PHYS 212 Project Final Report: Measuring Spin-Echo with Earth Field Magnetic Resonance

Ozan Cem Baş, Arda Erkan and Havva Aslı Topçu

Physics Department, Bilkent University

(Dated: May 29, 2023)

This paper focuses on getting spin-echo measurements and possibly to calculate the hydrogen content of a sample by making use of Earth field nucleic magnetic resonance, which is a kind of low-field NMR. The main points that will be studied in this paper are the theory behind nucleic magnetic resonance, explanation of the setup that will be used and how it is made and finally, getting spin-echo measurements using this setup. The important emphasis in this project is to be able perform these on a budget that can be afforded by undergraduate students.

I. INTRODUCTION

Ever since the spin property of matter was observed in Stern-Gerlach experiments, scientific community found ways to manipulate and make physical use out of this property. With the combined effort of Isidor Rabi, Felix Bloch and Edward Milles Purcell, the relation of this property to absorption of RF signals and it was observed that this absorption occurs at different frequencies for different nuclei, which have laid the foundations of nuclear magnetic resonance [1]. Today, devices that depend on principles of nuclear magnetic resonance (or NMR for short) are indispensable tools imaging and understanding matter on a molecular level in disciplines like chemistry and medicine.

With all this being said, there are limitations on implementations of NMR. First of all, to get a measurement with this method, one needs an external magnetic field, and homogeneity of this magnetic field plays an extremely important to get meaningful results. Second one being, to get strong and differentiable measurement, it is usually necessary to make use of really strong magnets whose magnetic field strength can range up to 21 tesla. To overcome these obstacles, superconducting magnets are employed. These delicate instruments are generally quite expensive and requires a designated laboratory to function properly. On the other hand, there methods of getting NMR measurements called "low-field NMR" that can be employed that can be done using lower magnetic fields. The applications of such methods can be a solution to the problems of NMR mentioned above. Being relatively low-cost and highly portable, machines that employ low-field NMR can be quite useful for measurements where a full-sized NMR spectrometer cannot be used. The one that will be focused on in this paper is "Earth field NMR" that makes use of the Earth's magnetic field to get NMR measurements from water samples and observe the existence and concentration of hydrogen inside it.

II. THEORY

A. Larmour Precession

With a classical consideration, a particle constitutes two types of angular momentum: orbital angular momentum and rotational angular momentum. The quantum counterpart of these behave in a similar way, although one cannot talk about the rotation of a particle about itself. With this in mind, a charged particle that has a non-zero spin behaves like a magnet and has a magnetic moment calculated as,

$$\vec{\mu} = \frac{g_s q}{2m}\vec{S} \tag{1}$$

Where $\vec{\mu}$ is the magnetic moment, q is the charge, m is the mass, g_s is a dimensionless quantity called g-factor and $\vec{S}$ is spin [2]. This is usually expressed as,

$$\vec{\mu} = \gamma\vec{S} \tag{2}$$

Where $\gamma = \frac{g_s q}{2m}$ is called the gyro-magnetic ratio of the particle. In an environment where a particle is under constant and homogeneous magnetic field $\vec{B} = B_0\hat{k}$, the Hamiltonian of the particle is expressed as,

$$\hat{H} = -\vec{\mu}\cdot\vec{B} = -\gamma B_0 \hat{S}_z \tag{3}$$

where $\hat{S}_z$ is the spin angular momentum operator in the z-direction. And using this Hamiltonian in the Schrodinger's equation results,

$$i\hbar\partial_t\Psi = \hat{H}\Psi = -\gamma B_0\hat{S}_z\Psi = -\frac{\gamma B_0\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\Psi \tag{4}$$

Which has the following eigenstates Ψ_+ and Ψ_- with corresponding energies $E_+ = -\frac{\gamma B_0\hbar}{2}$ and $E_- = \frac{\gamma B_0\hbar}{2}$. Then, the general solution can be written as,

$$\Psi(t) = cos(\theta/2)e^{\gamma B_0 t/2}\Psi_+ + sin(\theta/2)e^{-\gamma B_0/2}\Psi_- \tag{5}$$

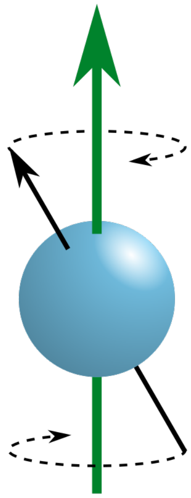

FIG. 1. An illustration showing this oscillating behavior of the particle

$$\Psi(t) = \begin{pmatrix} cos(\theta/2)e^{\gamma B_0 t/2} \\ sin(\theta/2)e^{-\gamma B_0/2} \end{pmatrix} \tag{6}$$

And calculating the expectation value $\left\langle \Psi \middle| \hat{S_x} \Psi \right\rangle$, one gets,

$$\left\langle \Psi \middle| \hat{S_x} \Psi \right\rangle = \frac{\hbar}{2} \Psi^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi = \frac{\hbar}{2} sin(\theta) cos(\gamma B_0 t) \tag{7}$$

As it can be seen, The expectation value of the x-component of the spin oscillates with a frequency,

$$f = \frac{\gamma}{2\pi} B_0 \tag{8}$$

Which is called the Larmor frequency of the particle and, the oscillating motion is called Larmor precession [3]. Larmor frequency depends on the applied magnetic field strength and to the gyro-magnetic ratio which is different for different nuclei. In particular, hydrogen in water has the gyro-magnetic ratio of $42.577 MHz$ [4]. This frequency will be used within the other calculations and the experiments.

B. Rotation Pulses and Their Timing

In the previous section, the behavior of a particle with $\frac{1}{1}$ spin under constant magnetic field was explored. But this is only the behavior of a single particle with no account for interactions with the external world. In a real physical system, like an ensemble of particles with spin, the particles interact with each other and the environment. Some of these are thermal interactions or precessing spins with different phases interacting. These interactions cause the system to lose the total magnetization M in the x-y plane and be polarized with the external magnetic field on the z-direction in the absence of any excitation signal. From equation 7, it is apparent that the amplitude of the precession is 0 for $\theta = 0$ or $\theta = \pi$, depending on the direction of the magnetic field. Therefore, to measure this oscillatory behavior, an initial excitation is necessary. Revisiting equation 7, it can be seen that the Received spin echo has the highest amplitude when $\theta = \frac{\pi}{2}$. So ideally, a signal should be sent to rotate the total magnetization 90° around the x or y axis. This is usually done with an electromagnetic pulse that is applied to the sample through a coil.

To quantify the amount of rotation and determine the duration and the frequency of this signal, one needs to examine the particle evolve under the new Hamiltonian,

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t) \tag{9}$$

Where $\hat{H}_0$ is the time invariant part of the Hamiltonian and $\hat{V}(t)$ is the time dependent part, which represents the rotation signal. Assume that the signal is a sinusoidal wave sent in the x-direction. Then,

$$\hat{V}(t) = -\vec{\mu} \cdot \vec{B}(t) = -\gamma B_1 sin(\omega_1 t) \hat{S}_x \tag{10}$$

And,

$$\hat{H}(t) = -\gamma B_0 \hat{S}_z - \gamma B_1 sin(\omega_1 t) \hat{S}_x \tag{11}$$

Where B_1 is the amplitude of the signal and ω_1 the frequency of the signal. Let he initial state be $\psi(t) = c_1(t)|0\rangle + c_2(t)|1\rangle$ with $c_1(0) = 1$ and $c_2(0) = 0$. If this state is allowed to evolve under this time dependent Hamiltonian it is seen that the probability of finding either of states fluctuate with time and this is an instance of a quantum mechanical Rabi problem. The final probability of obtaining $|1\rangle$, that is $|c_2(t)|^2$, can be written as,

$$\frac{\Omega_0^2}{\Omega_0^2 + \Delta^2} sin^2[\frac{\sqrt{\Omega_0^2 + \Delta^2} t}{2}] \tag{12}$$

Where $\Delta = \omega_0 - \omega_1 = \gamma B_0 - \gamma B_1$ is called the detuning. Ω_0 is the Rabi frequency and depends on the energy separation between two states,

$$\Omega_0 = \gamma B_1 \tag{13}$$

As shown in figure 2, the maximum amplitude of probability is decreases with increasing detuning. Therefore, to get the maximum efficiency the rotation pulse should ideally have the same frequency with the natural frequency of the particle, so that, $\Delta = 0$. That is,

$$\omega_1 = \omega_0 \tag{14}$$

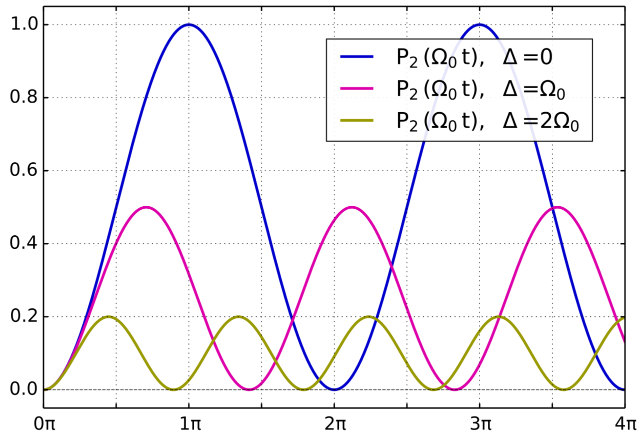

FIG. 2. A few examples of Rabi oscillations for the same Ω_0 but different detunings. The y-axis shows the probability of finding the state in the second state.

If the initial state $\psi_i n = |0\rangle$, then the 90° rotated state is $\psi_r ot = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. So, the probability of finding the second state in this rotated state is $|c_2(t)|^2 = \frac{1}{2}$.

Referring to figure 12, to get the times where this condition is satisfied,

$$\frac{1}{2} = sin^2(\frac{\Omega_0 t}{2}) \tag{15}$$

$$t_{\frac{\pi}{2}} = \frac{\pi}{2\Omega_0} = \frac{\pi}{2\gamma B_1} \tag{16}$$

These signals are called "$\frac{\pi}{2}$ pulses" for they rotate the state $\pi/2$ degrees around the y or x axis, depending on the direction of the magnetic field component of the electromagnetic wave.

C. Computational Theory

After the setup is built and sample is placed inside the setup, audio-frequency signal will be send and measurements will be taken. However, the measured signal cannot be interpreted by naked eye. To get a spectral analysis, one needs to find out the the different frequencies that are present in the signal. To do so, the Fourier transform of the signal needs to be calculated. Fourier transform is a mathematical transformation that states the function of interest can be written as an infinite sum of periodic functions $e^{i2\pi\xi t}$ with different frequencies ξ, and the values of these frequency components can be expressed as,

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(t)e^{-i2\pi\xi t}\, dt \tag{17}$$

Where $|\hat{f}(\xi)|$ the amplitude of a specific frequency, and $arg(\hat{f}(\xi))$ is the phase of that frequency. However, as no measurement in real life is truly continuous, one needs to use Fourier transform for real life signals.

The discrete Fourier transform (or DFT for short) of a signal $x[n]$ for $n = 0...N-1$ is expressed as,

$$X[k] = \sum_{n=0}^{N-1} x[n]e^{\frac{-2\pi k}{N}n} \tag{18}$$

Where $X[k]$ is the frequency component for the frequency $\frac{k}{N}$ for $k = 0...N-1$. Once again, one needs to calculate the absolute value of $X[k]$ or the $arg(X[k])$ for the amplitude and phase information.

III. METHODOLOGY

The methodology section will be presented in two parts: theoretical, experimental and computational.

A. Theoretical Methodology

When the experiment setup is ready, it is crucial for the measurements to give the correct signal to the sample and at the correct duration. As explained in the theory section, it is a must to send the excitation signal at the correct frequency, which would be the Larmour frequency of the hydrogen atom, the one within the water molecule in particular. This frequency is given as,

$$f = \frac{\gamma}{B_0} \tag{19}$$

where $\gamma/2\pi$ is $42.577 MHz/T^-1$ [4]. B_0 in the case of this experiment is the effective magnetic field strength of Earth at the location of the experiment. The location of the experiment is the Bilkent University EE building which has the coordinates 39.87211378063743 degrees in north and 32.75063494672253 degrees in east at 938 meters in altitude. At this location the magnetic field strength of Earth is $47,998.1nT$ [5]. The mutiplication of these values gives the Larmour frequency as $f = 2043.6Hz$.

The duration of the signal should be $t_{\pi/2}$ which is given as,

$$t_{\pi/2} = \frac{\pi}{2\gamma B_1} \tag{20}$$

where γ is the gyro-magnetic ratio and B_1 is the amplitude of the magnetic field that the coil generates. The net magnetic field that the coil generates cannot be calculated precision, but a good estimate can be calculating

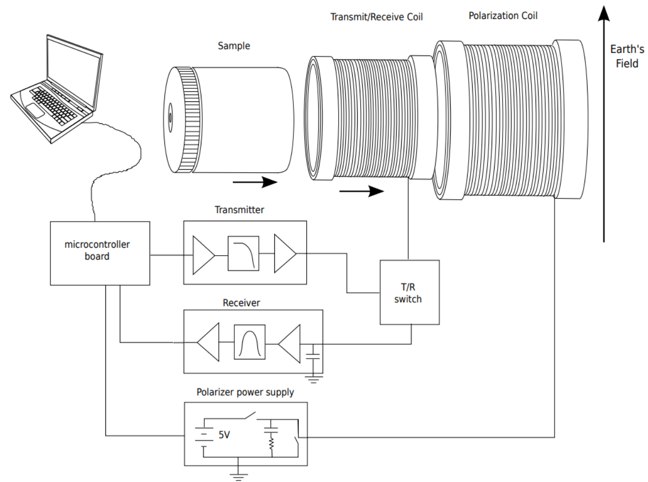

FIG. 3. The schematics of the experimental setup that will be used [6]

by using the approximation of an ideal solenoid. Therefore, the magnetic field strength is calculated as a fuction of the voltage applied as,

$$B_1(V) = 1.2566 \cdot 10^{-6} \frac{3100}{0.1} \frac{V}{310} = 1.2566 \cdot 10^{-4} V \quad (21)$$

For the experiments, the voltage at the coil is measured and the corresponding $t\pi/2$ duration is calculated.

B. Experimental Methodology

The working principle of an NMR measurement is through first aligning the nuclear spins of the sample with the external magnetic field, which is in this case the Earth's magnetic field. When performing an NMR with a high magnetic field, this polarization produced by the magnets would be enough to get measurements. However, in the low field case, one needs to further polarize the nuclei using an external magnetic field source before getting a measurement. This is performed by the polarization coil that can be seen in the figure 3. After this polarization period, the current in the polarization coil is cut and pulses of different length audio-frequency signal is sent through the transmit/receive coil and the resulting response is measured and amplified with the receiver circuit. A functional model build for Earth field NMR measurements was made by Carl A. Michal, which we will be replicating [6]. All the specifications of the experimental setup are present in his article. First, the coils will be wound. After ordering correct circuit elements with accordance to the article, the circuit elements will be soldered together. Finally the code for the timing of the coils and sending the audio signal will be written and uploaded to the arduino board.

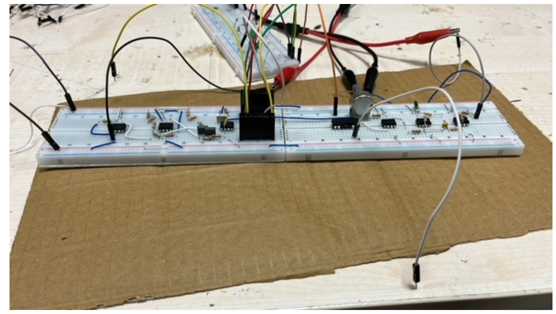

FIG. 4. The completed circuits.

First step of performing the experiments is building the setup. This is done in three parts: the building of the coils, the building the circuits and preparing the Arduino code. The coils were wound by a professional as seen in figure 5.

FIG. 5. The image of the coils that were used in the experiments

After the arrival of the necessary circuit elements, the circuits are built onto the breadboards.

To prevent electromagnetic interference, both coils and the circuit boards are wound with multiple layers of aluminum foil and these shieldings were grounded. While working on the physical components of the experiment, the an Arduino code was written to do the following instructions in an indefinite loop:

- Give signal to relay 1 and cut off the signal of the relay 2.
- Wait for T1 milliseconds.
- Cut off the signal of the relay 1 and give signal to relay 2.
- Wait for T2 milliseconds.

FIG. 6. The circuits elements.

Where the location of the relay 1 and 2 are marked on the figure 8. After the experimental setup was complete, the necessary terminals of the circuits are connected to the power lines, Arduino and to the signal generator and the coils are connected to the circuit. To see the code that is used in the Arduino, see the appendix.

FIG. 7. The complete experiment setup.

C. Computational Methodology

Most often than not, sending only one pulse is not enough to get a clear enough measurement due to noises. Therefore, in a single NMR measurement, several pulses

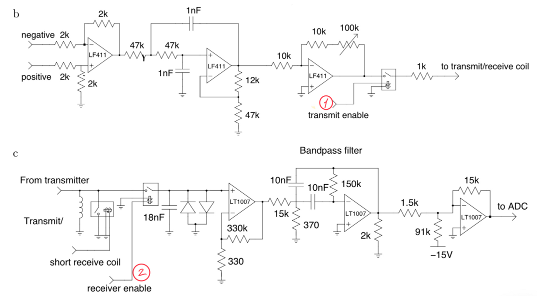

FIG. 8. The scheme of the circuit that were built. The marks 1 and two indicate the relay 1 and relay 2.

are sent and the obtained measurements are averaged in order to reduce the effects of noise, which needs to be done computationally. Also, to obtain the final spectrum, the Fourier transform of the measurements will be calculated.

IV. RESULTS

The experiments were carried out as explained in the earlier chapters. The setup is connected to the power supply and to the signal generator. The reading are taken into a flash drive directly from the oscilloscope as in figure 9.

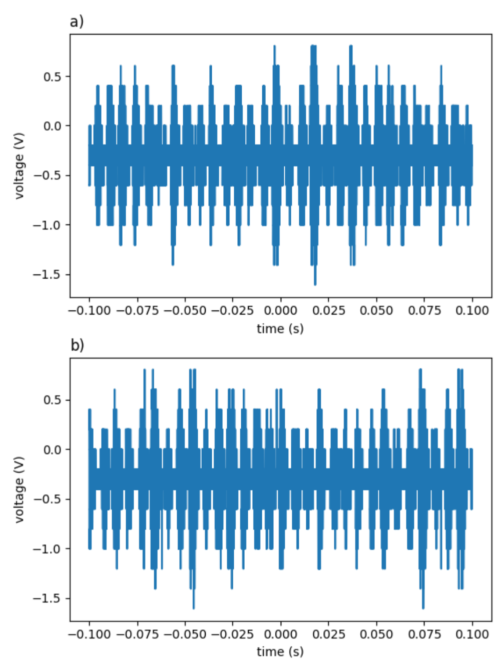

FIG. 9. a) The readings from the output without a sample, b) the readings with a sample.

The obtained measurements are then processed computationally by taking the Fourier transform of the data,

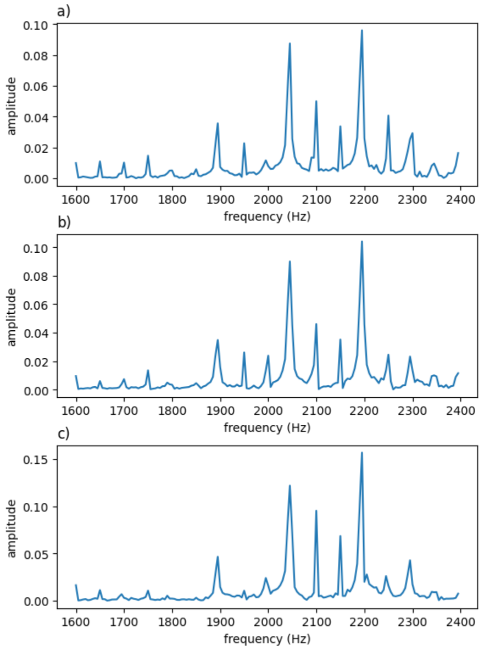

FIG. 10. a) The spectrum without a sample, b) the spectrum with a sample, c) the difference of the spectrums of two cases.

As seen in figure 10, the most significant peaks appear at $2043Hz$ and $2195Hz$. The appearence of the peak at $2043Hz$ was expected and wanted, since that would be the spin echo in the sampled case as in figure 10(b). However, in the conditions of the complete isolation of the input signal, when there is no sample present, that peak should not be present. This means there is a voltage leaking to the output as seen in figure 10(a). Never the less, the difference of the two spectrums shown in figure 10(c) has still a peak on the $2043Hz$, which can be considered as the obtained spin echo. Altough, it is reliability of this result is not clear, and the results that were expected to be seen is not observed. To see the code that has been used to generate these plots and pursuing the transformations, see the appendix.

V. DISCUSSION

In this section, the problems faced in the project in all steps will be explained and further explanations on the results will be presented.

Upon another examination of the resulting spectrum in figure 10, it can be seen that there are many other peaks at various frequencies other than $2043Hz$ and an even larger peak at $2195Hz$. Since these cannot be the the spin echo or the signal that is sent, they have to be noise.

Throughout the building of the setup, several problems were faced. the most significant one being the presence of noise. Appearance of noise anywhere in the circuits causes major consequences, for the noise is amplified further which reduces signal-to-noise ratio significantly. Therefore, we took every measure to keep the noise to a bare minimum. Here are the precautions taken to do so:

- Using low-noise op-amps
- Attaching decoupling capacitors between the terminals of the power supply
- Winding the circuits and the coils with aluminum foil and then grounding these shieldings
- Turning the all the paired cables like power and signal cables into twisted pairs
- Increasing the supplied plus and minus voltage to the op-amps and decreasing the gain of some of the op-amps in order to prevent saturation due to the noise
- Using really fast, signal type relays with electromagnetic shielding
- Using various filters in order to limit the high frequency noises

These helped to limit the noise quite effectively. However, one of the more significant causes of noise still remains, that is the circuits being on a breadboard. Breadboards have internal resistances and capacitances which could be causing some noise. A possible solution would be to solder the whole circuit onto a strip-board. Unfortunately, this solution could not be applied due to the extended trouble-shooting and prototyping, high complexity of the circuit and time limitations. However, even if this solution was applied, it likely would not solve the peak at $2195Hz$. This is because the noise is expected to have a $1/f^{\alpha}$ decay in power spectral density, which is clearly no the case as seen on the figure 11.

Only alpha-noise that can be readily seen on the PSD is $\alpha = 0$ at a really low amplitude. Therefore, such a specific frequency cannot be environmental noise. Another cause of this noise may be the intrinsic noise of the op-amp used in the receiver circuit. Once again this is hard to confirm, for the time limitations and also the rising cost of the project. So, the presence of this unexpected peak at $2195Hz$ cannot be resolved.

VI. ACKNOWLEDGEMENTS

We thank Ergin Atalar for his assistance throughout the project, Metin Kayabaşı for his help on building the circuits and Şakir Duman for building us the stand that we use to put our coils on.

VII. APPENDIX

A. The Arduino Code

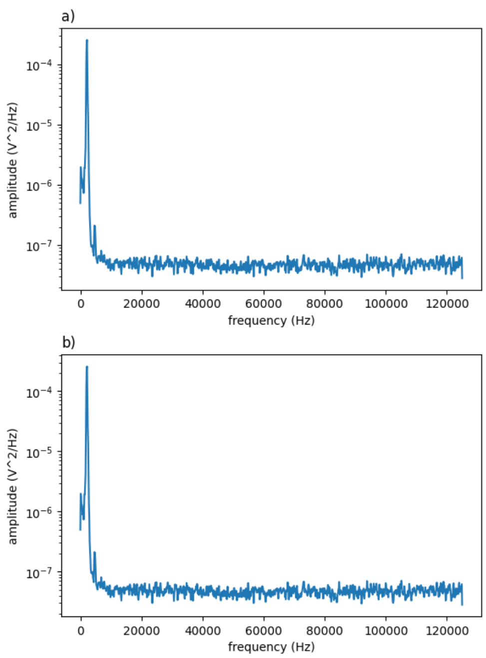

FIG. 11. a) The power spectral density without a sample, b) the power spectral density with a sample.

```
 const int outPin10 = 10;
const int outPin9 = 9;
const int inPin = A0;
int T1 = 14;
int T2 = 1000;

void setup() {
  // put your setup code here, to run once:
  pinMode(outPin10, OUTPUT);
  pinMode(outPin9, OUTPUT);
  pinMode(inPin, INPUT);
  Timer1.initialize(1000); // miliseconds as period
}

void loop() {
  // put your main code here, to run repeatedly:
  digitalWrite(outPin9, LOW);
  digitalWrite(outPin10, HIGH);
  delay(T1);
  digitalWrite(outPin10, LOW);
  digitalWrite(outPin9, HIGH);
  delay(T2);
}
```

B. The Python Code

```
    import numpy as np
import scipy as sp
import scipy.fftpack as fftp
import scipy.signal as signal
import pandas as pd
import matplotlib.pyplot as plt

without_sample = pd.read_csv("without_sample.csv"
with_sample = pd.read_csv("with_sample.csv", head

volt_wos = without_sample["Volt"].values
volt_ws = with_sample["Volt"].values
t_wos = without_sample["second"].values
t_ws = with_sample["second"].values

sample_period = t_wos[1] - t_wos[0]
sample_freq = 1/sample_period
len_freq = len(t_wos)
mp = len_freq//2 -1

ft_wos = fftp.fft(volt_wos)/len_freq
ft_ws = fftp.fft(volt_ws)/len_freq

ft_wos = ft_wos[:mp]
ft_ws = ft_ws[:mp]

f_array = fftp.fftfreq(len_freq, sample_period)
f_array = f_array[:mp]

index_1600 = int(1600/(f_array[-1]/len(f_array)))
index_2400 = int(2400/(f_array[-1]/len(f_array)))

f_array_adj = f_array[index_1600:index_2400]
ft_wos_adj = ft_wos[index_1600:index_2400]
ft_ws_adj = ft_ws[index_1600:index_2400]

plt.figure()
plt.subplot(211)
plt.plot(t_wos, volt_wos)
plt.title("measurement without sample")
plt.xlabel("time (s)")
plt.ylabel("voltage (V)")
plt.subplot(212)
plt.plot(t_ws, volt_ws)
plt.title("measurment with sample")
plt.xlabel("time (s)")
plt.ylabel("voltage (V)")

plt.figure()
plt.subplot(131)
plt.plot(f_array_adj, abs(ft_wos_adj))
plt.title("FFT without sample")
plt.xlabel("frequency (Hz)")
plt.ylabel("amplitude")
plt.subplot(132)
plt.plot(f_array_adj, abs(ft_ws_adj))
plt.title("FFT with sample")
plt.xlabel("frequency (Hz)")
plt.ylabel("amplitude")
plt.subplot(133)
plt.plot(f_array_adj, abs(ft_wos_adj-ft_ws_adj))
```

```
plt.title("differences of FFTs")
plt.xlabel("frequency (Hz)")
plt.ylabel("amplitude")

psd_volt_ws = signal.welch(volt_ws, sample_freq, nperseg=2048)
psd_volt_wos = signal.welch(volt_wos, sample_freq, nperseg=2048)
l_psd = len(psd_volt_wos[1])

plt.figure()
plt.subplot(211)
plt.semilogy(psd_volt_ws[0], psd_volt_ws[1])
plt.title("PSD without sample")
plt.xlabel("frequency (Hz)")
plt.ylabel("amplitude (V^2/Hz)")
plt.subplot(212)
plt.semilogy(psd_volt_ws[0], psd_volt_ws[1])
plt.title("PSD with sample")
plt.xlabel("frequency (Hz)")
plt.ylabel("amplitude (V^2/Hz)")

plt.show()
```


[1] E. M. Banwell, Colin N.; McCash, *Fundamentals of Molecular Spectroscopy* (McGraw-Hill College, 1994) Chap. 7 Spin Resonance Spectroscopy, pp. 214–242.

[2] B. B. C. Joachain, *Physics of Atoms and Molecules* (Longman Pub Group, 1982).

[3] D. J. Griffiths and D. F. Schroeter, *Introduction to Quantum Mechanics*, 3rd ed. (Cambridge University Press, 2018) pp. 219–220.

[4] R. D. Foltz, *CRC Handbook of Chemistry and Physics:A Ready-Reference Book of Chemical and Physical Data* (CRC Press Inc, 2000).

[5] U. D. of Commerce, NCEI Geomagnetic Calculators.

[6] C. Michal, A low-cost spectrometer for nmr measurements in the earth's magnetic field, Measurement Science and Technology **21**, 105902 (2010).