BLOCH EQUATION COMPUTATIONAL SIMULATION AND LOW FIELD STRENGTH NMR

Harvard College CHEM 10

Abel Bellows

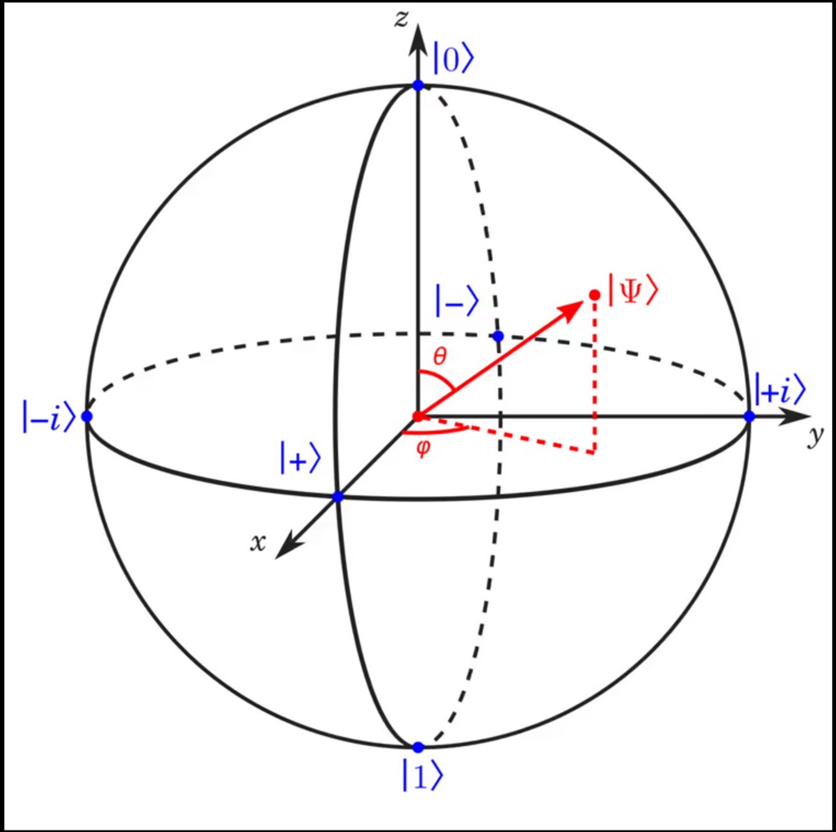
Content

Basics of Spin

- Fundamental particles have "Spin."
- Spin can be measured in x,y, and z directions.
- The nuclei of atoms also have spin.

Bloch Sphere

- Spin state can be represented as a linear combination of x,y, and z spin wavefunctions.
- Represented as vectors with head on a unit sphere.
- Bloch Sphere



Bloch Sphere

$$\frac{N_m}{N} = \exp\left(\frac{-E_m}{k_B T}\right) \Big/ \sum_{m=-I}^{I} \exp\left(\frac{-E_m}{k_B T}\right)$$

$$\approx \frac{1}{2I+1}\left(1 + \frac{m\hbar\gamma B_0}{k_B T}\right),$$

$$M_0 = \gamma\hbar \sum_{m=-I}^{I} m N_m$$

- The relative population of protons in spin state m (N_m) is given by the Boltzmann distribution.
- At $T = 398K$ spins are evenly distributed
  - $thermal\ E \gg \hbar m\gamma$

- The net magnetization ($\boldsymbol{M_0}$) of the sample is the sum of the magnetic moments of the protons in the population
- $\boldsymbol{M_0}$ is a vector on a Bloch Sphere.

$$\frac{d\mathbf{M}(t)}{dt} = \mathbf{M}(t) \times \gamma \mathbf{B}(t).$$

- $\frac{dM(t)}{dt}$ in external magnetic field B is given by the torque applied to M(t) by B.

$$\omega_0 = -\gamma B_0.$$

- If $B(t) = B_0$ M processes with frequency equal to w_0

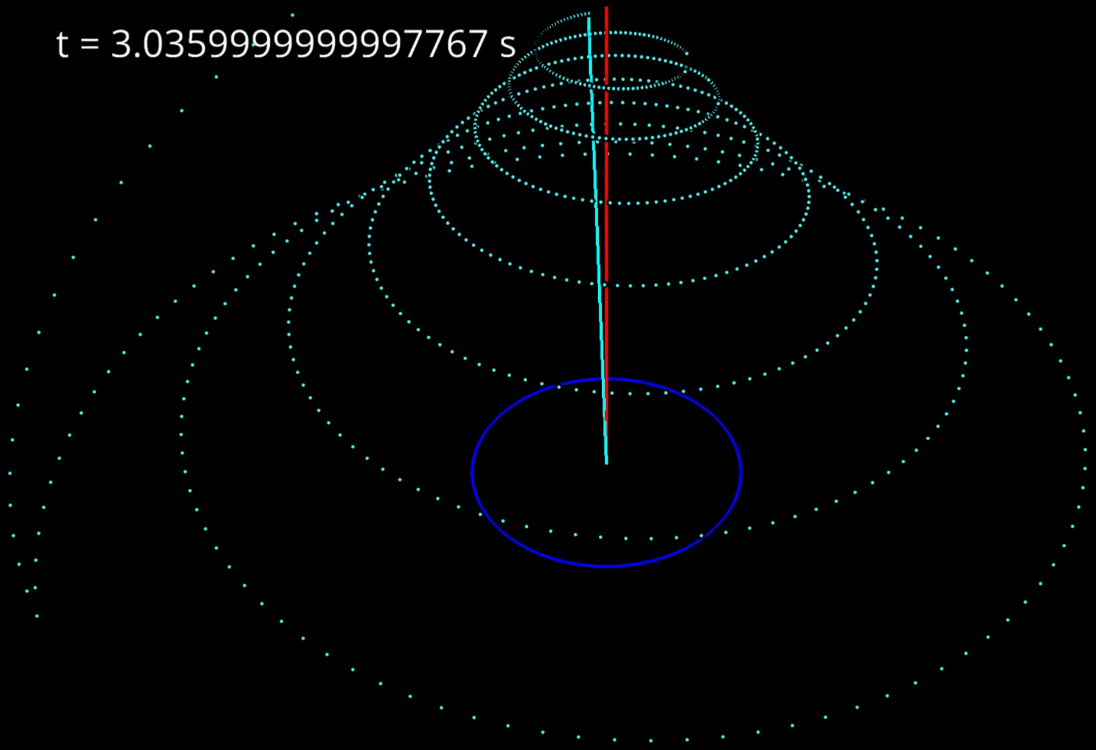
In a completely stable system, $\boldsymbol{M}$ would process around $\boldsymbol{B}$ without decay.

Since "thermal equilibrium must be re-established," the Bloch Equations give us a way to model how $\boldsymbol{M}(t)$ returns to equilibrium.

$$\frac{dM_x(t)}{dt} = \gamma\Big[\mathbf{M}(t) \times \mathbf{B}(t)\Big]_x - R_2 M_x(t)$$
$$= \gamma\Big[M_y(t)B_z(t) - M_z(t)B_y(t)\Big] - R_2 M_x(t),$$
$$\frac{dM_y(t)}{dt} = \gamma\Big[\mathbf{M}(t) \times \mathbf{B}(t)\Big]_y - R_2 M_y(t)$$
$$= \gamma\Big[M_z(t)B_x(t) - M_x(t)B_z(t)\Big] - R_2 M_y(t),$$
$$\frac{dM_z(t)}{dt} = \gamma\Big[\mathbf{M}(t) \times \mathbf{B}(t)\Big]_z - R_1\Big[M_z(t) - M_0\Big]$$
$$= \gamma\Big[M_x(t)B_y(t) - M_y(t)B_x(t)\Big] - R_1\Big[M_z(t) - M_0\Big],$$

R_1: Spin-lattice relaxation rate constant (**how fast does the spin distribution return to Boltzmann**)

R_2: Spin-spin relaxation rate constant (**How fast do the spins relax in the plane transverse to B**)



Bloch Procession

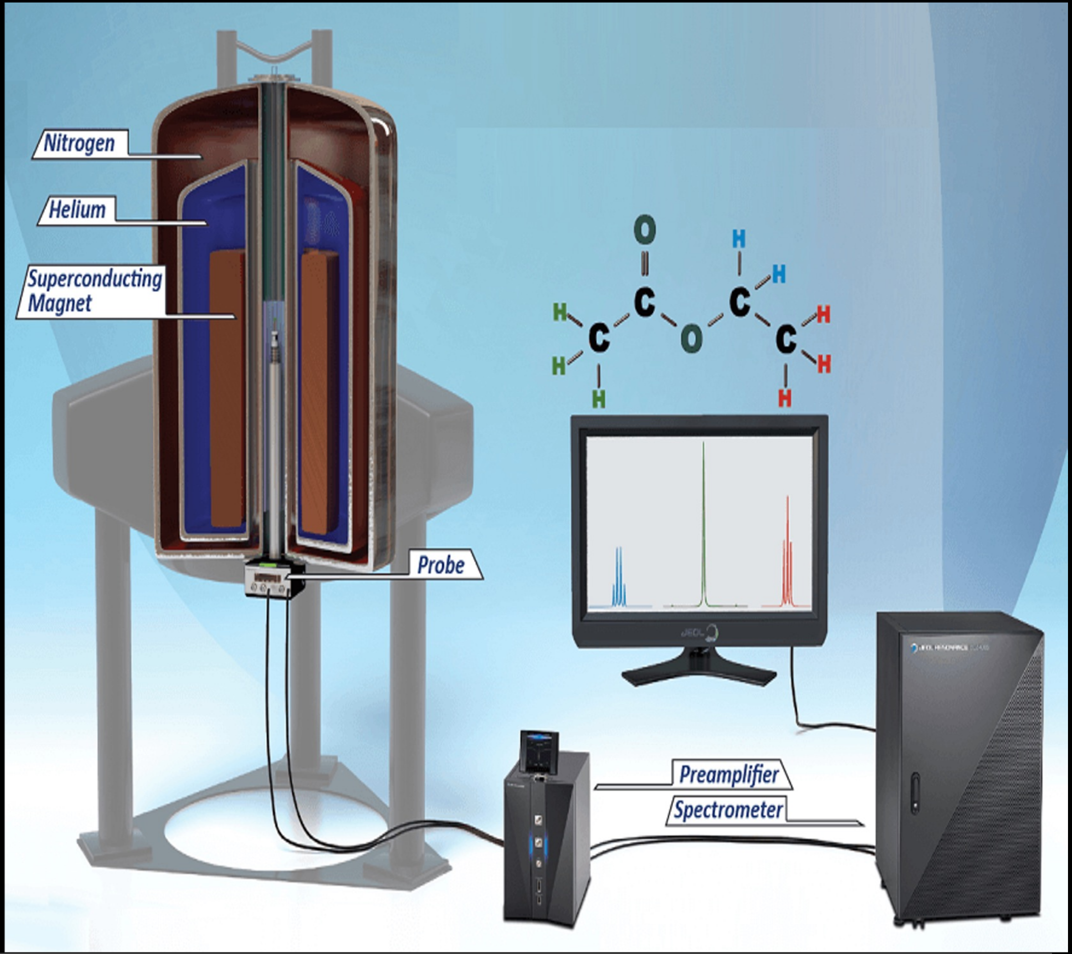
Green: $\boldsymbol{M}$
Red: $\boldsymbol{B_0}$

How can we use Bloch Procession to study molecules?

- $R1$ and $R2$ are determined by the chemical environment around a nucleolus. If we could measure the procession of **M**, we could learn about a nucleus' position in a molecule.

NMR Machines

- A sample is placed in a strong B field of around 10T
- The effective B field is temporarily changed by applying an RF pulse
- The RF pulse knocks down $\boldsymbol{M}$
- $\boldsymbol{M}$ processes around B according to the Bloch Equations.
- The changing emf is converted into an electric signal



Fast Fourier Transform (FFT) of Free Induction Decay (FID) signal is the NMR spectrum. Its peaks reveal the chemical structure of a given molecule.

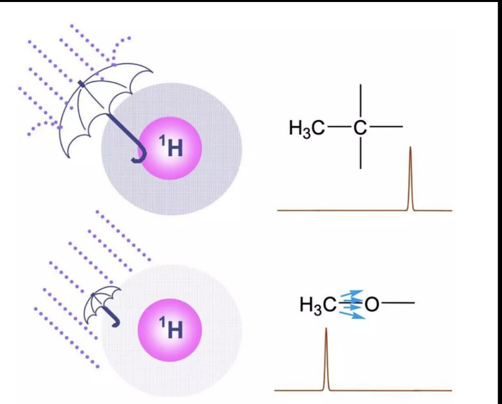
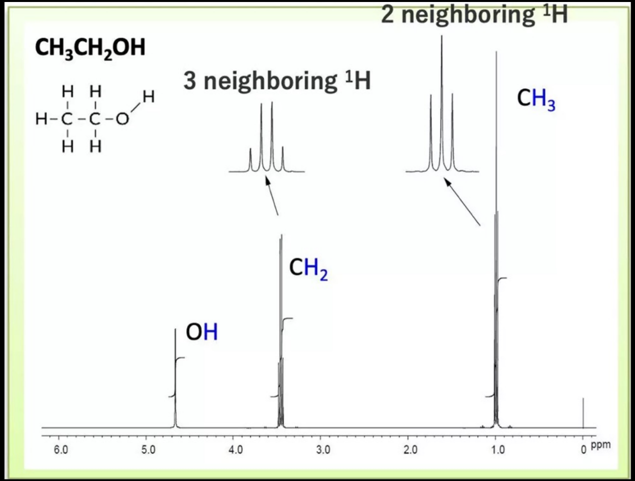


Fig. 2 Difference of strength of shielding the magnetic field



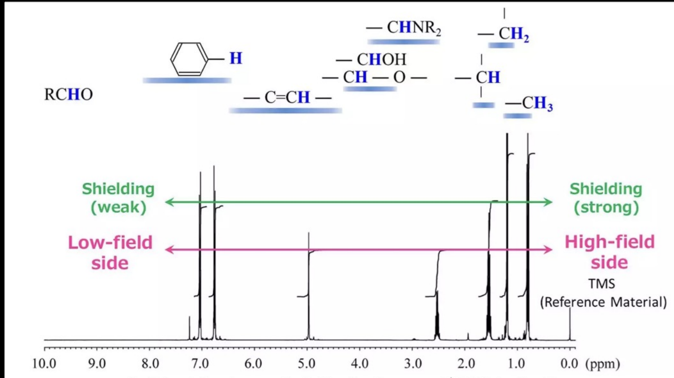


Fig. 3 Correlation diagram of typical functional groups and ¹HNMR signal positions

Computational Bloch Equation/NMR Simulator

- Demonstrates behavior of processing $\boldsymbol{M}$ in NMR machine
- Configure all aspects of the device including $B\_DEV, M, T1, T2$
- Send RF pulses with specified $\mathrm{B}_{\mathrm{effective}}$
- Source code and detailed instructions at https://github.com/abellows50/CHEM10_NMR_PROJECT

README

NMR Machine Simulator

Purpose

To demonstrate the macroscopic behavior of M in an NMR machine and to make clear the workflow of NMR analysis, I constructed a simulator of Bloch Equations. The user can configure all aspects of the device including B_DEV, M, T1, T2, and can send RF pulses with a specific applied magnetic field.

Usage

Python Enviroment Configuration

To setup the python enviroment, first create your venv by running `python3 -m venv venv` then activate your venv by running `source venv/bin/activate`. Install all of the required packages by running `pip3 install -r requirements.txt`.

Start the program

To run the simulator run `python3 NMR_SIM.py`. You may want to use a screen split function so that you can see all 4 windows at one time.

Configure simulation

To configure enromental variables of the simulator, use the `config` command in the command console. You can configure the magnetic field of the device (`B_DEV`), T1 and T2 (`T1` and `T2`), and net starting magnetization (`M`) with the following commands

1. `config B_DEV <Bx> <By> <Bz>`
2. `config M <Bx> <By> <Bz>`
3. `config T1 <value>`
4. `config T2 <value>`

Start the simulation

You can start the simulation by running `start`. You can pause the simulation by running `pause`.

Initiating radio pulse

You can initiate a radio pule with the following commands: `pulse <duration>` or `pulse <duration> <Bx> <By> <Bz>`

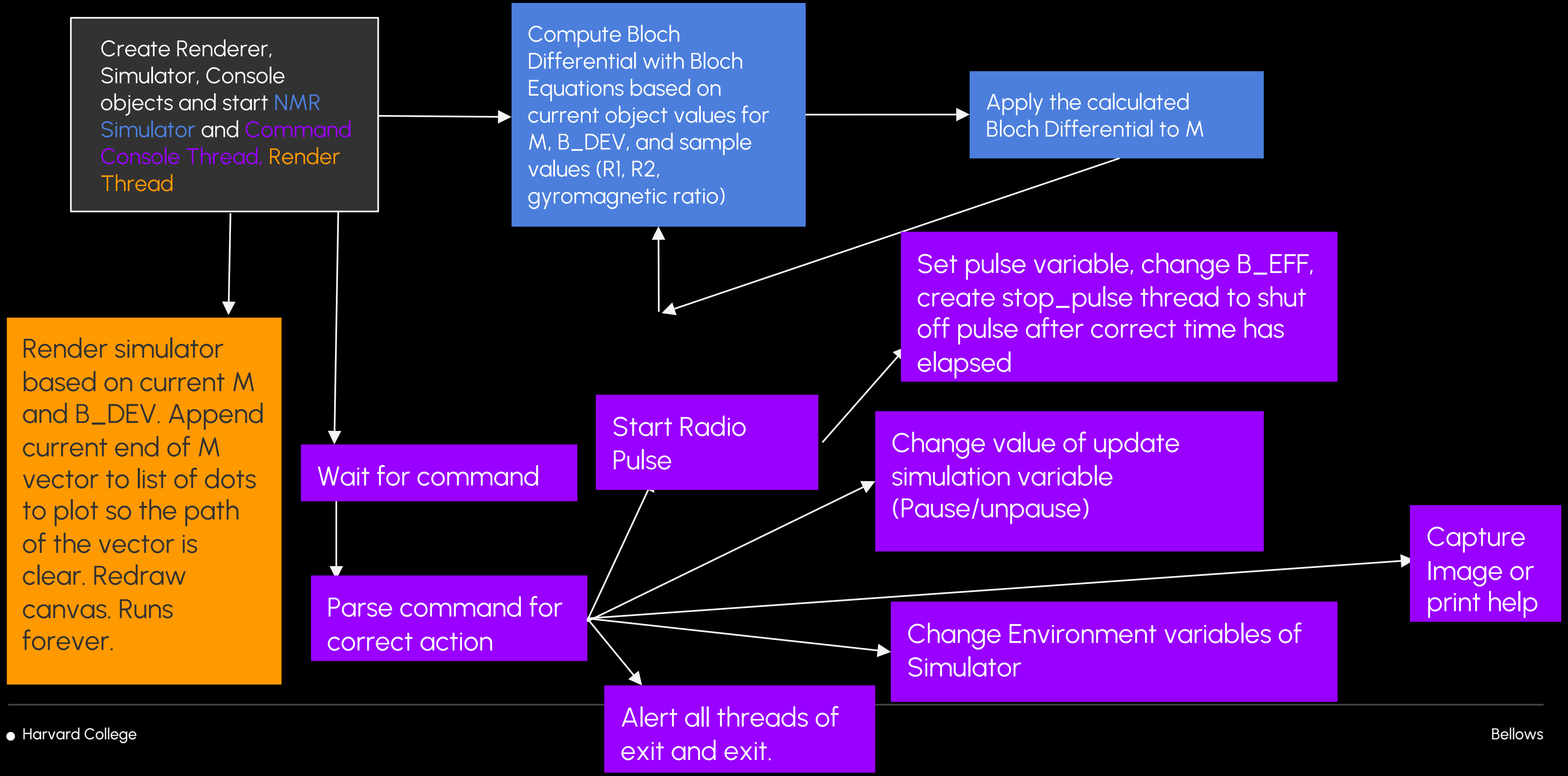
Capture a photo of the simulation

You can capture a photo of the current frame by running `capture <filename>.png`

Fourier Transform to see the final NMR spectrum

Viewing the FID graph run `fft <t1> <t2>` to initiate an fourier transform with the data between t=t1 and t=t2.

Flow Chart of Code



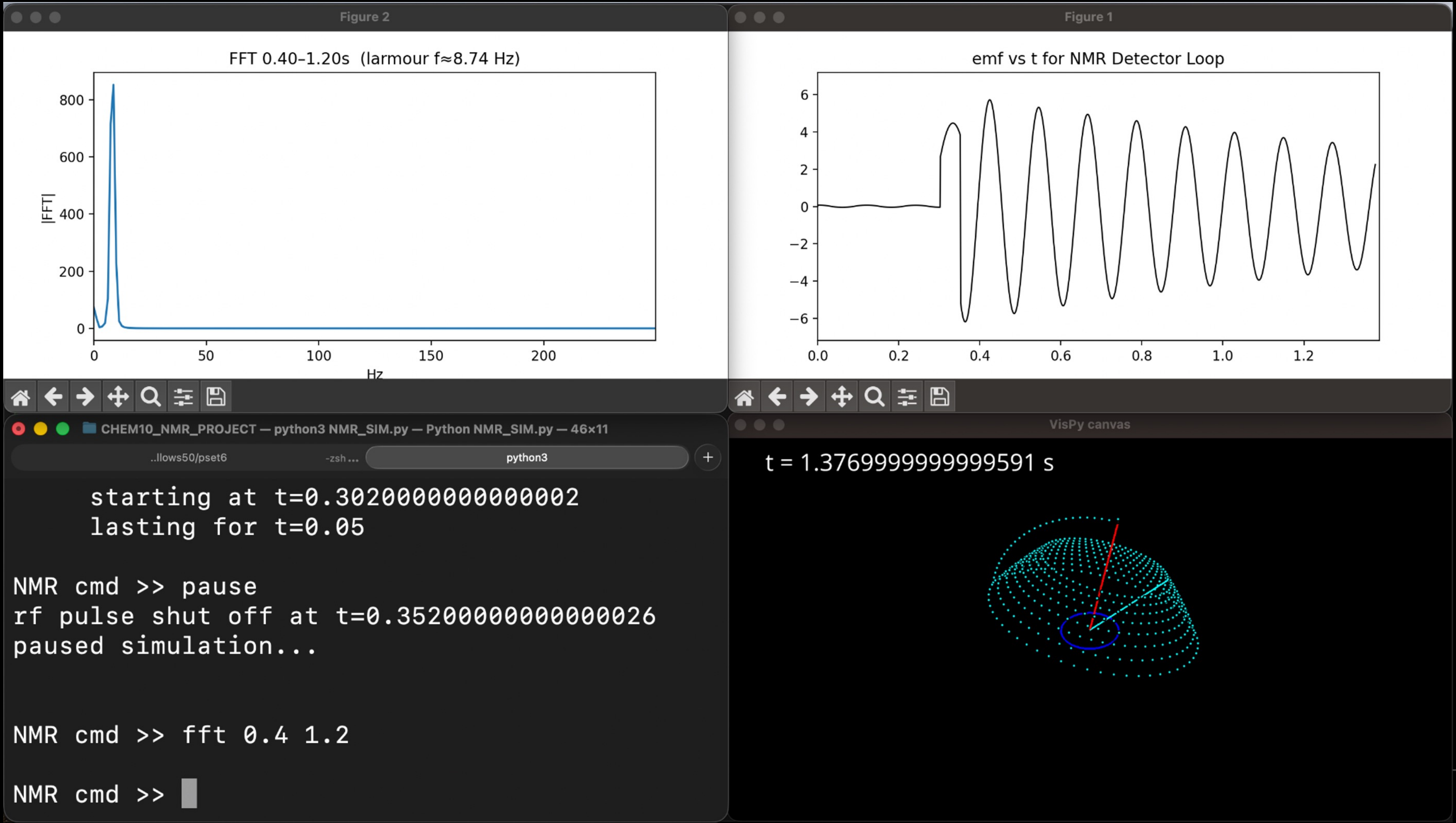


Figure 2
FFT 0.40–1.20s (larmour f≈8.74 Hz)
|FFT|
800
600
400
200
0
0
50
100
150
200
Hz
Figure 1
emf vs t for NMR Detector Loop
6
4
2
0
−2
−4
−6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
CHEM10_NMR_PROJECT — python3 NMR_SIM.py — Python NMR_SIM.py — 46×11
..llows50/pset6
-zsh ...
python3
starting at t=0.3020000000000002
lasting for t=0.05
NMR cmd >> pause
rf pulse shut off at t=0.35200000000000026
paused simulation...
NMR cmd >> fft 0.4 1.2
NMR cmd >>
VisPy canvas
t = 1.3769999999999591 s

Physical Attempt

Using Andy Nicol's Hackaday "Nuclear Magnetic Resonance for Everyone," I built a basic low field NMR machine.

Coil: When connected to power supply the coil acts as an electromagnet with magnetic field not aligned with Earth's magnetic field. When activated, local field increases by 1 mT.

When connected to Detector, rotating magnetic fields are converted to voltage oscillations,

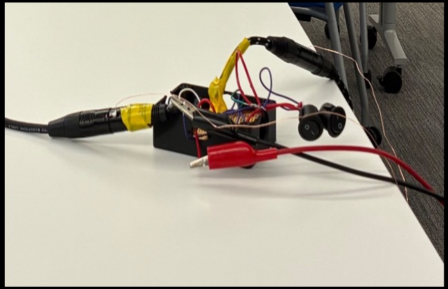
Control box switches whether Detector or Power is connected to coil

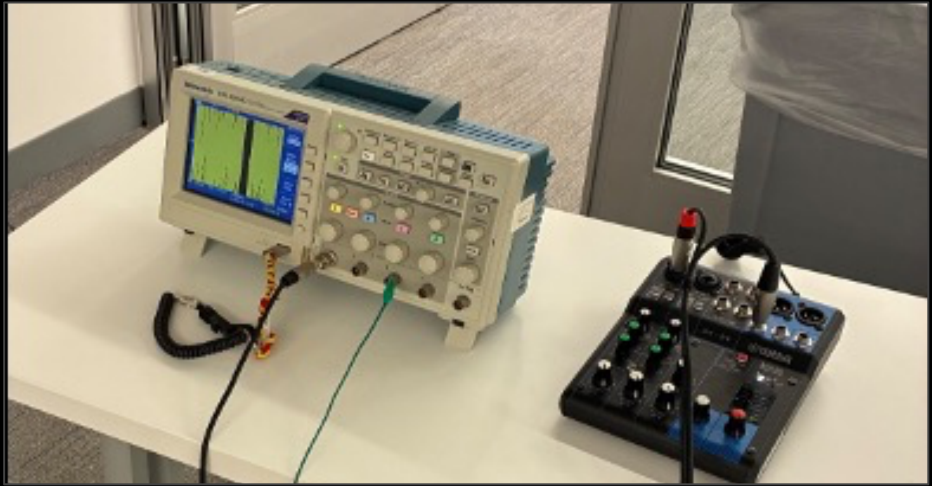
Power supply

Audio amplifier: 100x gain

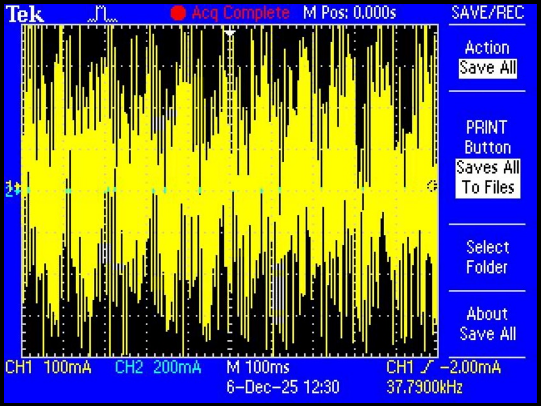
Oscilloscope displays signal

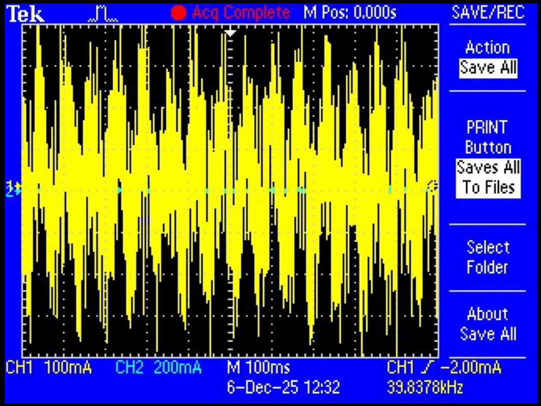
Clockwise from top left: control Box, coil with water sample, amplifier and oscilloscope detector



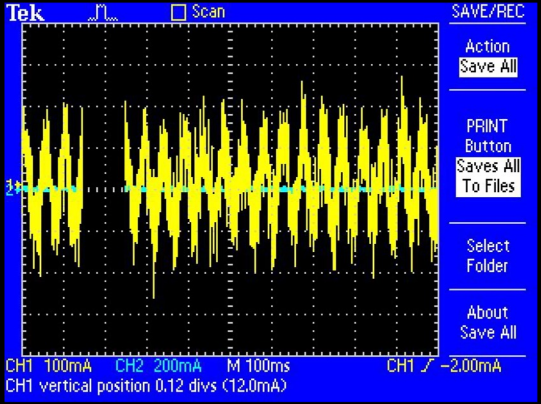


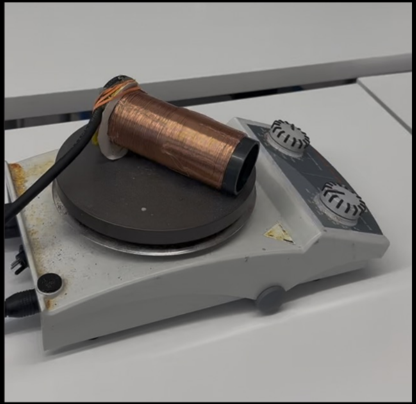
Results with a magnetic stirrer under the coil to create a string rotating magnetic field.



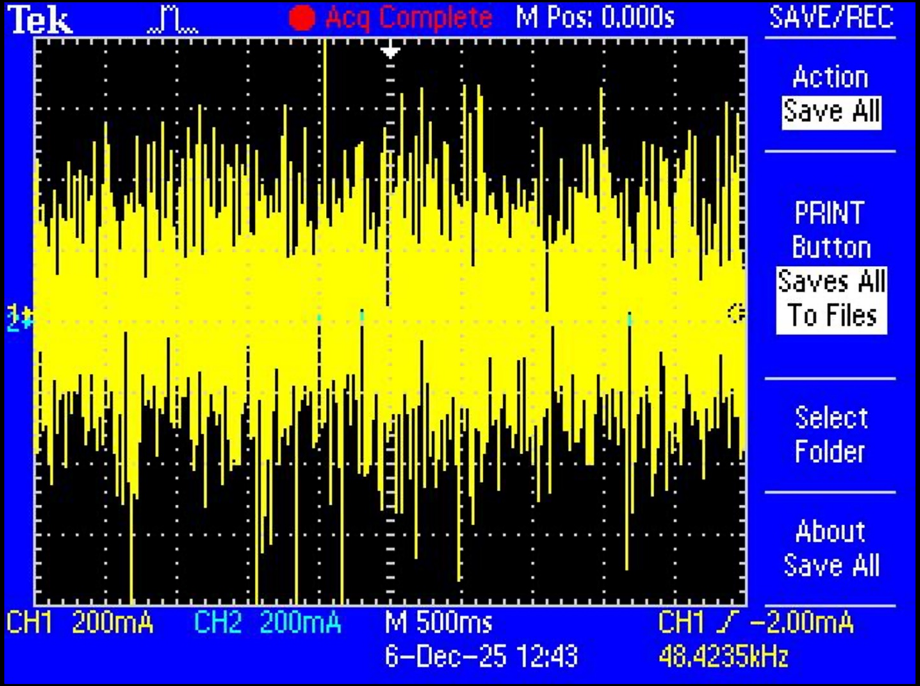


Voltage vs Time graphs for low, medium, and high speeds on the magnetic stirrer. Clockwise from top left.





Water sample after a 12 second polarization at 4 Amps and 17 V. There is too much noise to see the FID signal or get a clear fft.



Sources of noise:

- RF noise inducing current in coil
- Weak connections
- Crossed wires inducing current
- Static electricity buildup
- Random thermal fluctuations
- Faulty equipment

Mitigation

- Increase magnetic field strength to increase signal strength
- Use faraday cage around apartus
- Ground more effectively

Works Cited

JOHN CAVANAGH, WAYNE J. FAIRBROTHER, ARTHUR G. PALMER III, MARK RANCE, & NICHOLAS J. SKELTON. (n.d.). CLASSICAL NMR SPECTROSCOPY. Protein NMR Spectroscopy (Second Edition) Principles and Practice.

Kaseman, D. (2013, October 2). Relaxation. Chemistry LibreTexts. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Spectroscopy/Magnetic_Resonance_Spectroscopies/Nuclear_Magnetic_Resonance/NMR_-_Theory/Relaxation

Liao, Dr. S., Dourmashkin, Dr. P., & Belcher, P. J. W. (n.d.). Faraday's Law of Induction. MIT Physics 8.02 Electricity and Magnetism. https://web.mit.edu/8.02t/www/802TEAL3D/visualizations/coursenotes/index.htm

Nave. (n.d.-a). Nuclear Magnetic Resonance. Retrieved November 16, 2025, from http://hyperphysics.phy-astr.gsu.edu/hbase/Nuclear/nmr.html#c1

Nave. (n.d.-b). Nuclear Spin Polarization. Retrieved November 16, 2025, from http://hyperphysics.phy-astr.gsu.edu/hbase/Nuclear/spinpol.html#c1

Nave. (n.d.-c). Nuclear Spin Relaxation. Retrieved November 16, 2025, from http://hyperphysics.phy-astr.gsu.edu/hbase/Nuclear/spinrel.html#c1

Newman, M. (n.d.). Bloch sphere | Prefetch. Retrieved December 8, 2025, from https://prefetch.eu/know/concept/bloch-sphere/

NMR Basics for the absolute novice. (n.d.). JOEL Solutions for Innovation. Retrieved December 8, 2025, from https://www.jeolusa.com/RESOURCES/Analytical-Instruments/NMR-Basics

WileyPLUS - NMR spectroscopy and nuclear spin. (n.d.). Wiley Plus. Retrieved December 8, 2025, from https://www.johnwiley.net.au/highered/chemistry2e/wileyplus/basics/nmr/

Acknowledgements

- Khaled: Thank you for spending so many hours advising me in this project and for providing wisdom and support throughout the journey
- Andrew: Thank you for helping me clarify my ideas and realize what was possible for this project.
- Professor Park and Professor Xu: Thank you for showing how magical and beautiful Quantum Mechanics is and for inspiring all of this work.