Simulation of the Liverpool Qmeter Module to Predict Nucleon Target Polarizations

Colin Crovella

May 2020

Contents

Abstract

Polarized nucleon targets provide useful measurements for the study of spin structure and other observables. To maximize their usefulness it is necessary to measure their polarization. We discuss how polarization can be indirectly measured using the Liverpool Qmeter Module. In order to predict results for future experiments, and to optimize parameters of the circuit, we develop a simulation of the Liverpool Qmeter system which can take simulated data as an input and generate a signal approximating what the real device would output. We then demonstrate how to simulate the behavior of a type of target (deuteron) and use this data in our Qmeter simulation.

1 Introduction

The use of polarized nucleon targets in scattering experiments provides a way to study the spin structure of the nucleon, the structure of the nucleon's excited states, the electromagnetic structure of the nucleon, and more [1]. A common type of such targets is ammonia which has a relatively low dilution factor (ratio of free protons to total nuclei) [3]. It is therefore necessary to be able to measure the polarization of a nucleon target. One such method is by using Nuclear Magnetic Resonance. The implementation explored in this study is the Liverpool Qmeter Module, in which the polarized target is placed in the inductive part of an LC circuit. The target creates a frequency-dependent change in the inductance (and therefore impedance) of the circuit, peaking at its resonant frequency. If certain conditions are fulfilled, a measurement of this change in impedance across a range of frequencies (by means of measuring the voltage) provides information about the polarization of the target [2].

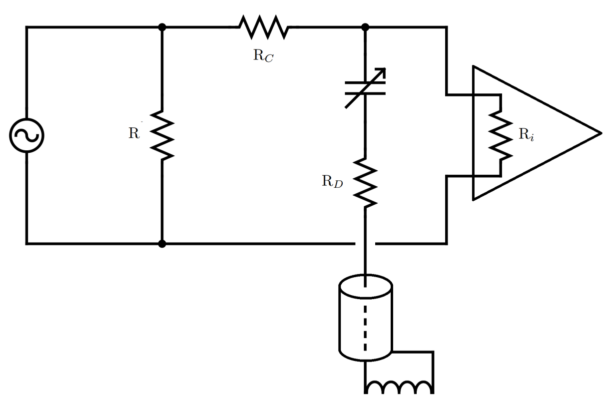

Figure 1: A diagram of a simple Qmeter circuit.

Figure 1 shows the principle behind the Qmeter circuit, where R_C is the constant current resistor, R_i is the amplifier input impedance, and R_D is the damping resistor. For this implementation to be effective, it is necessary that R_C be large compared to R, and the damped tuned circuit's impedance must be small compared to R_C and large compared to R_i [2].

To further develop this technique's usefulness, it is desirable to test it upon different types of polarized targets. However, this requires building the circuit, which is at the moment a complicated task, as well as having access to these materials. This makes it difficult to train new users and to test different types of materials. Therefore, this project seeks to develop a software simulation of the signal. This enables us to test new types of polarized targets in a theoretical sense, without a full lab setup. For example, while the simulation was originally written for a proton target, we can approximate how a deuteron target may respond instead. The deuteron is of interest as it is a spin-1 particle, as opposed to the spin-1/2 proton. This means that a deuteron is tensor-polarizable, while a proton is only vector-polarizable. Tensor-polarized targets allow the study of information beyond what is available to vector-polarized ones, such as the structure functions in spin-1 decomposition of hadronic tensor. However, various factors make it difficult to obtain a high level of precision with tensor-polarized targets, so there is as yet very little data on them [4].

Given this difficulty, some theoretical exploration of a deuteron target may inform future experiments as methods improve. Therefore, this study seeks to describe the methods and circuitry of the Liverpool Qmeter, show how a simulation of its output signal can be constructed (given a type of target material), and use this simulation to explore a hypothetical deuteron target used in the Liverpool Qmeter.

2 Theory

2.1 Nucleon Polarization

To make a polarized nucleon target, the target is doped with free radicals to provide a source of unpaired electrons. A magnetic holding field at low temperature polarizes the electrons which then couple to the nucleon (proton, deuteron, etc). Radiation in the microwave frequency range causes the electrons and nucleons to flip their spins. As a result the nucleon tends towards a particle orientation, becoming polarized. The long relaxation time ($\sim 10^3$ s) of the nucleons compared to the electrons ($\sim 10^-3$ s) allows the electrons to recouple to other protons. This creates a high level of polarization. [1]. This technique is referred to as Dynamic Nuclear Polarization (DNP).

An RF magnetic field is applied perpendicular to the holding field. The RF induces spin-flip transitions in the nucleons by adding energy proportional to the frequency of the RF. There will be a resonant frequency at which these transitions are maximized [3]. There will be a spectrum of the intensity of the transitions across a range of frequencies which peaks at the resonant frequency. The shape of this spectrum (hence referred to as the "lineshape") can be approximated mathematically by convoluting the density of states with a Lorentzian [4].

2.2 NMR Measurement

The magnetic susceptibility of a material is, qualitatively, a measure of how susceptible a material is to be magnetized in an applied magnetic field. Formally it is defined using the equation below:

$$\mathbf{M} = \chi \mathbf{H} \tag{1}$$

where $\mathbf{M}$ is the material's magnetization, $\mathbf{H}$ is the applied magnetic field strength, and χ is therefore the magnetic susceptibility.

A polarized nucleus has a complex magnetic susceptibility:

$$\chi = \chi' - i\chi'' \tag{2}$$

This modifies the inductance L of the system:

$$L_p = L(1 + 4\pi\eta\chi) \tag{3}$$

where L_p is the new inductance, L is the original inductace, and η is the system's filling factor.

The real part of χ is referred to as the dispersive part of the signal (χ'), while the imaginary part is referred to as the absorptive part (χ'').

The nuclear polarization can be shown to be proportional to the following quantity:

$$\int_0^\infty \chi''(\omega) d\omega \tag{4}$$

So, if it is possible to measure the absorptive part across a large enough domain, one can obtain a fairly accurate measurement of the nucleon's polarization [2].

As previously mentioned, the target's intensity of transitions will peak at a resonant frequency. The magnetic susceptibility is a reflection of this phenomenon, so it should display the same behavior. Therefore, to measure polarization it is not necessary to measure such a large range of frequencies as 0 to ∞. Rather, since we know the spectrum will be clustered around the resonant frequency, we may simply measure the range of this spectrum and treat the rest of the frequency range as having zero effect on the quantity given by Equation 4.

The Qmeter measures the absorptive part by placing the nucleon target in the inductive part of an LC circuit. This creates a frequency-dependent change in the inductance L_p of the circuit. By modulating the frequency it is possible to observe this change in L_p over a range in frequencies. This indirectly allows us to measure the quantity in (4), since χ and L_p are related as given in (3).

3 Hardware Implementation

This section will explore the design of the Liverpool Qmeter from a hardware standpoint.

There are two output signals which are of interest to us:

- Phase output. This is used primarily to calibrate the phase trim cables, which adjust the phase difference between the input RF and output RF. See "phase trim ports" in Figure 1.

- Magnitude output. This is the output RF which responds across a range of frequencies to a change in system impedance, allowing us to measure $\chi''(\omega)$ and therefore polarization.

The device has several inputs and outputs which are visible from the outside.

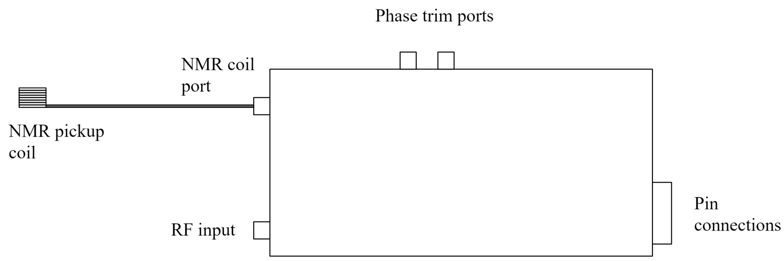

Figure 2: An outside view of the Qmeter and its relevant inputs/outputs.

- RF input. This receives an RF signal whose frequency is modulated. In the case of the proton signal, the resonant frequency is 213 MHz, so our RF input modulates from 212.75 MHz to 213.25 MHz. This puts 213 MHz at the center.
- NMR Pickup coil. This is how the target enters the inductive part of the LC circuit. The target is situated inside this coil.
- Phase trim ports. These are connected by a coaxial cable of variable length. This is used to align the phase of the output signal. The total length of this cable should be $\frac{n\lambda}{2}$, where λ is the wavelength of our resonant frequency.
- Pin connections. Our output signals are fed into these analog pins which can then be read by our other hardware.

The Liverpool Qmeter design consists primarily of five printed circuit boards or "PCBs". Each of these PCBs accomplishes a different task. The diagram below roughly demonstrates how signals travel from board to board.

As can be seen, there are several steps to obtaining the phase and magnitude signals:

- RF signal enters through the RF input port. Not shown, for the sake of simplicity, is how the RF signal enters PCB 1.
- PCB 1 contains a tuning capacitor and the inductor which includes our nucleon target. The tuning capacitor is tuned so that our LC circuit has the same resonant frequency as our target.
- PCB 2 receives the input RF and the RF from our LC circuit. These are used together for phase detection, as there will be a phase difference between these signals which should be minimized for the absorptive part detection.
- PCB 3 amplifies the phase detection signals.

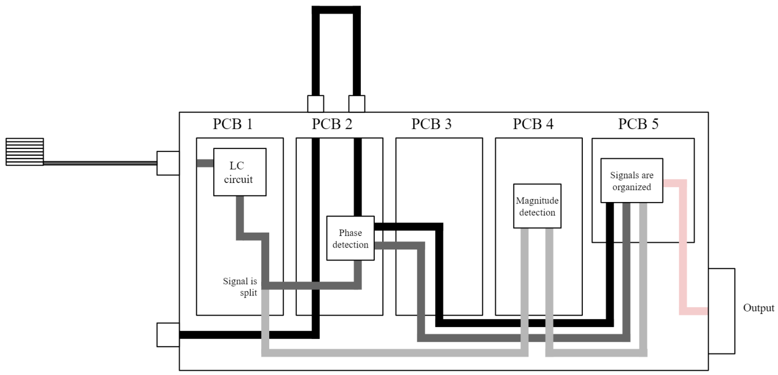

Figure 3: A simplified view of the Liverpool Qmeter circuitry.

- PCB 4 receives the RF from our LC circuit and uses a balanced ring modulator for magnitude detection.
- PCB 5 bundles the phase detection and magnitude detection signals to be fed to our pin outputs, which interface with other hardware and allow us to read the signals.

This description is simplified and omits many details for clarity. A more detailed description of the Qmeter circuitry is found in [2].

4 Qmeter Simulation

Simulating the Liverpool Qmeter entails the following steps:

1. Read in data which describes the frequency-response of our target (ex. a proton or deuteron).
2. Read in data which describes our background signal.
3. Using the data describing our target and the data describing the background signal, calculate the impedance of this system, as well as the phase offset, both as a function of frequency.
4. Plot the voltage as a function of frequency, where voltage is calculated using the impendance term $Z(\omega)$ and phase term $\phi(\omega)$.

The exact equation for our calculation of voltage is a complex form of Ohm's law, given by

$$V(\omega) = IZ(\omega)e^{i\phi(\omega)} \tag{5}$$

A simulation of this type was written in Mathcad by Geoff Court and Michael Holden [5]. Their program used measurements of a proton signal as the input to step 1 above. For this study, the original program was adapted into two forms: A Python script which uses the CERN Root Library, and a virtual interface for National Instruments' LabVIEW.

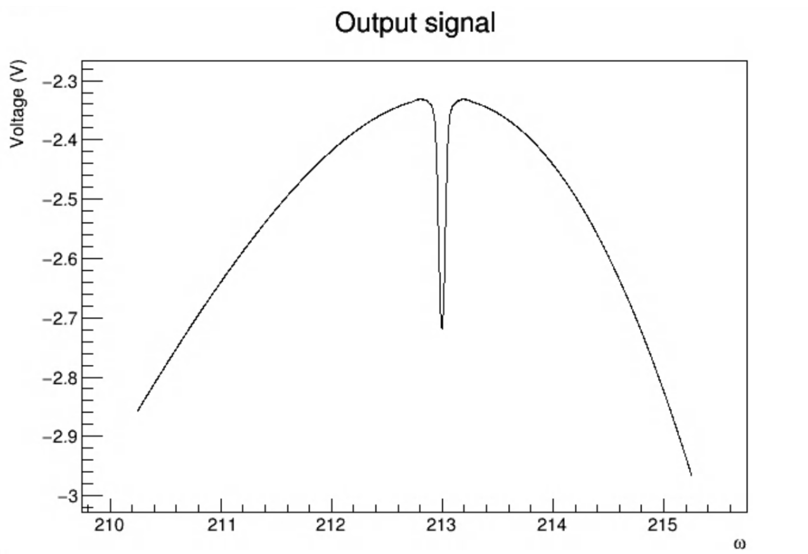

Figure 4: Output of the Python script using CERN ROOT.

Python was chosen for its ease of using complex numbers and array manipulation. The LabVIEW program actually interfaces with Python and runs a version of the Python script. LabVIEW's virtual interface system makes it easier to adjust the parameters of the simulation and quickly see the output respond to these changes. The Python/ROOT version is included for those without access to the proprietary LabVIEW (see section 7).

As can be seen in Figure 5, there are six main parameters which can be adjusted to observe changes in the circuit's output:

- *Input voltage* or U. This is the voltage of the RF signal. It is used here to calculate the current I in Equation (5).
- *knob*. This refers to the tuning capacitor of the circuit, which in reality is controlled with a physical knob. This adjusts the capacitance of the circuit.
- *trim*. In $\frac{n\lambda}{2}$, this is the value of $\frac{n}{2}$. See the section on Hardware Implementation (3).
- *eta*. The filling factor of the system (η) as seen in Equation (3).

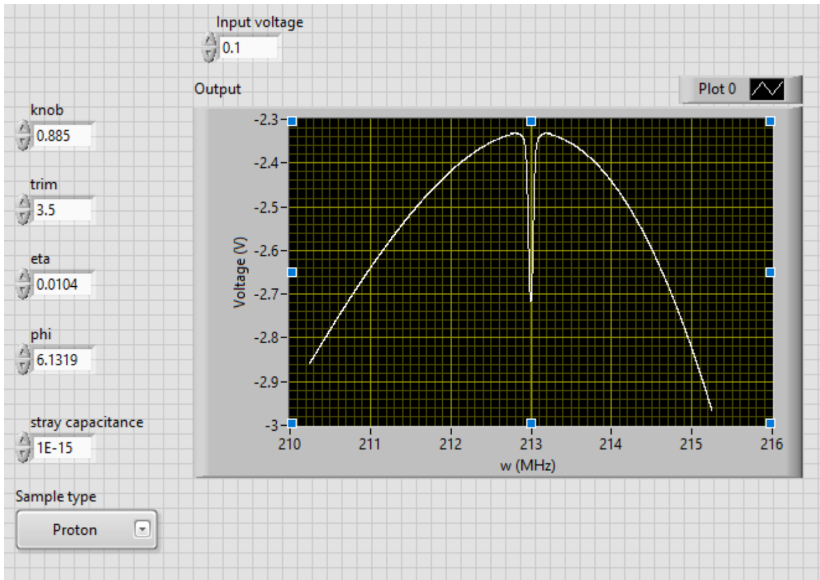

Figure 5: A view of the LabVIEW virtual interface.

- *phi* or ϕ. A value which offsets $\phi(\omega)$ as seen in Equation (5).
- *Stray capacitance* or C_{stray}. Any real-world build of the Qmeter will have some stray capacitance, and this is accounted for in the simulation. The value of 1 femtofarad is chosen as an order of magnitude estimate.

To fully demonstrate how each of these parameters affects the signal is difficult to convey concisely as there are many calculations which depend on other calculations and so forth. The actual circuit contains more elements than the circuit shown in Figure 1, so there are several series/parallel/etc. calculations which are used to create the final result. The following equations will walk through how our parameters are used to generate the output.

$\Gamma(\omega)$ has dimensions of $[LENGTH]^{-1}$ and is based on constants α and β which are estimates. It is used in the calculation of the target's impedance.

$$\Gamma(\omega) = \alpha + i\omega\beta \tag{6}$$

$C(\omega)$ is the capacitance of the tuning capacitor, which is based on the value of *knob*.

$$C(\omega) = (20 * 10^{-12})knob \tag{7}$$

$\chi(\omega)$, the magnetic susceptibility is generated based on the input data.

$L(\omega)$ is the inductance of the LC circuit which contains the target. This calculation mirrors Equation 3 but introduces $\mathscr{I}(\omega)$ to account for the coil current (this is also read in from one of the data files):

$$L(\omega) = L_0(1 + 4\pi\eta\mathscr{I}(\omega)\chi(\omega)) \tag{8}$$

$Z_0(\omega)$ is the impedance due to the cable which connects the circuits. It involves constants Z_{cable}, M, and D which are measurements relating to the cable's resistance, inductance, and capacitance.

$$Z_0(\omega) = \sqrt{\frac{2Z_{cable}\alpha + i\omega M}{i\omega D}} \tag{9}$$

$Z_L(\omega)$ is the impedance due to the inductance of the LC circuit. Since $L(\omega)$ is affected by the inductance of the target, the target is thereby affecting this value of impedance.

$$Z_L(\omega) = \frac{(R + i\omega L(\omega))(\frac{1}{i\omega C_{stray}})}{(R + i\omega L(\omega)) + (\frac{1}{i\omega C_{stray}})} \tag{10}$$

$Z_T(\omega)$ is a combination of the impedance from the cable and the inductor.

$$Z_T(\omega) = Z_0(\omega) * \frac{Z_L(\omega) + Z_0(\omega) * \tanh(\Gamma(\omega) * trim * \lambda)}{Z_0(\omega) + Z_L(\omega) * \tanh(\Gamma(\omega) * trim * \lambda)} \tag{11}$$

$Z_C(\omega)$ is the impedance due to the tuning capacitor in the LC circuit.

$$Z_C(\omega) = \frac{1}{i\omega C(\omega)} \tag{12}$$

Finally, $Z(\omega)$ is the total impedance of the system.

$$Z(\omega) = \frac{R_1}{1 + \frac{R_1}{r + Z_C(\omega) + Z_T(\omega)}} \tag{13}$$

$\phi(\omega)$ is calculated using a parabolic term with constants a, b, and c which are estimates, and the constant ϕ which our phase offset term.

$$\phi(\omega) = (a\omega^2 + b\omega + c) + \phi \tag{14}$$

The current I is calculated simply by Ohm's law:

$$I = \frac{U}{R} \tag{15}$$

It is important to note that the simulation is not inherently physical, but mathematical. That is, we do not have a 1:1 simulation of all of the resistors, capacitors, amplifiers, integrated circuits, etc. in the actual Qmeter. Rather, this simulation makes a reasonable approximation of the real signal by calculating the response of the circuit's impedance to changes in frequency, basing these calculations off of actual data. Therefore, there are factors which may cause a real-world experiment to differ from this simulation, including but not limited to the qualities of the aforementioned circuit components. This simulation does give the ability to make qualitative predictions about the shape of the signal.

5 Deuteron Simulation

As mentioned previously, the Qmeter simulation takes actual measurements as input, in order to simulate the effect of bringing that material into the circuit. This means that we can predict how a material which we do not possess physically may respond to the Liverpool Qmeter, as long as there is some way of obtaining these relevant measurements, or, in this case, simulating them.

The lineshape of the deuteron signal can be described by the following analytic function:

$$\begin{aligned}\mathscr{F} = \frac{1}{2\pi\mathscr{X}}\Big[2\cos(\alpha/2)\Big(\arctan\Big(\frac{\mathscr{Y}^2-\mathscr{X}^2}{2\mathscr{Y}\mathscr{X}\sin(\alpha/2)}\Big)+\frac{\pi}{2}\Big) \\ +\sin(\alpha/2)\ln\Big(\frac{\mathscr{Y}^2+\mathscr{X}^2+2\mathscr{Y}\mathscr{X}\cos(\alpha/2)}{\mathscr{Y}^2+\mathscr{X}^2-2\mathscr{Y}\mathscr{X}\cos(\alpha/2)}\Big)\Big]\end{aligned} \tag{16}$$

for $\mathscr{X}^2 = \sqrt{\Gamma^2 + (1-\epsilon R - \eta\cos 2\phi)^2}$, $\mathscr{Y}^2 = \sqrt{3-\eta\cos 2\phi}$, and $\cos(\alpha) = (1-\epsilon R - \eta\cos 2\phi)/\mathscr{X}^2$. R is the dependent variable of this function, and it is a dimensionless unit for frequency, centering the signal on our resonant frequency. The derivation of this function and the values of the constants are found in [4]. Given these values, our characteristic lineshape appears as in Figure 6.

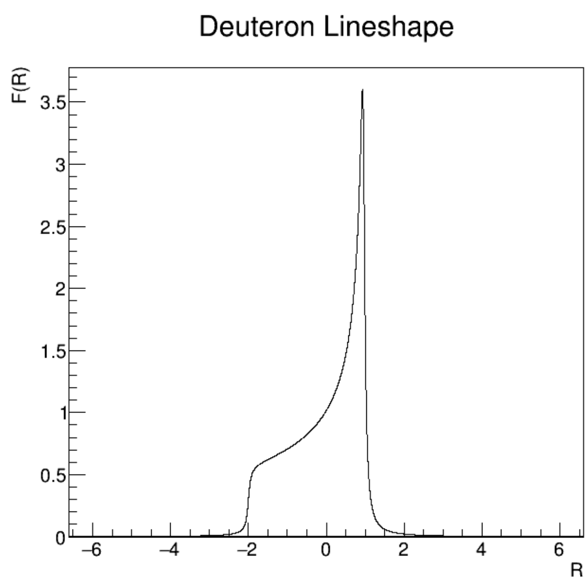

Figure 6: The analytic function for the lineshape of the Deuteron signal.

This lineshape is obtained by a convolution of the deuteron's energy states in a magnetic field with a Lorentzian [4]. There are two such transitions of the magnetic substate: $(0 \leftrightarrow 1)$ and $(-1 \leftrightarrow 0)$. The intensities of these transitions are referred to as I_+ and I_-, respectively. So our measurement of a deuteron will consist of a linear combination of lineshapes, weighted by the intensities I_+ and I_-. A typical example is shown in Figure 7.

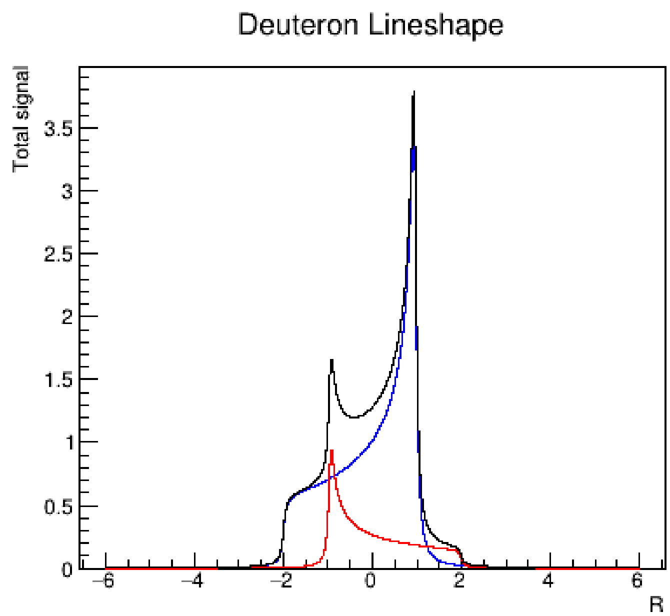

Figure 7: I_+ (blue) and I_- (red) form the shape of our expected signal.

The sizes of these peaks relative to each other is based on the polarization P of the sample and follows this relation:

$$P = \frac{r^2 - 1}{r^2 + r + 1} \tag{17}$$

where r is the ratio of the areas of the two peaks. Given that the total area of our combined signals should be proportional to P, we have what we need to generate data for the deuteron. We must also choose a calibration constant C_E in order for our data to be in the correct units; this will vary by system, so for our purposes it was chosen primarily to make the peaks large enough to easily see in the simulation (see $scale\_factor$ in *deuteron.py* in the source code, a link to which is given in Section 7).

For convenience, the generation of the deuteron signal has also been written into a LabVIEW virtual interface. One can set the polarization, run the program, and view how the theoretical signal changes. If the original Qmeter simulation is then run again, it will be updated to use the new deuteron data which has been generated.

With the data for the deuteron generated, all that remains is to run the Qmeter simulation using this data instead of the proton data which was generated for the original simulation [5].

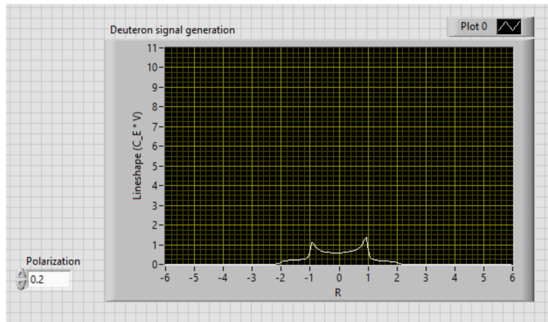

Figure 8: Signal with 40% polarization.

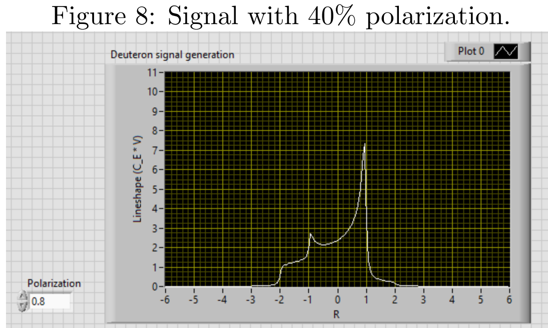

Figure 9: Signal with 80% polarization.

6 Results

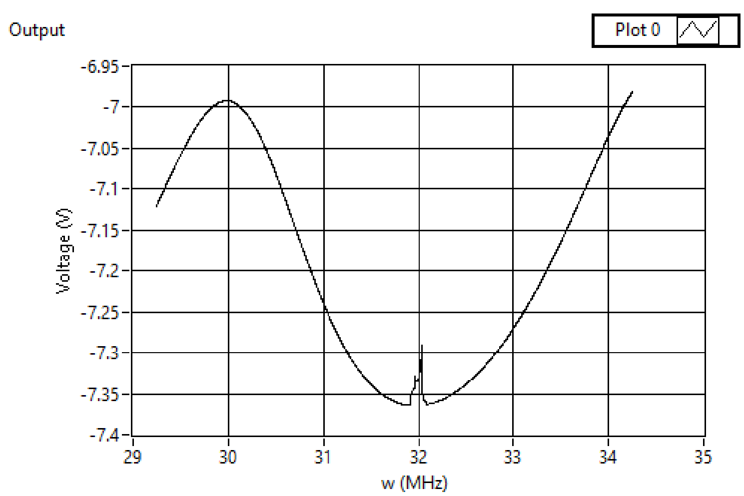

Figure 10: The Qmeter simulation with a deuteron at 80% polarization.

When running the simulation on deuteron data, it is necessary to adjust the parameter *knob* (see section 4) which adjusts the capacitance in the LC circuit, thereby tuning the resonance frequency of the circuit. The deuteron resonant frequency is around 32 MHz, and it was found that a *knob* value of 0.21 yielded decent results as pictured in Figure 10. The signal should be located in a region where the background signal is relatively flat.

A narrower range on the same data reveals the following plot:

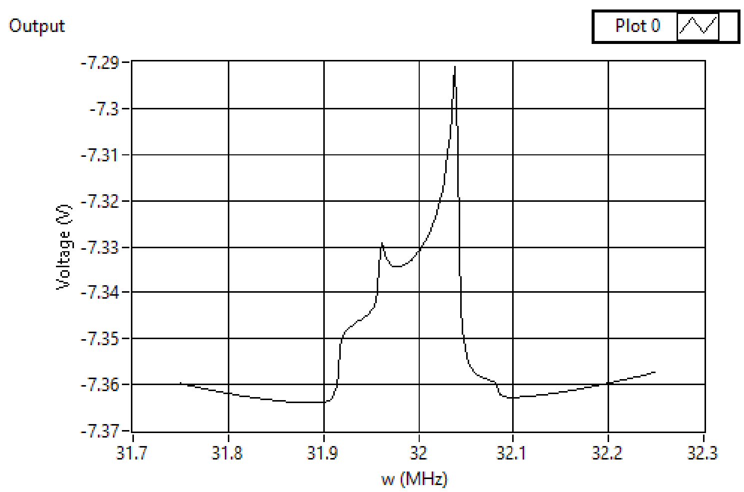

Figure 11: The Qmeter simulation with a deuteron at 80% polarization.

Adjusting to a lower polarization results in a smaller curve with more closely balanced peaks, as seen in Figure 12.

This simulation improves on purely simulating the lineshape, in that we may adjust various parameters of the circuit and observe the effect on the expected signal, even beyond the main controls provided in the LabVIEW interface. For instance, Figure 13 demonstrates the effect of changing L_0, the pickup coil inductance, to $50nH$ (all plots besides this used a value $L_0 = 30nH$). The resonant frequency of the circuit is no longer tuned to the target, and the background signal is noticeably less flat than in 12. This means that the simulation may be used to quickly test the effect of alternate circuit components, which may be used to improve these methods.

One limitation to this software is that noise is not factored into the calculation. As noted in [2], Qmeter measurements of nucleon targets face the issue of a poor signal-to-noise ratio. The coil current must be kept low to not disturb the spin-state populations, and in combination with typically low polarizations achievable in experiment, the signal is small enough that noise becomes a limiting factor on accuracy. The simulation is meant more for qualitative than quantitative purposes - i.e. adjust parameters or data and observing how the expected signal changes - but the addition of noise may increase the software's usefulness in replicating experimental conditions.

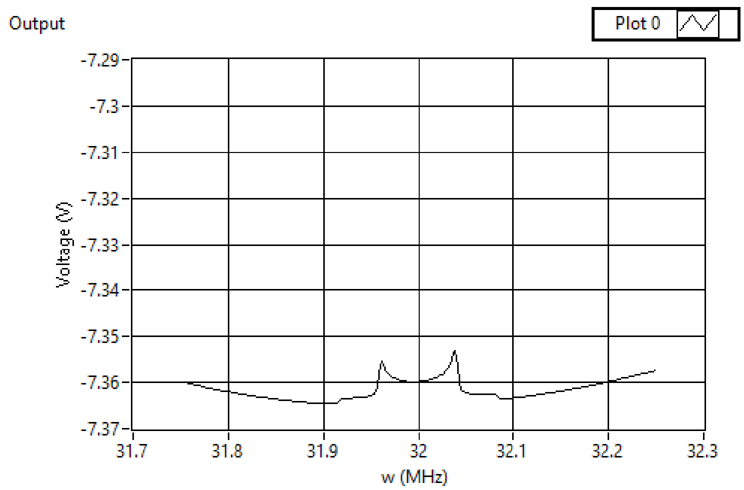

Figure 12: The Qmeter simulation with a deuteron at 10% polarization.

In addition, some parameters are not fully explored. One such example would be C_E, the calibration constant (see section 5) which allows the theoretical deuteron lineshape height to be converted into physical units. This was chosen not based on any real measurement, but rather by what value could create readable data for the purposes of this study. The calibration constant is found in experiment, so a real experiment on a deuteron target may help improve the realism of the simulation.

Another parameter which is not fully explored is the signal width. Whereas the calibration constant deals with the height of the signal, the signal width refers to how "spread out" the signal is across the frequency domain. As the simulation is currently written, there are parameters $W_h igh$ and $w_l ow$ which define the range of frequencies in which we expect to find our signal. The dimensionless signal data (which was generated as per the program in 5) is spread over this range of frequencies. However, there are factors in reality which may affect the signal width which are not accounted for in the simulation. The width of the signal is affected by the spin-spin relaxation rate [4].

7 External links

View the code for the Qmeter simulation on github: `https://github.com/crovellac/qmeter_simulation`.

For more info on the circuitry of the Qmeter, including blueprints and Computer-Aided-Design files, see: `https://confluence.its.virginia.edu/display/twist/Q-meter`.

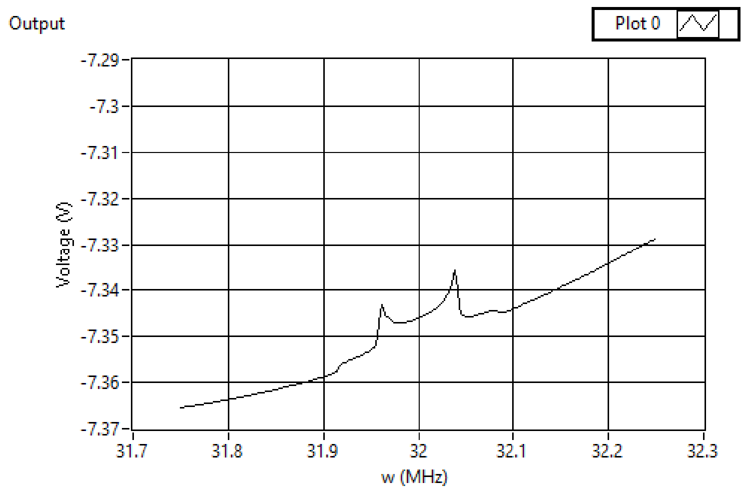

Figure 13: 10% polarization with L_0 changed from $30nH$ to $50nH$

References

[1] T. D. Averett, D. G. Crabb, D. B. Day, T. J. Liu, J. S. McCarthy, J. Mitchell, O. A. Rondon-Aramayo, D. Zimmermann et al., Nucl. Instrum. Meth. A427, 440-454 (1999)

[2] Ultra-Physics LTD. “Qmeter Manual.” Oliver Lodge Laboratory.

[3] J. Donaghy, ”Construction of an NMR Polarimeter for a Dynamically Polarized Nuclear Target” Deptartment of Physics, University of New Hampshire, Durham, NH, May 2011.

[4] D. Keller, ”Modeling Enhancement for Solid Polarized Targets”. University of Virginia, Charlottesville, VA, March 2018.

[5] G. Court and M. Holden, computer code S214NCC6.MCD, Physics Department, University of Liverpool, Liverpool, United Kingdom, August 1997.