

Pulsed Nuclear Magnetic Resonance and Spin Echo

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Goals

The main goal of this experiment is to determine the magnetic moment of the proton. By observing a resonance condition when applying an rf field to a collection of protons (i.e., a small container of water), the proton magnetic moment is determined from a measurement of the magnetic field strength and frequency.

Background

This experiment is an example of magnetic resonance - a class of experiments in which very small energy separations (typically 10^{-7} eV) of quantum mechanical states are determined by measuring the frequency of a sinusoidally varying magnetic field, which induces transitions between the states. Some examples of magnetic resonance experiments are: nuclear magnetic resonance [1, 4], nuclear quadrupole resonance [4] electron spin resonance [5], atomic beam magnetic resonance [6], and optical pumping [7]. These different experiments are distinguished by the systems under study i.e. atoms, nuclei, or solids, and by the method of detection of the resonance. Magnetic resonance has played an important role in almost every field of physics. Examples of the physical quantities measured in these experiments are given below.

Field of Research	Examples of Quantities Measured by Magnetic Resonance
Elementary Particles	Magnetic moments of the electron, proton, and neutron. Structure of positronium and muonium. Upper limit on the electric dipole moment of the neutron
Nuclear Physics	Nuclear magnetic dipole moments, electric quadrupole moments, magnetic octupole moments, and spins
Solid State Physics	Spin-lattice and spin-spin relaxation times. Knight shifts. Magnetic fields at the nucleus for ferromagnetic and anti-ferromagnetic solids. Energy level structure of paramagnetic ions in crystals and the structure of V_K centers
Atomic Physics	Fine and hyperfine structures. Zeeman and Stark effects. Lifetimes of excited states. Lamb shifts.
Biology	Structure of organic molecules and proteins (NMR), study of photosynthesis (EPR)
Medicine	Magnetic resonance imaging

In addition, through magnetic resonance it has become possible to measure magnetic fields to better than a part in 10^6 and to construct new time standards based on atomic resonance frequencies (The cesium atomic clock is presently used).

Nuclear Magnetic Resonance in Diamagnetic Substances

For a diamagnetic substance, such as water, the local magnetic field at the nuclei is only slightly lower (by a few parts per million) than an applied field. The nuclei interact with the applied magnetic field because of their magnetic moments. This is exactly analogous to the interaction of *atomic* magnetic moments with the external magnetic field, which gives rise to the Zeeman effect in atomic spectroscopy. The interaction energy is given by $E = -\boldsymbol{\mu} \cdot \mathbf{H}$, where \mathbf{H} is the applied magnetic field. The magnetic moment vector $\boldsymbol{\mu}$ can be

taken parallel to the angular momentum vector $\hbar\mathbf{I}$. The relationship between the two vectors is conventionally written as:

$$\boldsymbol{\mu} = \gamma\hbar\mathbf{I} = g\mu_N\mathbf{I}, \quad (1)$$

where γ is the ‘‘gyromagnetic ratio’’, μ_N is the nuclear magneton $\mu_N \equiv e\hbar/2M_p c$, M_p is the mass of the proton and g is a dimensionless nuclear g-factor. The magnetic moment is defined as $\boldsymbol{\mu} = g\mathbf{I}$, where I is the quantum number for the total angular momentum of the nucleus. If the magnetic field is taken in the z-direction, $\mathbf{H} = H\hat{\mathbf{z}}$, the interaction Hamiltonian can be written as:

$$\mathcal{H} = -g\mu_N H I_z. \quad (2)$$

The eigenvalues of the Hamiltonian are:

$$E_m = -g\mu_N H m, \quad (3)$$

where m is a quantum number that takes on the values in $I, I-1, I-2, \dots, -I$. The energy level diagram for $I = 1/2$ and $g > 0$ is shown in Figure 1:

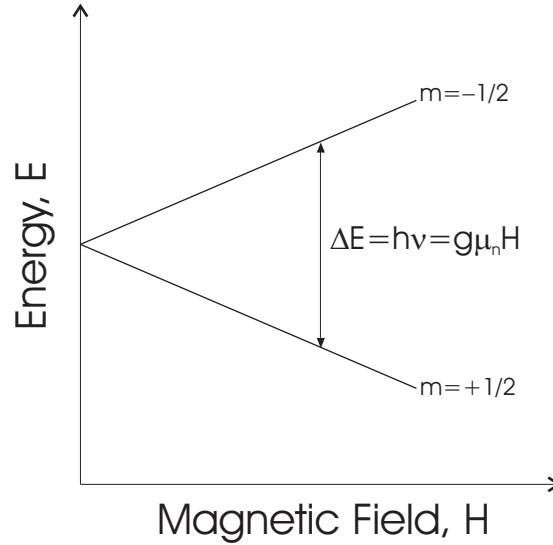


Figure 1: Energy levels of a spin 1/2 nucleus

Experimentally, we measure the frequency $\nu = g\mu_N H/h$. The detection of the resonance (equality of ν applied and $g\mu_N H/h$) is made possible by the fact that there is a slight excess of nuclei in the lower energy states. Because of this excess the application of an oscillating (rf) magnetic field of the correct frequency can lead to (1) absorption of energy from the circuit producing this field and (2) other effects due to the motion of the total magnetic moment of the sample.

The rf field induces transition from the $m = 1/2$ to the $m = -1/2$ state at a rate

$$R_{1/2 \rightarrow -1/2} = N_{1/2} W, \quad (4)$$

where $N_{1/2}$ is the number of nuclei in the $m = 1/2$ state. Similarly

$$R_{-1/2 \rightarrow 1/2} = N_{-1/2} W. \quad (5)$$

(The validity of the assumption of a time independent transition rate is discussed in Ref. 2). Therefore, the rate of absorption of energy is

$$\frac{dE}{dt} = N_{1/2} W h \nu - N_{-1/2} W h \nu = W h \nu (N_{1/2} - N_{-1/2}). \quad (6)$$

Since spins tend to go into a state of thermal equilibrium with the sample, $N_{1/2} \neq N_{-1/2}$ and therefore $dE/dt \neq 0$. Thermal equilibrium at temperature T implies that the ratio $N_{-1/2}/N_{1/2} = \exp(-\Delta E/k_B T)$,

where k_B is the Boltzmann constant. The rate at which thermal equilibrium is approached is characterized by the “spin-lattice relaxation time” T_1

$$\frac{dn}{dt} = \frac{n_0 - n}{T_1}, \quad (7)$$

where $n \equiv N_{1/2} - N_{-1/2}$, and n_0 is the value of n at thermal equilibrium.

The magnetic resonance signal is also characterized by a *width*. This width is *not* determined from the upper state lifetime, which is many times the age of the universe, but rather by the fact that the magnetic field seen by each nucleus in the sample is slightly different. This difference is sometimes due to the fact that the field generated by the magnet is not uniform. Even for a perfectly uniform applied magnetic field, however, there is a variation in the internal magnetic field seen by a given nucleus because the local field depends also on the field generated by neighboring nuclei. The spread in this local field can be expressed in terms of a spread in frequency $\Delta\omega$, which can, in turn, be expressed in terms of a time constant $T_2 = 1/\Delta\omega$, generally used in the literature

The rate equation formalism described in Eqs. (4 - 6) is based on the assumption that the applied rf magnetic field is very small and that the frequency and amplitude don't change in time. In cases where these assumptions don't hold the system can exhibit transient effects. For example, a very short pulse of the rf magnetic field can cause the system to “ring” even during times after the applied pulse is turned off. This ringing is analogous to the striking of a bell. Transient effects also occur when the rf field is swept rapidly through resonance. Under appropriate conditions, these transient effects can be observed in this experiment.

Apparatus

Overview

An overview of the experimental setup is shown in Fig. 2. In this experiment, a set of radio frequency (rf) pulses is applied to the pickup coil and the resulting precessing magnetic moment is picked up by the same coil. The radio frequency is generated by an oscillator, and switched on and off by an rf-switch controlled by a pulse generator. These pulses are then amplified by a 5 W rf amplifier before going to the probe circuit.

The probe circuit consists of the pickup coil and a pair of adjustable capacitors. (If you look into the magnet, you will see the pickup coil wedged between the pole pieces of the magnet. The adjustable capacitors are mounted inside a box on the front of the magnet.) The probe circuit is configured in such a way that with appropriate adjustment of the capacitors, the impedance of the circuit when “looking into it” is 50 Ω . By matching the impedance of the probe circuit to the characteristic impedance of the coaxial cables carrying the signal, and the other components in the circuit (amplifiers, etc), one can insure that all of the power generated by the power amplifier is transferred to the probe circuit, and any signal generated by the probe circuit is efficiently transferred to the detection circuitry.

The precessing magnetic moment induced by the applied pulses generates a voltage across the pickup coil, which is amplified by the low noise amplifier before being “mixed” with the signal from the oscillator. This “mixed-down” signal, which is at a frequency equal to the difference between the oscillator frequency and the frequency of the precessing spins is filtered and amplified further before going to the oscilloscope.

Details of the Circuit

rf Signals, Coaxial Cables, and Impedance Matching: To fully understand the operation of the apparatus, it is important to understand a few things about radio frequency electronics. One important distinction between radio frequency signals and *audio* (low frequency) signals, is that the distances between components in a radiofrequency circuit can be a significant fraction of the wavelength. Remember that the wavelength λ of a signal is related to the frequency f by $\lambda = v/f$, where v is the speed of the signal (equal to the speed of light c when the signal propagates through a vacuum). For a frequency of $f = 20$ MHz, the wavelength is 15 m.

In this experiment, *co-axial cables* are used to convey rf signals. These cables have a *characteristic impedance* of 50 Ω , which is the ratio of the voltage to the current in the cable when a traveling wave is propagating through it. When a device is connected to the end of the cable some fraction of the signal will be reflected off the device back through the cable, depending on the impedance of the device. If the device

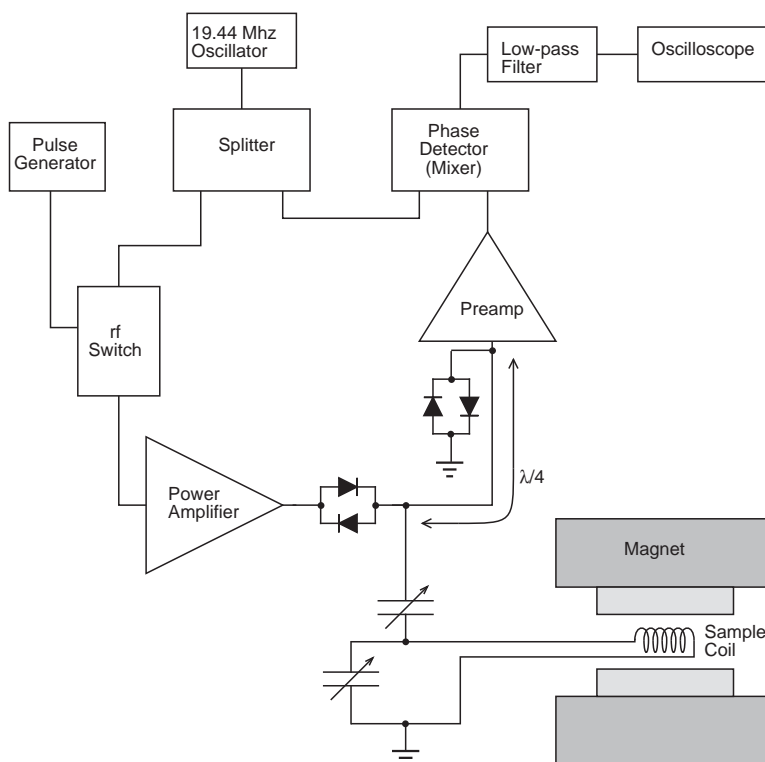


Figure 2: Overview of experimental setup.

has an impedance of 50Ω (i.e., if its impedance is *matched* to the cable), then there will be no reflection and all the power in the signal will be absorbed by the device. In general (but not always), when dealing with rf-signals, one uses 50Ω coax cables and devices with 50Ω input and output impedances.

Power Splitters: If one wants to run an rf signal to two components, one often uses a *power splitter*. The purpose of using the power splitter is to split the signal while maintaining an impedance of 50Ω .

Low-Pass Filter: This device simply absorbs (or reflects) any frequencies in the signal that are above the “cut-off frequency”. The only signals passing through the device are those with frequency below the cut-off frequency.

Mixers: A Mixer is a 3 port device (it has 3 connectors). When signals are sent to two of the ports, the mixer effectively multiplies these signals together and sends the product out the third port. As an example, suppose that two signals of frequencies ω_1 and ω_2 are entering two of the input ports respectively (remember that $\omega = 2\pi f$ is the “angular” frequency). Assume that these signals can be described by $\cos(\omega_1 t)$ and $\cos(\omega_2 t)$. The output of the mixer will have a signal proportional to $\cos(\omega_1 t) \cos(\omega_2 t)$. It can be shown using trigonometric identities that

$$\cos(\omega_1 t) \cos(\omega_2 t) = \cos[(\omega_1 + \omega_2)t]/2 + \cos[(\omega_1 - \omega_2)t]/2. \quad (8)$$

Thus, a mixer produces a signal consisting of frequencies equal to the sum and difference of the frequencies at the inputs.

A mixer can also be used as a *rf switch*. If an rf-signal is presented at one input and a dc (constant voltage) signal is presented at the other input, the output will consist of an rf signal whose amplitude is proportional to the size of the dc signal. In particular, if the dc signal has zero voltage, then no rf will exit the mixer. By turning on and off the dc voltage, one can switch the rf signal on and off.

Mixers are used for two purposes in this experiment. They are used to produce rf pulses by combining the signals from the rf-oscillator and a pulse from the pulse generator. A mixer is also used to reduce the frequency of the precessing nuclear spins (something close to 19.44 MHz) to a frequency equal to the *difference* between the precession frequency and the oscillator frequency (see Fig. 2). The mixer also produces the sum frequency, but this frequency is removed by the low-pass filter.

Crossed Diodes: *Crossed diodes* consists of 2 diodes in parallel, but pointing in opposite directions (see Fig. 2). For purposes of this discussion, a diode, when forward biased, has the properties that no current will pass through the diode if the voltage across the diode is less than about 0.6 V, and that if current *is* passing through the diode, the voltage across the diode is 0.6 V. For the purposes of this experiment, the crossed diodes can be considered to behave in the following way. If the magnitude of the voltage at one side of the pair of crossed diodes is significantly less than 0.6 V, then the crossed diodes act like an open circuit (the signal cannot pass through, and the impedance as viewed by the incoming signal is infinite). If the incoming signal is much larger than 0.6V, then the crossed diodes act simply like a wire with essentially no attenuation of the signal. One function of the crossed diodes shown in Fig. 2 is the following (another function will be described below): The crossed diodes at the input of the preamplifier insure that *during* the rf pulses, the voltage at the input of the preamplifier never exceeds 0.6 V, thus protecting the preamplifier from being damaged by the large amplitude rf pulse. The crossed diodes at the output of the power amplifier prevents any noise from the amplifier from getting into the detection circuit when the rf pulse is off, but allows the rf pulse itself to get through with very little attenuation.

$\lambda/4$ coaxial cable: A length of coaxial cable that is a quarter of a wavelength long ($\lambda/4$) has the following interesting property. If a device with impedance Z_{output} is connected to one end of the cable, then the impedance looking into the other end of the cable Z_{input} will be given by

$$Z_{\text{input}} = \frac{Z_0^2}{Z_{\text{output}}}, \quad (9)$$

where $Z_0 = 50 \Omega$ is the characteristic impedance of the cable. Thus, if one end of the cable is shorted ($Z_{\text{output}} = 0$), one will see infinite impedance looking into the other end. In the experiment, the $\lambda/4$ line is used in the following way: During the pulse, the pair of crossed diodes at the input of the preamplifier effectively shorts the amplifier input to ground. This end of the $\lambda/4$ cable therefore has zero impedance. The other end of the $\lambda/4$ cable therefore has infinite impedance, and has no influence on the signal from the power amplifier (it's as if the $\lambda/4$ cable were not connected). After the pulse is turned off and the nuclear spins are producing a signal, that signal sees an impedance of 50Ω looking into the $\lambda/4$ cable, and infinite impedance looking into the crossed diodes at the output of the power amplifier. The signal therefore travels down the $\lambda/4$ line and is efficiently coupled into the preamplifier.

General Operating Procedures

Check the circuit: Verify that the circuit is connected as shown in Fig. 4. The dashed box labeled “circuit box” contains the components laid out on the bench top. The dashed box labeled “probe tuning box” is a metal box with two knobs and two connectors on it located next to the magnet.

Tune the probe circuit: Turn on the power to the circuit (the two 15 V power supplies located in the rack). Don't turn on the power to the power amplifier yet (that's a 24 V power supply).

The capacitors C_1 and C_2 need to be adjusted to optimally match the probe coil to the transmitter and receiver. This means that the probe circuit must have 50 Ohms as seen by a 20MHz signal that enters the

circuit. One way to determine if the probe circuit has 50 Ohms is to look at the signal reflected from the probe circuit. If there is no rf reflected from the probe circuit, then it is properly matched. To measure the reflected rf, we use a device called a *directional coupler*. Figure 3 shows the circuit used to do this. To put this circuit together, disconnect the cable marked with a “D” in Fig. 4 from the mixer (the other

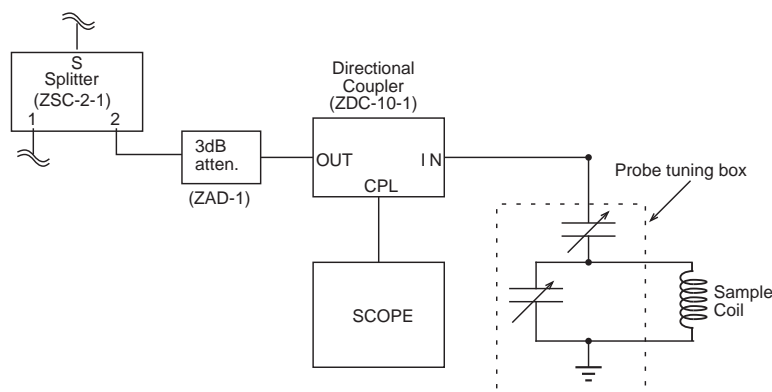


Figure 3: Circuit used for tuning the probe impedance.

end is connected to a 3dB attenuator), and connect it instead to the “OUT” port of the directional coupler (Fig. 3). Connect the “IN” port of the directional coupler to the scope. Be sure that this signal is properly terminated with 50 Ω . To terminate the signal, attach a “T” connector to the scope and a 50 Ω terminator to one side the the T connector. Connect the cable from the directional coupler to the other side of the T connector. Once you obtain a signal on the scope, adjust the capacitors (knobs on the probe tuning box) to minimize this signal. As the signal gets smaller and smaller, you will have to change the vertical scale on the scope to see it. Once you have minimized the signal, reconnect it as shown in Fig. 4.

Configure the pulse generator: Connect the output of channel 1 of the pulse generator to channel 1 of the scope (be sure it is terminated with 50 Ω s). Set the scope to trigger on channel 1 at a voltage of about 0.2 V. Configure the pulse generator to produce single pulses of about 2 μ s duration and about 10 times per second. To configure the pulse generator follow the steps outlined below. The menu buttons are the buttons immediately to the right of the display. In the steps below, the menu buttons are followed by “:”. “TM:” stands for the “Top Menu” button. First, turn on the pulse generator (if it’s already on, turn it off, and then back on). Then push the following sequence of buttons:

1. “On” button above Channel 1 output.
2. “Pulse” button (under “function”).
3. “Burst” button (under “run mode”).
4. 1-Cycle:
5. -more-: Trigger Interval: 100 ms (you can enter the “100” using the numeric keypad). This is the time interval between pulses.
6. TM: Freq/Period/Delay Menu: Period: 1 mS
7. TM: Pulse Parameter Menu: Width: 2 μ s. This is the duration of the pulses.
8. TM: Amplitude/Level Menu: Low: 0 V, High: 1.4V

Once you setup the pulse generator, you can save the configuration by pressing the “save” button. If you want to change a parameter, such as the pulse width or pulse separation go to the appropriate menu and either type in a new value on the numeric keypad or turn the wheel to change the value.

Check the rf pulses: Connect the output of the rf switches (the mixers) to the oscilloscope instead of to the input of the power amplifier. Don't forget that a $50\ \Omega$ terminator should always be used when looking at rf signals with the oscilloscope. View the pulses on the scope. They should be of about $1\ \mu\text{s}$ duration and have a peak-to-peak voltage of about 400 mV (or 0.4 V). Now increase the pulse duration until it is about $5\ \mu\text{s}$.

Finish assembling the rf circuit Now turn on the power to the power amplifier and reconnect the rf pulses to the input of the power amplifier. Connect the output of the low frequency amplifier (Ortec 4660) to channel 1 of the scope (no $50\ \Omega$ terminator is necessary here).

Load the sample Place the sample into the probe coil, which is wedged between the poles of the magnetic. Start with a sample of water with $\sim 0.05\text{M FeClO}_3$ (in the drawer under the circuit).

Turn on the magnet:

- a Turn on the cooling water.

The valve is located to the left of the sink and labeled "NMR (red) magnet". Be sure water starts running into the sink when the valve is opened.

- b Turn on the power supply.

First make sure that the "current" knob is turned completely counter-clockwise. Next be sure the voltage knob is turned all the way clockwise. Now, slowly turn up the current to about 16 A (this should be about 23 V). Note that the current should always be ramped down to zero before turning off the power supply.

When the current is close to 16 A, look at the signal on the scope for the presence of the NMR signal.

Questions

Observation of the "Free Induction Decay" (FID)

The signal you observe on the scope is a "Free-Induction Decay" (FID). Study the behavior of this signal as a function of various experimental parameters, such as magnetic field and pulse duration. Make qualitative observations and record some signals onto the computer. Attempt to explain your observations. You may need to consult some of the references (e.g., [3]). What is responsible for the decay of the FID signal?

The magnetic moment of the proton

Based on the principles described in the Introduction, determine the proton magnetic moment using a sample of water. Adjust the current until the oscillations in the signal are as low a frequency as possible (this means the the spins are precessing at the same rate as the 19.44 MHz oscillator). Measure the magnetic field at the location of the sample using the gauss meter. From these results, calculate the magnetic moment of the Proton.

Observation of the "spin-echo"

The pulse generator can be configured to produce two pulses of unequal length. To do this perform the following steps:

1. Make sure the power amplifier is turned off.
2. Connect the output of both channels of the pulse generator to the input of the resistive power combiner, and the output of the power combiner to the scope. Make sure the signal into the scope is terminated with $50\ \Omega$ s, and both channels of the pulse generator are turned on.

3. Push the button “Ch1/Ch2” between the “On” buttons above the two output channels. This allows you to configure Channel 2.
4. Follow the same steps you used (described above) to configure channel 1 (except for Channel 2).
5. Push “Burst Button”, then “-more-: Delay: $\langle \text{time} \rangle$ ”, where “ $\langle \text{time} \rangle$ ” is the time interval between the two pulses. This time interval should be several times the duration of the FID signal (say, 20-40 ms).
6. Adjust the amplitude of the pulses: Since the power combiner will reduce the amplitude of each pulse, you need to readjust the amplitudes of the pulses. Observe the pulses on the scope and adjust the amplitude (“High”) to about 1.4 Volts.

Now observe the signal on the scope. One should see an FID after each pulse plus a “spin-echo”, which occurs a time after the second pulse equal to the time between the two pulses. Adjust the magnet current to produce oscillations of the signal that have a period significantly larger than the pulse durations. Vary the width (duration) of the first pulse so that the FID after the first pulse is the maximum. Then vary the width of the second pulse so that the echo is a maximum. Note how the size of the FID after the second pulse is related to the size of the echo as you vary the width of the second pulse. Can you explain this behavior?

Now increase the time between the pulses and record the amplitude of the resulting echo. You may have to use the delayed trigger on the scope to view the echo. Record the resulting echos as a function of pulse separation. You will notice that for long times, the echo gets smaller. Estimate the “echo lifetime”: that is, the time between pulses in which the echo is half the amplitude it is for short times. This lifetime is a measure of “ T_2 ”. Repeat this experiment for pure water. Note that for pure water, you must reduce the repetition rate of the experiment to about once per second in order to see a big signal. Does the value of T_2 depend on the concentration of Ferric Chloride? What is responsible for the “decay” of the echo signal (measured as a function of the pulse separation)? Make a plot of the echo size as a function of pulse separation for two different concentrations of Ferric Chloride.

The effect of the local environment on the nuclear magnetic resonance

The ability to detect the resonance requires some energy flow from the electronic circuit to the nuclear spins and to the molecular environment. The strength of this “relaxation” process (characterized by the constant T_1) can be adjusted in water by adding various amounts of a paramagnetic salt, in this case ferric chloride. Estimate the value of T_1 of water containing the following concentrations of ferric chloride: zero, 0.01, 0.05, 0.1, and 0.5 molar (moles/liter). (For pure water the relaxation time T_1 is in the range of seconds). To make this measurement, setup a two pulse experiment with the time interval between pulses equal to several times the FID duration. Now adjust the pulse durations so that the FID after the second pulse is a minimum. If the period of oscillations of the signal is much larger than the pulse durations, it should be possible to make the FID after the second pulse much less than the FID after the first pulse. With this pulse duration, record the FID after the second pulse as a function of interval between pulses. The rate of this recovery is a measure of T_1 . Plot the size of the FID signal after the second pulse as a function of pulse separation. Compare this with what you expect theoretically.

Measurement of the magnetic moment of ^{19}F .

The magnetic moment of ^{19}F is close to that of protons. To make this measurement, remove the water sample from the probe coil and replace it with a sample of Teflon. Then adjust the magnetic field until a signal is observed (the value of the current should be around 17A). Measure the magnetic field at which the resonance occurs with the gauss meter.

Determine the decay time of the signal (save some traces to the computer). How does this compare with what you observed for water? Now attempt to observe a spin-echo. Do you see one? Why or why not?

Observation of the “Stimulated Echo”

Another interesting experiment is the observation of the *stimulated echo*. In a stimulated echo, one first applies two 90° pulses spaced time T_{12} apart, followed by another pulse at time $T > T_{12}$. In addition to the

usual spin-echos (how many would you expect there to be in this case), there will be a stimulated echo at time $t = T + T_{12}$.

To produce the required pulse sequence, first connect the output of the power combiner to the scope (as for spin-echo). Then configure Channel 1 to produce two pulses instead of one. Push the following buttons to do this:

1. “Burst” button (under “run mode”).
2. N-Cycles: 2
3. Adjust the period between pulses to be a few times the FID duration. Push “TM: Freq/Period/Delay Menu: Period: \langle time \rangle ”

To set up this experiment, it may be easier to increase the inhomogeneity of the magnet to decrease the duration of the FID and echo signals. Ask the instructor to help you do this.

When you get a signal you will see several spin-echos as well as the stimulated echo. Adjust the duration of the first two pulses and the third pulse to maximize the stimulated echo.

Make a measurement of the lifetime of the stimulated echo (by increasing the time between the first first two pulses and the third pulse (keeping the time between the first two pulses constant), and record the size of the echo signal as a function of this time. How does this graph compare with the spin-echo lifetime results?

What is going on in the stimulated echo experiment, to explain you lifetime measurements ? You can try looking in Slichter for an explanation of the stimulated echo.

References

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Using the DOS based program “GETWFM”:

This is the recommended procedure to save files, since it has features that make saving data more convenient. This software, however, only lets you save one scope channel at a time. Do the following to run this program:

1. Start a DOS window (there should be an icon on the desktop to do this)
2. Navigate to the directory where you want to save the data
3. Type “GETWFM” at the DOS prompt
4. The program should start. How to use it should be self explanatory.

Using the Tektronix software “OpenChoice Desktop”:

1. Use ”OpenChoice Desktop” icon on the desktop to run the software
2. Hit the button ”Select Instrument” on the left
3. Choose the one from the list and press ”OK” button
4. Now you have a choice of the tabs on top of the screen. For data capturing, press ”Waveform Data Capture”
5. Press ”Get Data” on the left
6. Once the data is captured and plotted in a scope-like screen, it can be saved by pressing ”Save As” button.

Data can be saved in three different formats: one ‘txt’ format, and two ‘cvs’ formats. The difference between ‘cvs’ formats is that ‘multiple cvs’ saves the data from two channels into two different files, wether the simple ‘cvs’ puts all the data into one file. If you wish to save both channels it is suggested you save them in a single file. Mathematica can read the individual channels saved this way.

Appendix C: Analysing the data

To plot and analyze the data, it is convenient to read it into a data analysis programs such as “Mathematica” or “Matlab”. Routines have been written in both Mathematica and Matlab to read the two types of files listed above. These routines can be found in directories on the PC associated with the NMR experiment.