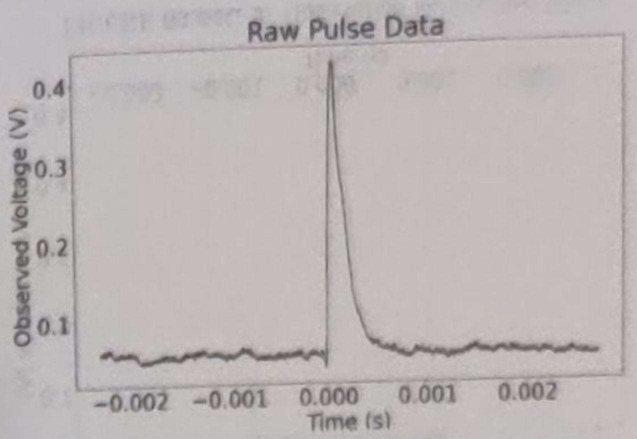


FIGURE 03.04H.2: Observation for Light Mineral Oil.

1259 π pulse followed by $\frac{\pi}{2}$ pulse w/ $\tau = 0.0007$ s

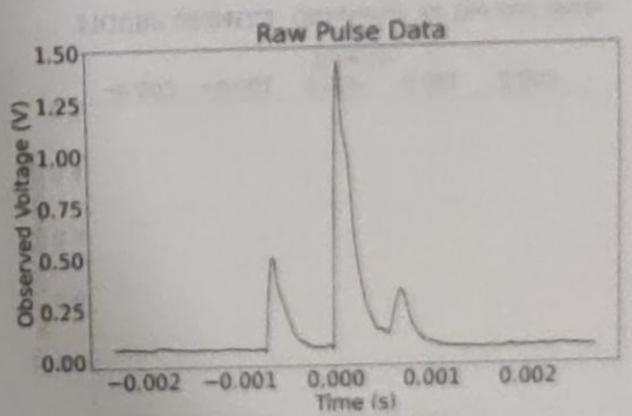


FIGURE 03.04H.3: Observation for Light Mineral Oil.

1300 Presumably, Spin Echo observed.

1301 Changing sample to Heavy Mineral Oil and repeating

1302 Heavy Mineral Oil inside Machine.

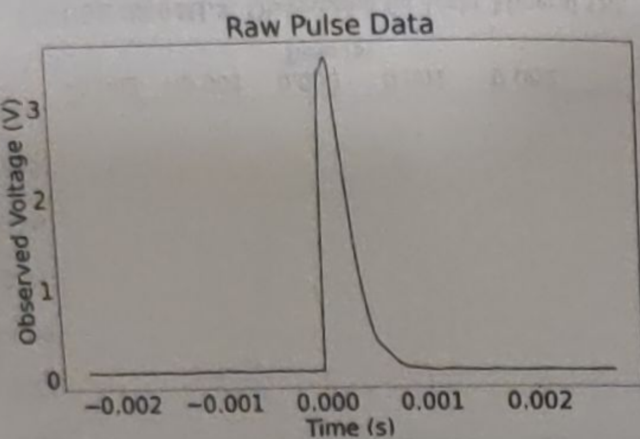


FIGURE 03.04I.1: Observation for Heavy Mineral Oil.

B02 π-pulse

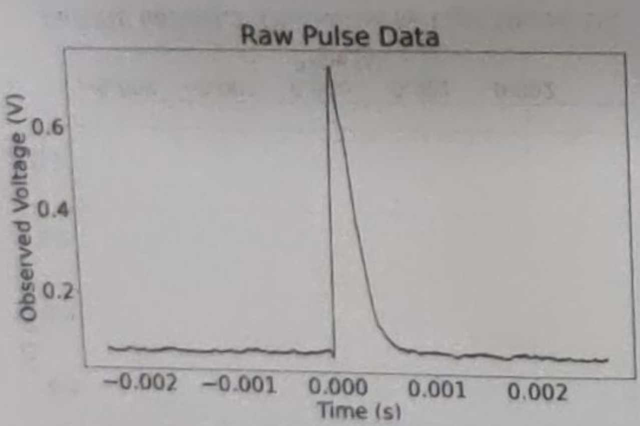


FIGURE 03.04I.2: Observation for Heavy Mineral Oil.

B03 π followed by π/2 pulse

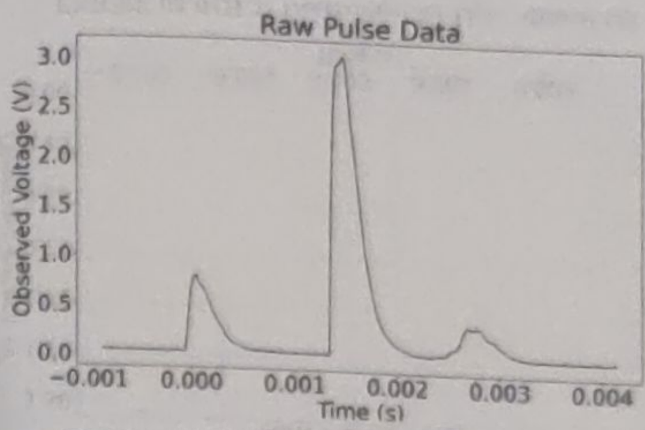


FIGURE 03.04I.3: Observation for Heavy Mineral Oil.

303 Data collected. Need to process images and paste them into book.

30 3 Objectives for today / tmorw:

1. Finish Writing Background Theory
2. Write up lit review on applications
3. Data Analysis

1304 May need to email supervisor for an extension, we'll see.

1305 Checking lab manual incase any details were missed.

1307 There is some interesting discussion on using the PS2 controller to "keep the spins alive."

1310 Lets see if we can keep the spins alive and do some sort of unitary operation like in a Q Algorithm.

317 Additional measurement at $\tau = 0.0014$ s

→

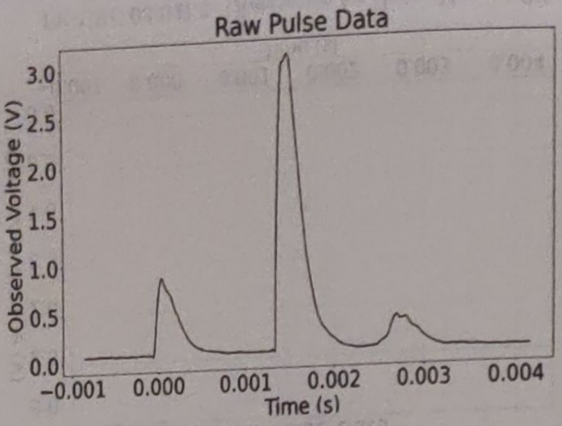


FIGURE 03.04J.1: Playing around with pulses to see if we can implement a unitary gate. This is more just exploration with no expectation of results.

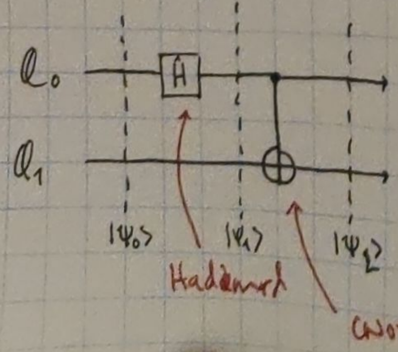
1318 Running only $\frac{\pi}{2}$ pulse and seeing if we can extend FID.

1324 Interesting effects observed, but not much worth reporting.

1325 Main interesting change was that, apparently, the magnetic fi[eld] gradient in the $+z$ direction had some small value. After ch[anging] changing this f_R changed to $f_R = 20.85558$ MHz. However, due to time constraints, we will still analyze old data.

1326 We may do this because that data was still taken consistently and any comparative analysis will still be self consistent.

1327 Back to exploring. Consider the following Q Algorithm / circuit



1329 Where $\boxed{\hat{H}}$ is the Hadamard operator w/ unitary matrix

$$\hat{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

and $\oplus$ is a "CNOT" or Controlled Not operator. This may also be ~~written~~ called a controlled pauli $\hat{X}$ operator

$$\hat{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

1331 We may examine this circuit w/ initial ket at $|\psi_0\rangle$

$$|\psi_0\rangle = |00\rangle$$

For $\hat{H}$ acting on Q_0

$$\hat{H}|0\rangle \mapsto \tfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$
$$\hat{H}|1\rangle \mapsto \tfrac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

So $$|\psi_1\rangle = \frac{|00\rangle + |01\rangle}{\sqrt{2}}$$

1347 Now the CNOT gate works as follows

Q_1 — if $Q_0 = |0\rangle$: $|0\rangle \mapsto |0\rangle$, $|1\rangle \mapsto |1\rangle$
if $Q_0 = |1\rangle$: $|0\rangle \mapsto |1\rangle$, $|1\rangle \mapsto |0\rangle$

Then $$|\psi_2\rangle = CNOT(|\psi_1\rangle) = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

Notice this is β_0 ie, a Bell state or an EPR pair.

1349 We obviously cannot do such manipulations in ~~the~~ this lab, however, we can model a CNOT gate as follows.

If we model our groundstate as pre π-pulse, then π-pulse $= \hat{X}$ gate

→

$\longrightarrow$

~~...~~

1351 I would like to see if we can take a measurement and if the state was ~~?~~ in $|0\rangle$ or $|1\rangle$.

1352 An ideal π-pulse has no FID, but this is not ideal. If we interrogate the spin w/ a $\frac{\pi}{2}$ pulse, we may see ~~see~~ a difference b/w a $|0\rangle$ and $|1\rangle$.

1354 Data obtained looks normal (spin Echo). ~~looks long~~ ~~?~~ ~~a~~ when ~~l_π then a $l_{\pi/2}$~~.

$\uparrow$
$|1\rangle$

$$l_\pi - \tau - l_{\pi/2} - \boxed{\pi}$$

We may also try $l_\pi - \tau - l_\pi - l_{\pi/2} - \boxed{\pi}$

1358 Nothing observed (need a better way to implement).

1359 ~~Maybe~~ we can try a $\hat{H}$ gate

$$\hat{H} = \frac{\hat{X} + \hat{Z}}{\sqrt{2}} \qquad \hat{X}\hat{Z} = [\,\cdot\,][\,\cdot\,]$$

$= ~~[\ldots]~~$

~~?~~ $\hat{X} = \hat{H}\hat{Z}\hat{H}$

Not today ~~a~~, ~~?~~ will think more, for now need to get back on track.

1400 Done for today, turning off equipment. Taking ~~a~~ op-amp circuit to debug.

1402 Signing out of lab ~~?~~

5-03-04

1920 Signing in.

1923 ~~Lo~~ Objectives:

1. Discuss Applications of NMR from a few papers.
   - ↳ NMR (MRI) in Medicine
   - ↳ Quantum computing.

1927 Given my background, I will first start w/ a review for Quantum (α) Computing.

1927 From [6] it was reported that "143 is the largest number yet factorized by a Quantum Algorithm." what does this actually mean and what does it have to do w/ NMR?

1937 In general, the problem of factoring is not so glorious, it is what one of the first things we're taught in our schooling. Factoring 36 for instance is not so impressive: (1, 36), (2, 18), (3, 12), (4, 9) and (6, 6). However, most of modern encryption is built on the idea that it is really really hard to factor prime numbers. For composite numbers (like 36) we may use techniques such as the Seive or Erathones or Probablistic Factoring Algorithms to achieve factorizations. ~~ta~~ It is also not so difficult to check if a number is idead prime. Wilson's Algorithm, for instance, is a deterministic test that can verify a number is prime in $O(n^2)$ time complexity.

~~How~~

2011 However, as the size of the numbers scale, it becomes increasingly complex to factorize these numbers. Encryption methods (for instance RSA or SHA256) take two large primes and ~~factorize the~~ multiply them to obtain a composite number with only two factors (other than one and itself), which are two primes.

2020 "When an integer reaches more than 100,000 or so digits, it becomes too complex to ~~factorize~~ ~~Classically~~ solve using classical computing methods." [6]. Quantum Computers on the other hand have some "slick tricks" which they can use to overcome this hurdle.

2023 Shor's Algorithm, probably the most famous Quantum Algorithm ~~other~~ ~~only~~ (apart from maybe Grover's Algorithm) utilizes ~~the~~ special ~~ext~~ features exclusive to Quantum Computing like entanglement to leverage the "Quantum Advantage"

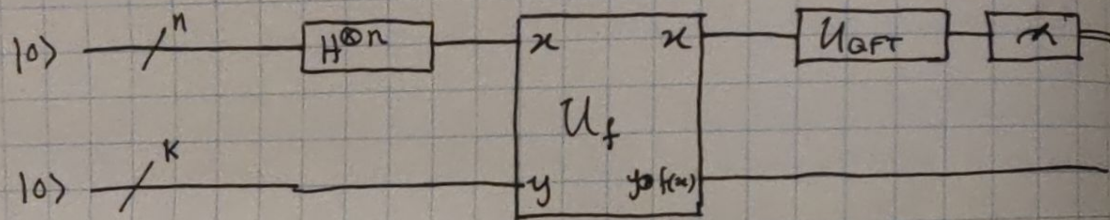
→

2024 Shor's Algorithm effectively works as follows:

Let $N = ab$, select c such that c is coprime to $M = (a-1)(b-1)$.
Now, compute d such that $c \cdot d \bmod M = 1$

Choose d which is coprime to N $(\gcd(d,N) = 1)$. Then $f_{N,d} = d$
which is periodic with period p. Then, we may find that
Either $\gcd(d^{p/2}+1, N)$ or $\gcd(d^{p/2}-1, N)$ is a factor of N.

2044 And the corresponding circuit diagram [7]:



2054 I will not be going in depth into how the Ansatz or Oracle work in this case.

2105 It was found, as highlighted by the article, that in 2001, E. Farhi proposed an algorithm known as AQC or Adiabatic Quantum computing.

2107 Unlike Shor's Algorithm, AQC relies on quantum adiabatic processes which all possible solutions to the factoring problem are encoded as Eigenstates to our problem Hamiltonian.

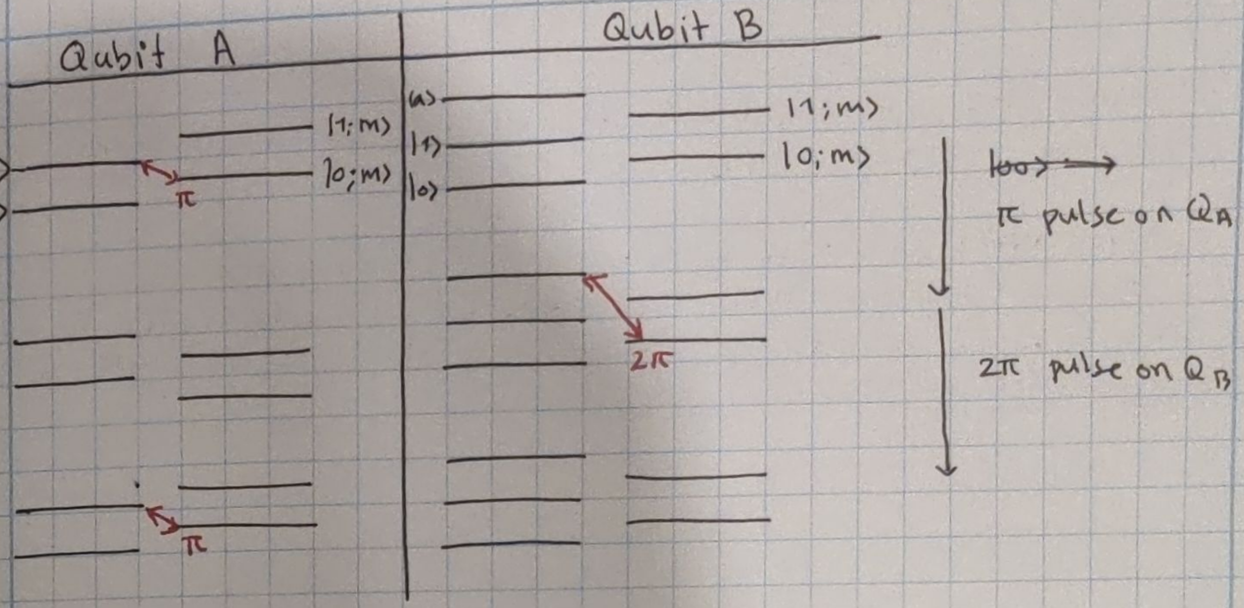
2111 In the Physical implementation, NMR is used to gradually evolve the Hamiltonian to solve the factoring problem

2137 I realize now that this article does not go nearly in depth enough to explain how NMR works in this context, so I will attempt to supplement.

2140 One implementation of gate operations utilizes the energy spin states to encode our Qbit implementation.

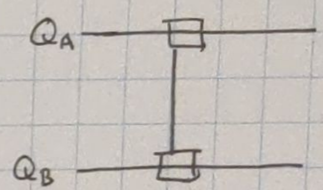
2141 Consider the following implementation of a CZ gate.

142



$|00\rangle \rightarrow |00\rangle \longrightarrow |00\rangle \longrightarrow |00\rangle$
$|01\rangle \rightarrow |01\rangle \longrightarrow |01\rangle \longrightarrow |01\rangle$
$|10\rangle \longrightarrow |00;m\rangle \longrightarrow -|00;m\rangle \longrightarrow |10\rangle$
$|11\rangle \longrightarrow |01;m\rangle \longrightarrow |01;m\rangle \longrightarrow -|11\rangle$

=



2158 Note the above is ~~here~~. for a Trapped Ion system. Notice the use of π and 2π pulses to manipulate b/w energy states and moving states (denoted by the m). In this way we can use NMR-esque techniques to implement 2-qubit gates and other unitary operations.

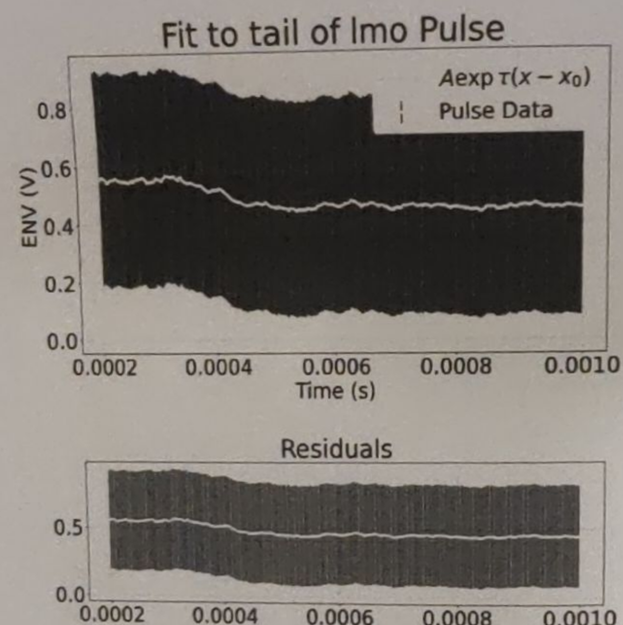
2243 signing out. AT

2025-03-05

1417 Signing in

1419 Continuing Analysis of collected data on LMO, HMO, and d-H_2O from yesterday (2025-03-04).

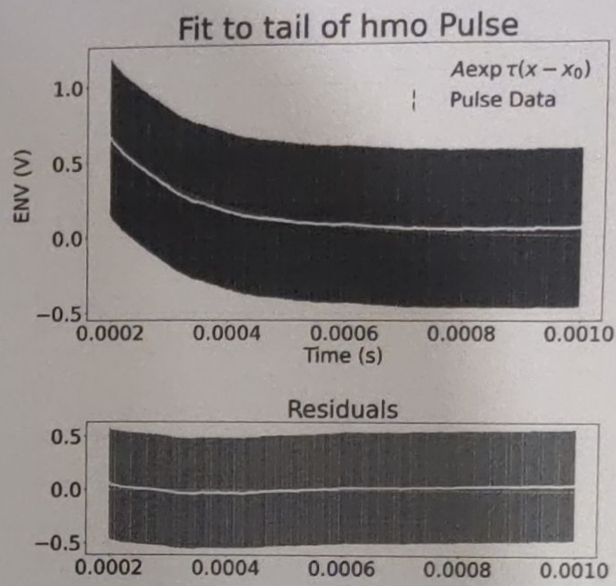
1425 I have realized an error in my data collection, I only took one τ for each measurement, making it impossible to properly fit T_1 and T_2. I can still get an estimate using my FID code from earlier perhaps.



03.05

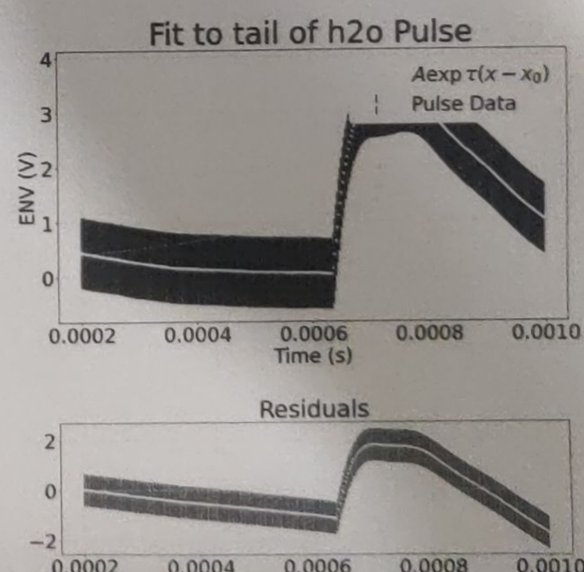
FIGURE 03.04A.1: $A = 125.02730736861422 \pm inf$, $\tau = -159.21440895422927 \pm inf$, $x_0 = -0.711144259571313 \pm inf$ $\chi^2_{red} = 2.0$

1445 Note that due to personal time constraints most of these plots are not optimized. Especially Fig 03.05C.1 seems to be fit to the wrong dataset.



03.05

FIGURE 03.05B.1: $A = 0.0 \pm 9000.0$, $\tau = -5456.4 \pm 90.0$, $x_0 = 0.0 \pm 200.0$, $\chi^2_{\text{red}} = 0.003$



03.05

FIGURE 03.05C.1: $A = 0.650974392642326 \pm 1436422.7844434683$, $\tau = 2345.446650108936 \pm 224.61004122688507$, $x_0 = 0.0003897026532702442 \pm 937.2177888340759$, $\chi^2_{\text{red}} = 2.0$

1510 Finally I will briefly discuss what I should've done.
Namely 1 kind. set 5 C pendulums and varied them

1511 This would have given me sufficient data to properly calculate
T_1 and T_2 as currently my datasets, and ~~test~~ time are too
restricted to get meaningful results.

1513 I will comment that the uncertainties in Fig 03.05A.1,
Fig 03.05B.1, and Fig 03.05C.1 are quite unrealistic. Here,
my methodology was simply based off of the noise and taking the
min and max of these noisy ~~[illegible]~~ areas.

1517 Likely, taking ~~and~~ another ~~#~~ FFT and taking the higher
order parameters may have been a better method for such
analysis of uncertainties.

1521 One primary error was ~~[illegible]~~ not realizing I had an ~~[illegible]~~ incorrect
resonance condition early on. This lead to rushed final data
collection, ~~and~~ ~~Th~~ Should ~~have~~ have been more time, I would
have realized my mistake sooner and taken more data

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
"""
Created on Tue Feb 25 10:25:15 2025

@author: Aditya K. Rao
@github: @adirao-projects
"""

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import toolkit as tk
import toolkitnew as tkn

def load_data(csvname):
    # ch1 is ENV out
    # ch2 is Q out
    # ch3 is I out

    df = pd.read_csv(csvname, names=['Time', 'ENV', 'Q', 'I'], skiprows=2)
    df_units = {'Time':'s', 'ENV':'V', 'Q':'V', 'I':'V'}
    return df, df_units

def pulse(x, y0, x0, w0, h, tau):
    if x<=x0:
        return 0

    elif x<=w0:
        return h

    else:
        return h*np.exp((x-w0)*tau)+y0


def fiteqn(t, M0, T1):
    return M0*(1-np.exp(-t/T1))

def get_uncert(df):
    df_ = df.where(df['Time']<0)
    df['uENV'] = df_['ENV'].max()-df_['ENV'].min()
    df['uQ'] = df_['Q'].var()
    df['uI'] = df_['I'].var()

    return df


def fidcalc(df, units, name):
    df = df[df['Time']<0.001]
    df = df[df['Time']>=2e-4]

    meta = {'title':f'Fit to tail of {name} Pulse',
            'xlabel':'Time (s)',
            'ylabel':'ENV (V)',
            'fit-label': r"$A\exp{\tau(x-x_0)}$",
            'data-label': "Pulse Data",
            'loc':'upper right',
            'save-name':f'{name}fid'}
```

```
tkn.quick_analyze(df['Time'], df['ENV'], yerr=df['uENV'], fit_type='exp',
                  res=True, chi=True, guess=(1.75, -100, 0.00025),
                  meta = meta, show=True, save=True, dataout=True,
                  params=('A', r'\tau', 'x_0'), rounding=False)


def t1calc(df, units, name):
    df = df['Time']<0.001
    df = df[df['Time']>=2e-4]
    vpulse = np.vectorize(pulse)

    meta = {'title':f'Fit to tail of {name} Pulse',
            'xlabel':'Time (s)',
            'ylabel':'ENV Voltage (V)',
            'fit-label': r"$M_0(1 - \exp{-\frac{t}{T_1}})$",
            'data-label': "Pulse Data",
            'loc':'upper right',
            'save-name':f'{name}.png'}

    tkn.quick_analyze(df['Time'], df['ENV'], xerr=df['uENV'], fit_type='custom',
                      model_function_custom = fiteqn, res=True, chi=True,
                      meta = meta, show=True, save=True, dataout=True,
                      params=('A', r'\tau', 'x_0'))


def t2calc(df, units, name):
    df = df[df['Time']<0.001]
    df = df[df['Time']>=2e-4]
    vpulse = np.vectorize(pulse)

    meta = {'title':f'Fit to tail of {name} Pulse',
            'xlabel':'Time (s)',
            'ylabel':'ENV (V)',
            'fit-label': r"$A\exp{\tau(x-x_0)}$",
            'data-label': "Pulse Data",
            'loc':'upper right',
            'save-name':f'{name}'}

    tkn.quick_analyze(df['Time'], df['ENV'], xerr=df['uENV'], fit_type='exp',
                      res=True, chi=True, guess=(1.75, -100, 0.00025),
                      meta = meta, show=True)


if __name__ == '__main__':


    hmo = ['../Data/hmo1.csv', '../Data/hmo2.csv', '../Data/hmo3.csv']
    lmo = ['../Data/lmo1.csv', '../Data/lmo2.csv', '../Data/lmo3.csv']
    h2o = ['../Data/h2o1.csv', '../Data/h2o2.csv', '../Data/h2o3.csv']

    for sample_nam, sample_dat in zip(('hmo', 'lmo', 'h2o'), (hmo, lmo, h2o)):
        for data_type, data_path in zip(('pi2', 'pi', 'pipi2'), sample_dat):
            df, units = load_data(data_path)
            df = get_uncert(df)
            df = df.dropna()

            if data_type == 'pipi2':
                pass
```

```
    #tIcalc(df, units, sample_nam)

elif data_type == 'pi2':
    fidcalc(df, units, sample_nam)
```

```python
# -*- coding: utf-8 -*-
"""
Created on Tue Jan 23 12:34:34 2024
Updated on Mon Oct 14 21:22:09 2024
Updated on Mon Feb 10 09:51:03 2025
Updated on Sat Mar 01 21:03:54 2025
Updated on Mon Mar 03 14:45:13 2025

Lab Toolkit

@author: Aditya K. Rao
@github: @adirao-projects
"""
import numpy as np
from scipy.optimize import curve_fit
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec
import os
import math
import textwrap

#from uncertainties import ufloat

font = {'family' : 'DejaVu Sans',
        'size'   : 30}

plt.rc('font', **font)

def fit_data(xdata, ydata, fit_type, override=False,
             override_params=(None,), uncertainty=None,
             res=False, chi=False, uncertainty_x=None,
             model_function_custom=None, guess=None):

    def chi_sq_red(measured_data:list[float], expected_data:list[float],
            uncertainty:list[float], v: int):
        if type(uncertainty)==float:
            uncertainty = [uncertainty]*len(measured_data)
        chi_sq = 0

        # Converting summation in equation into a for loop
        # for i in range(0, len(measured_data)):
        #     chi_sq += (pow((measured_data[i] \
        #           - expected_data[i]),2)/(uncertainty[i]**2))

        for m, e, u in zip(measured_data, expected_data, uncertainty):
            chi_sq += ((m-e)/u)**2

        chi_sq = (1/v)*chi_sq

        return chi_sq


    def residual_calculation(y_data: list, exp_y_data) -> list[float]:
        residuals = []
        for v, u in zip(y_data, exp_y_data):
            residuals.append(u-v)

        return residuals
```

```
def model_function_linear_int(x, m, c):
    return m*x+c

def model_function_exp(x, a, b, c):
    return a*np.exp(b*(x-c))

def model_function_log(x, a, b):
    return b*np.log(x+a)

def model_function_linear_int_mod(x, m, c):
    return m*(x+c)

def model_function_linear(x, m):
    return m*x

def model_function_xlnx(x, a, b, c):
    return b*x*(np.log(x)) + c

def model_function_ln(x, a, b, c):
    return b*(np.log(x)) + c

def model_function_sqrt(x, a):
    return a*np.sqrt(x)

model_functions = {
    'linear' : model_function_linear,
    'linear-int' : model_function_linear_int,
    'xlnx' : model_function_xlnx,
    'log' : model_function_log,
    'exp' : model_function_exp,
    'custom' : model_function_custom
    }

try:
    model_func = model_functions[fit_type]

except:
    raise ValueError(f'Unsupported fit-type: {fit_type}')


if not override:
    new_xdata = np.linspace(min(xdata), max(xdata), num=100)


    if type(uncertainty) == int:
        abs_sig =True
    else:
        abs_sig = False

    if guess is not None:
        popt, pcov = curve_fit(model_func, xdata, ydata, sigma=uncertainty,
                        maxfev=20000, absolute_sigma=abs_sig, p0=guess)
    else:
        popt, pcov = curve_fit(model_func, xdata, ydata, sigma=uncertainty,
                        maxfev=20000, absolute_sigma=abs_sig)
    param_num = len(popt)
```

```python
    meta = {'title' : 'INSERT-TITLE',
            'xlabel' : 'INSERT-XLABEL',
            'ylabel' : 'INSERT-YLABEL',
            'chisq' : 0,
            'fit-label': "Best Fit",
            'data-label': "Data",
            'save-name' : 'IMAGE',
            'loc' : 'lower right'}

main_fig.set_title(meta['title'], fontsize = 46)
if len(uncertainty_x)==0:
    main_fig.errorbar(xdata, ydata, yerr=uncertainty, #xerr=uncertainty_x,
                      markersize='4', fmt='o', color='red',
                      label=meta['data-label'], ecolor='black')
else:
    main_fig.errorbar(xdata, ydata, yerr=uncertainty, xerr=uncertainty_x,
                      markersize='4', fmt='o', color='red',
                      label=meta['data-label'], ecolor='black')

main_fig.plot(plot_x, plot_y, linestyle='dashed',
              label=meta['fit-label'])

main_fig.set_xlabel(meta['xlabel'])
main_fig.set_ylabel(meta['ylabel'])
main_fig.legend(loc=meta['loc'])

if res:
    res_fig.errorbar(xdata, residuals, markersize='3', color='red', fmt='o',
                     yerr=uncertainty, ecolor='black', alpha=0.7)
    res_fig.axhline(y=0, linestyle='dashed', color='blue')
    res_fig.set_title('Residuals')

if save:
    plt.savefig(f"figures/{meta['save-name']}")

if show:
    plt.show()

def block_print(data: list[str], title: str, delimiter='=') -> None:
    """
    Prints a formated block of text with a title and delimiter

    Parameters
    ----------
    data : list[str]
        Text to be printed (should be input as one block of text).
    title : str
        Title of the data being output.
    delimiter : str, optional
        Delimiter to be used. The default is '='.

    Returns
    -------
    None.

    Examples
    --------
    >>> r_log = 100114.24998716781
```

```
    >>> r_dec = 0.007422298127465114
    >>> data = [f'r^2 value (log): {r_log}',
                f'r^2 value (real): {r_dec}']
    >>> block_print(data, 'Regression Coefficient', '=')
    ============================ Regression Coefficient ============================
    r^2 value (log): 100114.24998718781
    r^2 value (real): 0.007422298127465114
    ================================================================================
    """
    term_size = os.get_terminal_size().columns

    breaks = 1
    str_len = len(title)+2
    while  str_len >= term_size:
        breaks += 1
        str_len = math.ceil(str_len/2)


    str_chunk_len = math.ceil(len(title)/breaks)
    str_chunks = textwrap.wrap(title, str_chunk_len)
    output = ''
    for chunk in str_chunks:
        border = delimiter*(math.floor((term_size - str_chunk_len)/2)-1)
        output = f'{border} {chunk} {border}\n'

    output=output[:-1]

    output+= '\n'+ '\n'.join(data) + '\n'
    output+=delimiter*term_size

    print(output)

def quick_analyze(xdata, ydata, fit_type, model_function_custom=None,
                  yerr=None, xerr=[], res=False, chi=False, guess=None,\
                  save=False, meta=None, dataout=False, params=None,
                  rounding=True, show=False):


    data = fit_data(xdata, ydata, fit_type=fit_type, uncertainty=yerr,
                    chi=chi, res=res, guess=guess,
                    model_function_custom=model_function_custom)

    plot_data(xdata, ydata, data['plotx'], data['ploty'],
              residuals=data['residuals'], uncertainty=yerr,
              uncertainty_x=xerr, res=res, save=save, meta=meta,
              show=show)

    if dataout:
        with open(f'figures/{meta["save-name"]}.dat', 'w') as f:
            for n, t, d in zip(params,  data['popt'], data['pstd']):
                if rounding:
                    d = round(d, -int(np.floor(np.log10(np.abs(d)))))
                    dp = len(str(d).split(".")[1])
                    t = round(t, dp)

                f.write(f'{n} : ${n} = {t} \pm {d}$\n')

            chisq = round(data['chisq'], \
```

```
        -int(np.floor(np.log10(np.abs(data['chisq'])))))
    f.write(r'chisq : $\chi^2_{\text{red}}$ = ' + str(chisq) + '\n')


def param_print(names, popt, pstd, latex=True):
    """
    Prints all parameters for easy input into a LaTeX document.

    Parameters
    ----------
    names : list[str]
        Symbols/Names of each parameter
    popt : list[float]
        Value of each parameter.
    pstd : list[float]
        Standard deviation/uncertainty associated with each parameter.
    latex : bool, optional
        Print in LaTeX format. The default is True.

    Returns
    -------
    None.
    """

    data = []
    for n, t, d in zip(names, popt, pstd):
        if latex:
            data.append(f'${n} = {t} \pm {d}$')

        else:
            data.append(f'{n} = {t} +/- {d}')
    block_print(title='Paramters', data=data)


def numerical_methods(method_type, args=None, custom_method=None):
    def gaussxw(N):

        # Initial approximation to roots of the Legendre polynomial
        a = np.linspace(3,4*N-1,N)/(4*N+2)
        x = np.cos(np.pi*a+1/(8*N*N*np.tan(a)))

        # Find roots using Newton's method
        epsilon = 1e-15
        delta = 1.0
        while delta>epsilon:
            p0 = np.ones(N,float)
            p1 = np.copy(x)
            for k in range(1,N):
                p0,p1 = p1,((2*k+1)*x*p1-k*p0)/(k+1)
            dp = (N+1)*(p0-x*p1)/(1-x*x)
            dx = p1/dp
            x -= dx
            delta = max(abs(dx))

        # Calculate the weights
        w = 2*(N+1)*(N+1)/(N*N*(1-x*x)*dp*dp)
```

```
    return x, w

def gaussxwab(N,a,b):
    x,w = gaussxw(N)
    return 0.5*(b-a)*x+0.5*(b+a),0.5*(b-a)*w

methods = {
'gausswx' : gaussxw,
'gaussxwab' : gaussxwab,
'custom' : custom_method
}

try:
    method = methods[method_type]

except:
    raise ValueError(f'Unsupported method-type: {method_type}')

return method(*args)


def interpolation_methods(method_type, args=None, custom_method=None):

    methods = {
    'custom' : custom_method
    }

    try:
        method = methods[method_type]

    except:
        raise ValueError(f'Unsupported method-type: {method_type}')

    return method(*args)
```

```python
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
"""
Created on Tue Feb 25 10:25:15 2025

@author: Aditya K. Rao
@github: @adirao-projects
"""

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import toolkit as tk
import toolkitnew as tkn

def load_data(csvname):
    # ch1 is ENV out
    # ch2 is Q out
    # ch3 is I out

    df = pd.read_csv(csvname, names=['Time', 'ENV', 'Q', 'I'], skiprows=2)
    df_units = {'Time':'s', 'ENV':'V', 'Q':'V', 'I':'V'}
    return df, df_units

def pulse(x, y0, x0, w0, h, tau):
    if x<=x0:
        return 0

    elif x<=w0:
        return h

    else:
        return h*np.exp((x-w0)*tau)+y0

def get_uncert(df):
    df_ = df.where(df['Time']<0)
    df['uENV'] = df_['ENV'].max()-df_['ENV'].min()
    df['uQ'] = df_['Q'].var()
    df['uI'] = df_['I'].var()

    return df

def get_t1(df, units, name):
    df = df[df['Time']<0.001]
    df = df[df['Time']>=2e-4]
    vpulse = np.vectorize(pulse)

    # data = tk.curve_fit_data(df['Time'], df['ENV'], uncertainty=df['uENV'],
    #                          fit_type='custom', chi=False, res=True,
    #                          model_function_custom=vpulse,
    #                          guess=(0.05, 0.00005, 0.0002, 1.75, -0.0001))
    data = tk.curve_fit_data(df['Time'], df['ENV'], uncertainty=df['uENV'],
                             fit_type='exp', chi=True, res=True,
                             guess=(1.75, -100, 0.00025))

    print(data['popt'])
```

```python
    meta = {'title':f'Fit to tail of {name} Pulse',
            'xlabel':'Time (s)',
            'ylabel':'ENV (V)',
            'fit-label': r"$A\exp{\tau(x-x_0)}$",
            'data-label': "Pulse Data",
            'loc':'upper right',
            'save-name':f'{name}.png'}

    # tk.block_print(data=[f"Chi:{data['chisq']}\pm", f"A:{data['popt'][0]}",
    #                      f"B:{data['popt'][1]}", f"x_0:{data['popt'][2]}"],
    #               title='Fit Parameters')
    tk.parameter_print(['A', r'\tau', 'x_0'], data['popt'], data['pstd'])

    print(r'\chi^2_{\text{red}}='+str(data['chisq']))
    print(f"T_1 = {np.abs(1/data['popt'][1])}")
    tk.quick_plot_residuals(df['Time'], df['ENV'],
                            data['plotx'], data['ploty'],
                            uncertainty=df['uENV'],
                            residuals=data['residuals'],
                            meta=meta)


def get_tinew(df, units, name):
    df = df[df['Time']<0.001]
    df = df[df['Time']>=2e-4]
    vpulse = np.vectorize(pulse)

    meta = {'title':f'Fit to tail of {name} Pulse',
            'xlabel':'Time (s)',
            'ylabel':'ENV (V)',
            'fit-label': r"$A\exp{\tau(x-x_0)}$",
            'data-label': "Pulse Data",
            'loc':'upper right',
            'save-name':f'{name}.png'}

    tkn.quick_analyze(df['Time'], df['ENV'], xerr=df['uENV'], fit_type='exp',
                      res=True, chi=True, guess=(1.75, -100, 0.00025),
                      meta = meta)

def get_fft(df):
    print('here')

    print(df['I'].head())

    i_dat = df['I'].to_numpy()



    #df.plot(x='Time', y='Q')

    i_fft = np.fft.rfft(i_dat)
    res = df['Time'].iloc[1] - df['Time'].iloc[0]
    #print(q_fft)
    #print(res)


    print(i_dat.shape[0])

    freq = np.fft.rfftfreq(i_dat.shape[0], res)
```

```
#freq = np.arange(0, i_dat.shape[0], res)

plt.plot(freq, np.abs(i_fft), color='black')

i_dat_new = i_dat - np.mean(i_dat)

i_fft_new = np.fft.rfft(i_dat_new)

i_fft_new_abs = np.abs(i_fft_new)

plt.plot(freq, i_fft_new_abs, color='black', linestyle='dashed')

#imax = np.max(i_fft_new_abs)

fmax = np.argmax(i_fft_new_abs)


print(freq[fmax])

print(20.9e6 + freq[fmax])
print(20.9e6 - freq[fmax])


plt.show()

if __name__ == '__main__':
    df_hmo1, units_hmo1 = load_data('../Data/heavyminoil.csv')
    #df_hmo1.plot(x='Time', y='ENV', legend=False, grid='on',
    #             title='Raw Pulse Data for Heavy Mineral Oil',
    #             xlabel='Time (s)', ylabel='ENV (V)', figsize=(14, 8))
    df_hmo1 = get_uncert(df_hmo1)

    #get_fft(df_hmo1)

    #print(df_hmo1.head())

    #t1_hmo1new = get_t1new(df_hmo1, units_hmo1, 'Heavy Mineral Oil')
    t1_hmo1 = get_t1(df_hmo1, units_hmo1, 'Heavy Mineral Oil')

    #df_lmo1, units_lmo1 = load_data('../Data/lightminoil.csv')
    #df_lmo1.plot(x='Time', y='ENV')
```

```python
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
"""
Created on Tue Mar 04 13:28:27 2025

@author: Aditya K. Rao
@github: @adirao-projects
"""

import pandas as pd

def load_data(name):
    df = pd.read_csv(f'{name}.csv', names=['Time', 'ENV', 'Q', 'I'], skiprows=2)
    return df

def get_uncert(df):
    df_ = df.where(df['Time']<0)
    df['uENV'] = df_['ENV'].max()-df_['ENV'].min()
    df['uQ'] = df_['Q'].var()
    df['uI'] = df_['I'].var()

    return df


def plot(df, name):
    sig = df.plot(x='Time', y='ENV', legend=False, grid='on',
                  title='Raw Pulse Data', color=['black'],
                  xlabel='Time (s)', ylabel='Observed Voltage (V)',
                  figsize=(14, 8)).get_figure()


    dif = df.plot(x='Time', y='I', legend=False, grid='on',
                  title='Raw Pulse Data', color=['black'],
                  xlabel='Time (s)', ylabel='Difference Voltage (V)',
                  figsize=(14, 8)).get_figure()


    sig.savefig(f'{name}sig')
    dif.savefig(f'{name}dif')

if __name__ == '__main__':
    # LMO : 56, 57, 58
    # HMO : 60, 61, 62
    # H20 : 64, 65, 66
    scope_files = ['56', '57', '58', '60', '61', '62', '64', '65', '67', '68']
    #scope_files = ['46', '47', '48', '49']
    for scp in scope_files:
        df = load_data(f"scope_{scp}")
        plot(df, scp)
```