Lab 1: Earth's Field NMR

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Galen Reed (GSI), Miki Lustig (Prof)

1 Introduction

In this lab, we will acquire spectra using an Earth's field spectrometer. This lab will cover basic NMR concepts such as acquiring free induction decays (FID), transmitter strength & flip angle calibration, B_0 strength and homogeneity, and basic NMR experiments such as pulse / acquire, spin echoes, and relaxation parameter measurements.

1.1 Hardware

The spectrometer consists of concentric B_1, gradient, and polarization coils (Fig 1). It is a pre-polarized MRI system in which a stronger, but inhomogeneous electromagnet is used to polarize the sample, and another, weaker and very homogeneous field is used for the signal detection. We will utilize the earth's field for signal detection, which at Berkeley's latitude, make an approximately a 65° inclination angle with the vertical and has a strength of about 0.5 Gauss. Our detection frequency is

$$f_0 = \gamma B_e / 2\pi \approx 2 \text{ kHz} \tag{1}$$

We are calling the axis of this field z, analogous to the B_0 in standard NMR / MRI systems; the solenoidal axis is defined as x (Fig 2). Notice how all of the coils are concentric and point along x (Figs 1, 2). In this respect this system is different from standard NMR / MRI systems in that the detection field (Earth's magnetic field) is perpendicular to the longitudinal (x) axis of the system (most systems use the detection field parallel to the solenoid axis). Recall that when we drive current through a solenoid, we produce a longitudinal magnetic field (use the right hand rule with your fingers wrapping around the coils in the direction of the current). The strength of this field is approximately

$$\vec{B} = \mu_0 N I \hat{x} \tag{2}$$

where I is the current and N number of coil turns per length (along x).

1.2 RF Coil

When we drive a low frequency AC field though the coil, we generate a field along x that also oscillates at the driving frequency. In the lab frame, this field can be written as

$$\vec{B_1} = B_1(t) \cos \omega t \ \hat{x}, \tag{3}$$

where ω is a tunable parameter and $B_1(t)$ is the amplitude modulation. The B_1 field can also be written in terms of complex exponentials as,

$$\vec{B_1} = \frac{1}{2} B_1(t) \left(e^{i\omega t} + e^{-i\omega t} \right). \tag{4}$$

In this case, it is only the right circular polarization is going to interact with the magnetization (The other component is "off-resonance") so the effective field that interacts with the magnetization is,

$$\vec{B_1} = \frac{1}{2} B_1(t) e^{-i\omega t}. \tag{5}$$

For this experiment, $B_1(t)$ is just an on/off control (i.e. a rect function in time). This is how we generate our RF pulses (Note, that RF is not really the right terminology here. 2KHz is well within the audio range). Recall the rotating frame treatment of RF pulses where we are allowed to express the pulse simply as

$$\vec{B_{1,rot}} = \frac{1}{2} B_1(t) \ \hat{x}. \tag{6}$$

We lose a factor of 2 in field strength per current because we use a linearly polarized RF field in $\hat{x}$, but this is unimportant in this case where efficiency is not a great issue.

Coil Parameter	Polarizing Coil	Gradient Coils (pgse,x,y,z)	B_1 Coil
Avg. coil diameter (mm)	170	105	84
Calc. mag. Field (mT/A)	3.13	N/A	30
Field gradient (mT/m/A)	N/A	2.38,0.31,0.28,0.28	N/A
Avg. Resistance (W) incl. cable	2.8	3.1/2.0/1.5/1.5	325
Tuning cap for 2300 Hz (nF)	N/A	N/A	9.7

Figure 1: The concentric coils of the Terra Nova unit

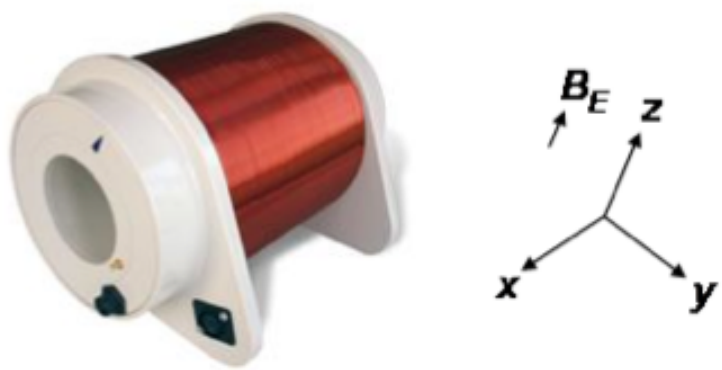

Figure 2: Basic geometry of the NMR spectrometer. The solenoidal axis is defined as x.

1.3 Polarizing Coil

The Terra Nova unit has a polarizing coil, which is just another solenoid along x. We apply a switchable DC current through this coil, and turn it on for some period and switch it off before we play the B_1 pulse and perform signal detection. The need for this coil is evident when we look at the Curie magnetization induced by a field with strength B_0:

$$M = N\mu \tanh\left(\frac{\mu B_0}{kT}\right) \tag{7}$$

This expression is specific to spin $S = 1/2$ particles. μ is the magnetic moment of a single nucleus ($\mu = \gamma\hbar S$), N is the number of nuclei in the sample, k is the Boltzmann constant, and T is the temperature in Kelvin. The tanh term (sometimes called P for polarization) just describes the fraction of the spins aligned with the B_0 vector, so equation 7 just says

$$\text{total magnetization } = (\#\text{ nuclei}) \times \left(\frac{\text{magnetic moment}}{\text{single nucleus}}\right) \times (\text{frac aligned with } B_0) \tag{8}$$

$P = \tanh(\mu B_0/kT)$ is 0 for $B_0 = 0$ (no field, no polarization), linearly increases with B_0 for a bit, and asymptotically approaches 1 when $\mu B_0 \gg kT$. For most NMR applications, this is no where near the case, and we are making all our images with $\mu B_0/kT$ pathetically small. The polarization coil operates with a peak current of 6 A generating a peak $B_p = 18.8$ mT giving $P = 6 \times 10^{-8}$. For comparison the Earth's field $B_e = 50\mu$T, and $P = 2 \times 10^{-10}$. A standard clinical scanner operating a 1.5 T will give $P = 5 \times 10^{-6}$, a big gain but sadly 6 orders of magnitude shy of 100% polarization.

We use B_p to make $P = 6 \times 10^{-8}$ instead of 2×10^{-10} which translates directly to a ~ 300 fold SNR increase over using the earth's field for polarization. However, we are performing all B_1 excitation and signal detection with B_p switched off, so how do we extract this gain from the polarization coil? It turns out the increased polarization will live for a little while after B_p is switched off. The z component of the Bloch equation is

$$\frac{dM_z}{dt} = \frac{1}{T_1}\left(M_z - M_0\right), \tag{9}$$

where T_1 is a time constant, M_z is the "current" z component of M, and M_0 is the equilibrium M (given by eq 7) that depends on the "current" B_0. Therefore, we have a time $\sim T_1$ before the polarized magnetization dies off back to the 2×10^{-10} induced by the earth's field. This is also why we have to leave B_p on for a few seconds before we do any detection: the magnetization will take T_1 seconds to approach the higher polarization induced by B_p.

Another concern with the polarization coil is that it generates the polarization in the wrong direction (we want it along z, but it generates it along x). However, this turns out to be not a big deal provided that B_p is switched off slow enough (or adiabatically) . Specifically, as long as the rate of change of B_p is much less than the Larmor frequency, the magnetization will track the field and will end up lined up with B_e, i.e. along z by the time we play the B_1 pulse.

2 Experiments

2.1 Pulse / Acquire FID

The most basic NMR experiment is the pulse / acquire, or pulse collect experiment consisting of an RF excitation followed by a data acquisition period. Our version of this basic sequence is *slightly* complicated due to the need for a polarization pulse. Fig 3 shows this sequence as we'll implement it. Following the polarization pulse, we play the excitation, and this is followed by a data acquisition period.

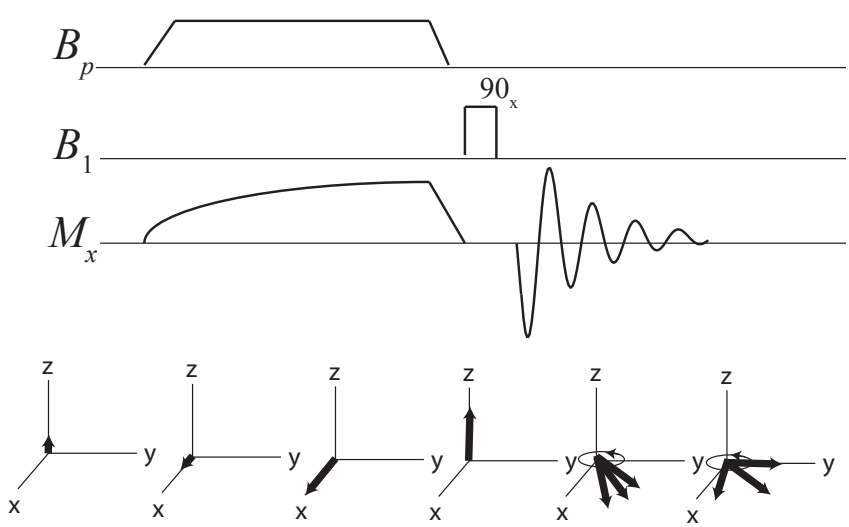

Figure 3: The pulse / acquire experiment.

The magnetization response after during readout is easily described by a Larmor frequency oscillation term and a decay envelope. The decay term is a combination of the "native" decay constant T_2 and another term which depends on the homogeneity of the sample. This term is called T_2^*, and is defined as

$$1/T_2^* = 1/T_2 + 1/T2', \tag{10}$$

where $T2' \propto \Delta B_0$ is proportional to the spread (inhomogeneity) of the field strength ΔB_0. Expression 10 is almost always dominated by the second term, so we can almost always ignore the T_2 contribution to the decay envelope of pulse / acquire experiments.

The signal encoded immediately following an RF excitation is

$$S(t) = e^{-i2\pi f_0 t} e^{-t/T_2^*}, \tag{11}$$

where we've defined $f_0 = \gamma B_0 / 2\pi$ as the Larmor frequency. Magnetic field inhomogeneity increases the damping, and also affects the spectral appearance. We can calculate the spectra analytically by taking a (half-sided) Fourier transform:

$$\begin{aligned} S(f) &= \int_0^\infty S(t) e^{-i2\pi f t}\, dt \\ &= \frac{-1}{1/T_2^* + i2\pi\,(f - f_0)} \end{aligned}$$

This curve is called the Lorentzian line shape, and it has some key characteristics which are more readily visible in magnitude:

$$|S(f)| = \frac{T_2^*}{\sqrt{1 + (2\pi T_2^*)^2\,(f - f_0)^2}} \tag{12}$$

This is just a spike centered at f_0 with some width which is due to damping. Note that the peak signal on resonance is T_2^*, and the full width at half maximum $(FWHM) \sim 1/T_2^*$ (see Fig 4, right). Therefore, we can see how magnetic field inhomogeneity ΔB_0 directly affects the data quality. For a well "shimmed" magnetic field, ΔB_0 is small, so T_2^* is big, so the $FWHM$ of the spectra is narrow and the spike is tall. When the homogeneity diminishes, our peak is blurred out (Fig 5). MRI image quality is always improved with long T_2^* / small ΔB_0 since the integrated signal over the readout (and thus the SNR efficiency) is higher.

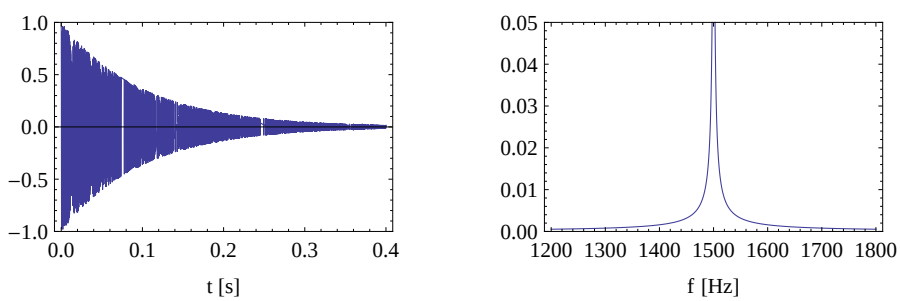

Figure 4: Pulse acquire FID with a long T_2^*: a well shimmed magnet

The Terra Nova uses the fact that the height of the spectra is proportional to T_2^* to perform automatic shimming. In other words, it automatically iterates the current in shim coils (DC coils that spatially alter B_0) in order to minimize ΔB_0 between pulse / acquire experiments.

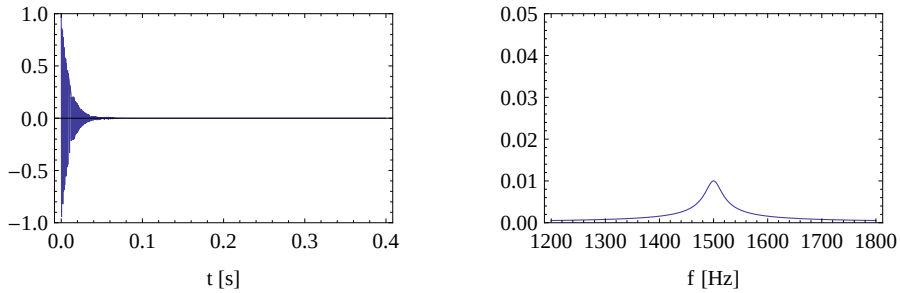

Figure 5: Pulse acquire FID with a short T_2^*: a badly shimmed magnet

2.2 Coil Capacitance Calibration

We can use some linear circuit analysis to optimize the efficiency of the transmitter (B_1 coil). The coil is itself a resonant circuit, and can be loosely approximated as a series LRC circuit. L is the inductor, which is just the coil itself. The circuit has a resonance with some width (proportional to R), and a resonant frequency centered at

$$\omega = \frac{1}{\sqrt{LC}}. \tag{13}$$

In order to maximize the efficiency of the transmitter, we will want to first measure the resonant frequency (via a pulse acquire experiment). The spectrometer automatically generates an ω versus C curve, and we manually set C to the proper resonance frequency. This is a tunable parameter by necessity since B_e can vary significantly as a function of geography.

2.3 90° Pulse Calibration

We ignored the amplitude of the signal response in our treatment in the pulse / acquire section, but the amplitude actually is a function of the polarization and flip angle:

$$S(t) = e^{-i2\pi f_0 t} e^{-t/T_2^*} M_z \sin\theta, \tag{14}$$

where θ is the RF pulse flip angle. Recall that this is just

$$\theta = \gamma \int_0^T B_1(t)\, dt \tag{15}$$

which is the "pulse area." For our spectrometer, the pulse is just a square function

$$B_1(t) = |B_1| \sqcap \left(\frac{t}{\Delta t}\right)$$

so

$$\theta = \gamma B_1 \Delta t$$

To calibrate the 90° pulse, the spectrometer plays pulse/acquire experiments at varying values of the pulse width Δt. What should the maximum value of the spectrum $S(f)$ look like as a function of Δt? Once we find the 90° pulse, then we know what a 180° is too: we just double Δt.

2.4 The Spin Echo

Say we want a measurement of the actual sample-specific T_2 (which varies with molecular structure, temperature, solvent viscosity, and a million other interesting parameters), and not the B_0 inhomogeneity-dominated parameter T_2^* which the pulse/acquire experiment gives us. It turns out we can extract this parameter with a 2-pulse experiment called the spin echo. A second RF pulse placed $TE/2$ after the first refocuses the magnetization dephased by T_2^*, and we get the signal back again at $TE/2$ after the second pulse. The echo is not full amplitude; it's actually modulated by the pure T_2 decay curve (but the echo grows and dies on either side by the old T_2^* envelope). The second pulse does not necessarily have to be a 180°, but this is the angle that maximizes the response.

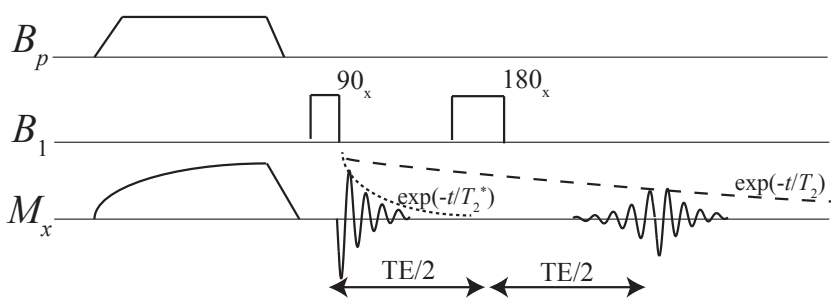

Figure 6: The spin echo experiment.

Figure 6 shows the basic spin echo experiment. As before, we use B_p to boost the SNR. Only the data after the second pulse is acquired. A single spin echo experiment doesn't give us a T_2 estimate, however. We have to repeat the experiment with multiple TE values in order to generate an exponential decay curve of the echo amplitudes.

The spin echo signal is a symmetric echo; what does this imply about the phase detection of the spectrum $S(f)$? It turns out there are many reasons to perform spin echoes besides estimating T_2. We can use the T_2 as a contrast generating mechanism for MRI. For materials with long T_2 (and systems with short T_2^* such as ours), there are large SNR benefits to acquiring spin echo versus pulse/acquire data.

2.5 The Carr Purcell Meiboom Gill (CPMG) Sequence

The CPMG experiment is a modification of the spin echo experiment. This time we play a spin echo train, and between each refocusing pulse we acquire the echo. Since each echo is modulated by a T_2 decay, we can perform a T_2 measurement in a single acquisition. However, there is a price to be paid for acquiring the measurement in a single scan, and it is sensitivity to flip angle. For a $90_x, 180_x, 180_x, 180_x, ...$ sequence, the 180s must be calibrated *perfectly* to generate a T_2 curve. As the blue dotted line in Figure 8 shows, when we are only 2° away from a perfect 180 (a 1% error in RF calibration), the signal response curve is vastly different from the pure T_2 decay curve after only a few echoes. This is because the error propagates between each echo. What do you think the actual % error in RF calibration is?

A clever way to address this instability is to play the 180° pulses with a phase advance of $\pi/2$ with respect to the initial pulse; i.e they are y pulses. In this way, the RF amplitude

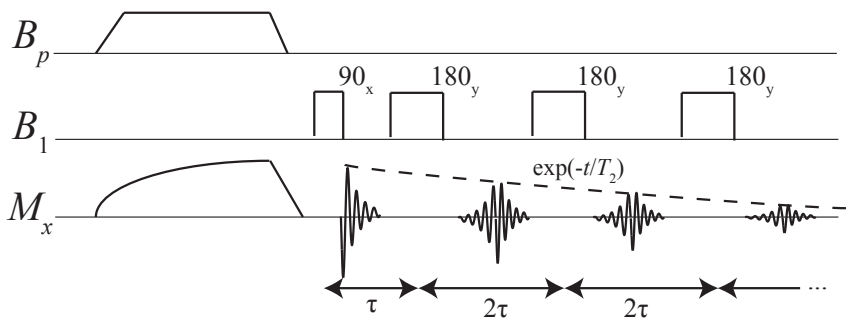

Figure 7: The CPMG experiment.

error does not corrupt the signal response (see Figure 8) since the errors are not cumulative in echo number. The CPMG experiment is the basis for the commercial "fast spin echo" (FSE) or "turbo spin echo" (TSE) scans which are used to obtain high resolution T_2-weighted images in nearly every clinical exam.

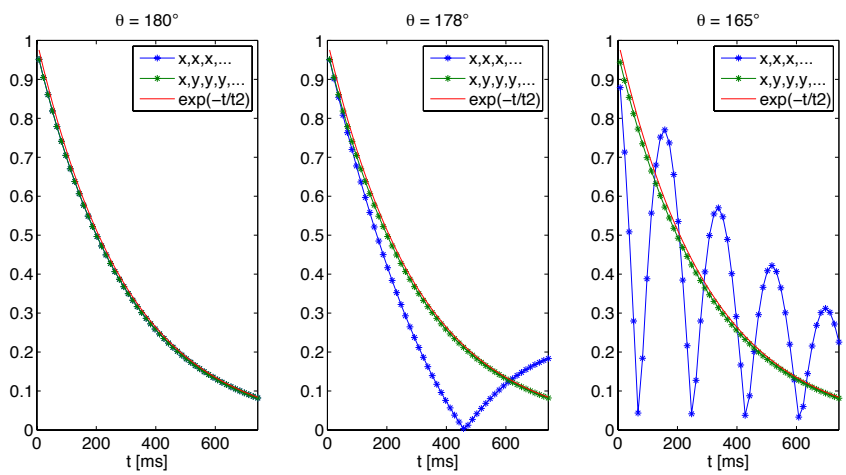

Figure 8: The ideal T_2 decay curve (red) is plotted with the signal response of the $90, 180, 180, 180, ...$ sequence using phase modulation $x, x, x, ...$ (blue) and $x, y, y, y, ...$ (green)