Earth's-Field NMR Gradient/Field Coil System

Operating Manual, student version (condensed)

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I. Introduction

I.A. Earth's-Field Nuclear Magnetic Resonance

Protons have mass, charge, and angular momentum, but in addition they possess magnetic moments; and the net magnetic moment of a suitably prepared sample of protons, placed in a static and uniform magnetic field, will precess at a characteristic frequency. This precessional motion in space is so real that it will induce, by Faraday's Law, an emf in a coil of wire surrounding the sample, and the resulting sinusoidal oscillations can be detected by ordinary electronic means. When the magnetic field strength is of order 50 μT, typical of the ambient geomagnetic field on earth's surface, the precession frequency is about 2100 Hz, conveniently located in the audible range of the frequency spectrum. This is the physical effect that is made accessible by TeachSpin's "Earth's-Field Nuclear Magnetic Resonance" apparatus.

This manual describes the function and use of a valuable addition to that EFNMR apparatus, the "EFNMR Gradient/Field Coil System", which markedly extend the quality and range of experiments that can be done in magnetic resonance. Here are the capabilities of the Coil System you are about to use:

- You will be able to use 'gradient coils', whose purpose is to make the ambient magnetic field strength much more uniform in space. The result will be NMR signals lasting much longer in time, no longer limited by the inhomogeneities in the local magnetic field.
- You will be able to use 'Helmholtz coils', whose purpose is to add to, or subtract from, the local magnetic field an accurately known and controllable field. The result will be a first-principles measurement of both the proton magnetic moment in absolute units and the local magnetic field strength in Tesla.
- You will be able to orient the Helmholtz-coil symmetry axis to lie along the direction of the local earth's field, and you'll be able to measure the consequences of any misalignment. The result will be a lesson in vector addition, and in the correction of systematic error.
- With the long-lasting precession signals that you will obtain, you'll be able to investigate a host of physical effects that influence the decay in time of free-precession signals. These are called "T_2 studies", and they are parallel to but distinct from the "T_1 studies" that are described in the EFNMR manual.
- With the variable magnetic field available from the Helmholtz coils, you will be able to bring into the 1600-2500 Hz tuning range of the EFNMR apparatus the nuclear precession signals from a variety of other nuclei. To your list of ^{1}H (protons) and ^{19}F (fluorine), you should be able to add the NMR signals from ^{31}P (phosphorus) and ^{2}H (deuterium, in heavy water).
- You will be able to create, and hear, one kind of "spin echo" by deliberate choice of magnetic-field gradients. The result will be a very clear physical demonstration of the difference between reversible and irreversible loss of sample magnetization, and the

closest you can come in the lab to the time-reversal operation.

- Finally, by another use of deliberate magnetic-field gradients, you will be able to map sample location in physical space to signal location in frequency space, and thereby understand and accomplish the process of one-dimensional magnetic resonance imaging (MRI).

This condensed version of the EFNMR Gradient/Field Coil System manual will teach you how to exercise all these new capabilities. It assumes that you have already gotten signals from the EFNMR apparatus, and that the EFNMR Gradient/Field Coil System has already been set up and used at your location. If you have used the EFNMR apparatus, but never with the EFNMR Gradient/Field Coil System added, then the expanded version of the manual for EFNMR Gradient/Field Coil System will be appropriate for your use.

I.B. Set-up of the EFNMR Gradient/Field Coil System

This manual assumes that you already have, and have used, the EFNMR apparatus within the EFNMR Gradient/Field Coil System, and want to use its extended capabilities along the lines laid out above. For our purposes, this means that you have installed the EFNMR "head" with its base, sample coil, and bucking coil, into the assembled EFNMR Gradient/Field Coil System, according to the installation instructions that were enclosed with the Coil System; and further, that you have the whole apparatus in a location such that you have gotten "free induction decay" or free precession signals using a sample of water, and that you have tuned the EFNMR sample-coil to make those signals visible on an oscilloscope. An operational definition of success, and the starting point for improvements, is a signal with identifiable frequency, and with duration of at least 50 ms. [In particular, you need to be sure that you can recognize a difference between the signal emerging from the EFNMR apparatus when the sample bottle is removed (the coil transient) and the signal when it is present (the longer-lasting free-precession signal).]

So you will now have the EFNMR head in its chosen location in space, elevated above a tabletop by the frame of the Coil System. Connect the EFNMR head to its controller in the usual way, attach the polarizing power supply that you have previously used, and confirm that you can still see a free-precession signal. You might want to use a tap-water sample, and a polarizing current of 3 A, and a polarizing duration of at least 4 s. You will need to have set the tuning of the sample coil to a value appropriate for the precession frequency expected for your location's magnetic field strength.

Connect also the Coil System's (grey 8-conductor) cable to the EFNMR Gradient/Field Coils controller box, which is designed to stand neatly atop your EFNMR controller box. Power up the Coil System by plugging its wall-transformer power supply into the ac line. At this stage you do not yet need a separate dc power supply to run the Helmholtz coils; for the next steps, you will be using the gradient coils only, and they are now energized.

You will also need a good compass and dip-needle, or the combination available from TeachSpin, since the first step in improving your signals will be to check the alignment of the axis of the Coil System along the direction of the local field.

I.C. Use of the EFNMR Gradient/Field Coil System

This section of the manual should take you from visible free-precession decay signals, with duration limited by field inhomogeneity, to beautiful free-precession signals with a duration of several seconds. You can accomplish this first by geometrical alignment, and then by gradient cancellation. There are two parameters to set geometrically (the azimuth and altitude of the Coil System's axis), and three parameters to set electrically (the strengths of the currents in three sets of gradient coils).

I.C.1. Geometrical alignment

To check the geometrical alignment, it's best to turn off the power to *both* the EFNMR and the EFNMR Gradient/Field Coils controllers. Now your sample is immersed in a vector field, the ambient magnetic field, and your task is to check if the symmetry axis of the gradient and Helmholtz coils is aligned along the local direction of this field. To do this, you'll be sensing the field's direction with a compass and/or a dip needle, and adjusting the Coil System's orientation in space.

Q1. Why should you use the compass and dip needle only *one at a time* in the vicinity of the apparatus?

You will want first to check the direction of the horizontal component of the magnetic field; your goal is to check if the orientation of the sample coil's axis is perpendicular to that component.

Q2. What's the right tool for checking the direction of the horizontal component of the magnetic field? Where in space would you want to place that tool?

You might improve this alignment by a small rotation of the entire Gradient/Field Coil System, frame and all, on the tabletop where you've placed it.

[For reference, an indicator plate on the Gradient/Field Coils shows TeachSpin's choice of axes of a Cartesian coordinate system whose origin is taken to be at the common center of the sample, the sample coil, and the Helmholtz coils. We've taken the z-axis to lie along the symmetry axis of the Helmholtz coils. We've taken the x-axis to lie along the axis of the sample coil, the symmetry axis of the sample bottles; this axis passes through two wooden 'axles' which attach the Coil System to its frame. Finally the y-axis is perpendicular to the x- and z-axis, and it passes through the center of the sample and the center of the xyz-indicator plate.]

You should be able to confirm alignment of the magnetic field's horizontal component to be perpendicular to the x-axis to within a few degrees of angle. But remember that the ambient field may be inhomogeneous, so it might vary from place to place in *direction* as well as magnitude; thus you should place your indicator alternately near both ends of the sample coil, and align in azimuth until your x-axis is as nearly perpendicular as possible to the average of these two readings of field direction.

Now you've dealt with the magnetic field's horizontal component, but there is still its vertical component to deal with.

Q3. In what plane is the vector **B** now sure to be found? With what tool will you sense the direction of **B** in that plane?

Your goal is to check the rotation of the Coil System around the wooden axles to ensure that its z-axis coincides with **B**'s direction. This adjustment in altitude can be accomplished by loosening the clamping screws at the hubs of the two axles, and hand-rotating the Coil System about the x-axis, meanwhile using your tool to sense the direction of **B**. Again the goal is to align the z-axis with **B**'s direction to within a few degrees of angle; again, you will want to position the tool near both ends of the sample coil, since inhomogeneities may give **B** different directions at these two locations. Don't forget to tighten the clamping screws after you've finished this adjustment.

I.C.2. Gradient cancellation

By the geometrical alignment, you have ensured that **B** has only a z-component at the center of the sample, so you could write $\mathbf{B}(x,y,z)$ as having $\mathbf{B}(0,0,0) = B_0\,\mathbf{z}$. But away from the center of the sample, **B** varies in magnitude and direction, and this inhomogeneity is the direct cause of the short duration of the free-precession signals you've been getting from the sample. This section tells you how the gradient coils of the EFNMR Gradient/Field Coil System can cancel out the three relevant gradients of the ambient field, thereby creating a field much more uniform in magnitude over the volume of the sample, and yielding free-precession signals of markedly longer duration.

You will be using the NMR signals themselves to accomplish these adjustments, so now turn the two controllers back on. In addition to the familiar settings for the EFNMR controller, you need to make some new settings on the Gradient/Field Coils controller: set the 'x-gradient step change' toggle switch to its uppermost 'off' position, and set the three ten-turn 'gradient adjustment' knobs to previously determined appropriate values. [If you lack these settings, start with all three dials at mid-range (at 5 on their 0-10 scales).] Now confirm that you can still get a precession signal out of the EFNMR pre-amplifier output, and note its duration (defined, operationally, as how long it takes for the signal to decay to half its initial size). This duration tells you something about how large the field gradients are, and that in turn tells you about how large an adjustment you might need to make on the gradient-adjustment knobs.

Here are some brief exercises in the quantitative consequences of a field gradient (more details can be found in Appendices 0 and 1).

Q4. Suppose that the field **B** had at the sample's center a magnitude of 50.00 μT; with what frequency would protons at the origin precess?

Q5. Suppose that the field's magnitude had a rate of variation in space of even 3 μT/m (along some direction); then at another point just 2 cm away from the origin, what field would protons in the sample bottle experience?

Q6. At what frequency would protons at this new location precess?

Q7. After (say) 0.19 s of precession time, how much would these precessing protons have gained in precession angle, compared to protons at the sample's center?

So protons in different regions of the sample get out of phase with each other in their free precession; they cease to cooperate fully in inducing emfs in the sample coil. Appendix 1 shows that a gradient of strength g will cause this dephasing to become serious in a time T, where T is given by

$$T \approx \frac{1}{c_p\, g\, S}$$

for a sample of extension ±S/2 with respect to the center. Here $c_p = 42.58$ Hz/μT is the gyromagnetic constant for protons (see Appendix 0 for notation). Thus an observation of the dephasing time T is a semi-quantitative indication of the size of the gradient you'll want to cancel out.

Q8. What value of T are you seeing for your signals? If this dephasing time is attributed solely to gradients, what characteristic strength of gradient do you infer?

The gradient coils are located in grooves cut into the wooden Helmholtz-coil forms, and they make possible the three independent and orthogonal adjustments needed; in the notation of Appendix 1, they adjust the three first-order spatial derivatives $\partial B_x/\partial x$, $\partial B_z/\partial y$, and $\partial B_z/\partial z$. That is to say, each of three sets of coils generates a field which has zero value at the origin, but whose z-component varies linearly in one of three coordinates across the volume of the sample. The design of the coils gives gradients of strength (250±2) μT/m per Ampere of current sent through each particular coil set, and the EFNMR Gradient/Field Coils controller contains three constant-current power supplies, each with nominal (bipolar) output range ±20 mA.

Q9. What are the extreme values of gradient strength thereby made accessible? If this range is accessed linearly over the 10-turn span of the dials, what change in gradient strength do you expect for each full turn of the dial?

Now here's the procedure: knowing (from the observed dephasing time) the approximate scale of the gradient change you might need, make a change of perhaps half that size to one of the three gradient adjustments. Acquire another free-precession signal, and note its *duration* (rather than its initial amplitude, which may not have changed). The duration might be longer, in which case you've made an improvement; or it might be shorter, in which case you can try a gradient change of the *opposite sign*; or it might not have made much difference, in which case you're being limited by the gradient in one of the other two dimensions -- so try an adjustment of another knob.

You're going to take repeated free-precession signals, and you'll be improving the signal's duration iteratively. Any improvement of any of the gradients makes the other two gradients even easier to adjust, since you have a longer-lasting signal and hence one sensitive to ever-smaller errors in the gradient adjustment.

As you improve the signal's duration, you might want once or twice to fine-tune the sample coil; this will affect the amplitude (not the duration) of the free-precession signal. As the signal improves in duration and magnitude, you might try adjusting the ten-turn tuning dial of the main-amplifier section in the EFNMR controller, since this will reward you with the lovely long-lasting *audible* version of the free-precession signal.

It is not necessary to make *perfect* adjustments; if all three gradients are correct to 0.1 μT/m, then the decay time will be of order 2 seconds, and your signals' duration will be limited by things other than gradients. For example, you'll be sensitive to imperfect geometrical alignment, if any; and the methods of section II.B. below will give you an alternative way to detect such misalignments. Also at the level of 0.1 μT/m you will be sensitive to slow *changes* in the gradients. Typically both the field values, and field *gradient* values, display changes on a time

scale of hours, perhaps due to temperature changes in the steel frames of typical buildings. It is worth recording what settings you have found for the gradient adjustments, as this will markedly reduce the effort required for gradient optimizations in the future. You can record either the nominal settings on the ten-turn indicators for the three dials, or the potential difference at the gradient-coil current-monitor outputs of the controller. Here a voltmeter will register the voltage drop across one of three 100 Ω (±1%) shunt resistors; the 'monitor selector' switch will allow you to record the three settings in turn. From the voltage drops across the shunt resistor, you can deduce the actual coil currents; from the coil currents and the gradient-coil constants of (250 μT/m)/(A), you can deduce the size of the gradients you have created, and thereby infer the size of the pre-existing gradients in the ambient field you have canceled out.

II. Experiments

II.A. The reality of magnetic-field gradients

This section of the manual assumes that you have successfully brought into operation the EFNMR apparatus inside the Coil System, and that you have achieved, by geometrical alignment and by gradient cancellation, a free-precession signal of long duration (of order 1 second) from a water sample. Here are some experiments aimed at a more quantitative study of gradients.

II.A.1. Is there really a magnetic-field gradient in space?

If you have a free-precession signal of duration about 1 s at frequency 2 kHz, then about 2000 full cycles of signal of useable size are available for you to measure. This should enable you to determine that frequency to about 0.5 Hz precision; section II.B. discusses some of the methods you might use to accomplish this. Here's a way to use that measured frequency to assure yourself that magnetic field gradients really are present in the ambient field.

Suppose that the $\partial B_z/\partial x$ adjustment you have made in your optimization corresponds to the addition of 2.3 μT/m of gradient; since that gives a long-lasting free-precession signal, you can infer that you have canceled out a pre-existing gradient in the ambient field, along the x-direction, of magnitude 2.3 μT/m.

Q10. If you were to translate the whole EFNMR Gradient/Field Coil System by 0.1 m along the x-direction, in how different a magnetic-field strength would you be putting the sample? By how much should this change the precession frequency of the protons, compared to your previous value?

To test this sort of prediction, you might translate the whole frame of the apparatus on the tabletop along the x-dimension, preserving its azimuthal alignment; you might want to take data at ±10 cm and ±20 cm relative to its original location. You should *not* need to change anything else about the apparatus; in particular, you can leave the three gradient adjustments right where they were originally optimized. But you should see precession frequencies that vary linearly with your translated x-position, and their variation with x-position should give you an (independent!) measurement of the gradient $\partial B_z/\partial x$. What's more, the *sign* of the gradient should now be clear, since you can tell unambiguously in which direction the field's magnitude increases.

It's not quite so easy to translate the whole apparatus along the y- or z-directions you have found, since these will in general not be convenient horizontal or vertical directions. But if you can create even approximate translations in y or z, you can by this same method verify that these gradients really exist, and you can also find their signs unambiguously.

II.A.2. What does a single gradient do to the signal?

Suppose you have 'optimized the gradients', ie. you have found those three gradient settings which give a nice long-lasting free-precession signal. Now what happens if you deliberately offset *one* of the gradients from its best value? We'll answer that question here "in the time domain", showing quantitatively the effect of a gradient offset on the free-precession signal.

Appendix 1 shows that if the sample is modelled as a cylinder of length L and diameter 2R, then the effect of a single gradient is to change the otherwise sinusoidal free-precession signal to the product of a sinusoid times an 'envelope function'. For a gradient of strength g along the x-direction, the envelope function is predicted to have form

$$\frac{\sin(\pi c_p g L t)}{(\pi c_p g L t)},$$

while for a gradient along the y- or z-direction, the envelope is predicted to have form

$$\frac{J_1(\pi c_p g \cdot 2R \cdot t)}{(\pi c_p g \cdot 2R \cdot t)}.$$

Here $J_1(x)$ is the Bessel function of order one, and c_p is the gyromagnetic constant 42.58 Hz/μT for protons.

Your goal is to create a gradient offset of a size that yields envelope functions which drop off quickly compared to the (approximately exponential) decay of free-precession signal you see in optimized fields, but not too quickly to see; you might aim for the envelope to decrease to half its original value in 0.1 - 0.6 s.

Q11. What gradient strength is required, along the x-direction, to give an envelope function dropping from 1.0 to 0.5 in just 0.30 s? What dial setting(s) would leave you with this gradient?

So record some free-precession signals under conditions in which (only) one of the three gradients is offset by a known amount from its optimum value, and see if the signals' envelopes resemble those predicted by theory.

Note in particular that these envelope functions 'pinch off to zero' in a finite time, at $\pi c_p g L t = \pi$ for an x-gradient or at $\pi c_p g \cdot 2R \cdot t = 3.8317$ for y- or z-gradients. A plot of the reciprocal of the pinch-off time vs. gradient setting ought therefore to be linear.

Q12. What would happen if you went *past* the optimum gradient setting? How can a plot like this help you to establish the optimum gradient setting?

Note also that the signal is *not* identically zero after the pinch-off time. The model predicts, and your signals ought to display, a *revival* of the free-precession signal.

Q13. What is the cause of this revival, physically speaking? [You should be encouraged to think about different regions of the sample doing different things,

and to think about the phase relationships of the emfs that they induce in the sample coil.]

II.B. Varying the magnetic field

Thus far you have used the Coil System's geometric and gradient capabilities to get a long-lasting free-precession signals, but you've not made any use of their largest feature, the Helmholtz-coil pair. These coils are intended to be used with an external stable adjustable direct-current supply (to be connected to the rear-panel connectors on the Gradient/Field Coil controller box). Their function is to create a field, adequately uniform in space over the sample volume, which can add to (or subtract from) the ambient value of the earth's field. The two 30-turn coils are connected electrically in series, and they are designed for use with continuous currents of up to ±3 A. Appendix 3 discusses the 'coil constant' k that can be deduced from their geometry and the Biot-Savart Law; you can use its methods to improve on an approximate value, $k \approx 90\ \mu T/A$.

The goal of this section is to measure the effects of the Helmholtz coil on the free-precession frequency. To see that such effects are expected,

Q14. Compute the field change you expect for a mere 1 mA current in the Helmholtz coils, and compute the precession frequency shift you expect in response. If you can measure frequencies to 1 Hz precision, what does this imply about the resolution in measuring (and stability) you'll need in the Helmholtz-coil current?

Your measurement of the Helmholtz-coil current can use the 'field coil current-monitor' outputs available on the front panel of the Gradient/Field Coils controller box. These give access to the potential difference created by the Helmholtz-coil current across an internal 0.100 Ω (±1%) shunt resistor.

With the total field at the sample subject to precisely known changes, you will get changes in the precession frequency that deserve to be measured to similar precision. There are several methods available for measuring the frequency of the slowly decaying, nearly sinusoidal free-precession signals:

- A frequency meter can count cycles directly, provided it is properly used. To use this method, you might have to use the output of the tuned amplifier to provide adequate amplitude during the whole duration of 1 second. You will also want to understand the triggering of the frequency meter; you'll want to set a triggering level at the zero-crossings of the signal. If you can count cycles reliably for a properly chosen 'gate time' of 1 whole second, you'll get frequency correct to ±1 Hz.
- Some digital oscilloscopes will display the frequency of a signal they acquire. To use this method, you'll need a 'scope which will acquire voltage samples at a rate of at least 5 kSa/s (to prevent aliasing) and which will acquire data for an adequate duration. The 'scope's algorithm will in effect count cycles-per-second and give a result. Best precision will come from a time record that includes the maximum possible number of cycles.
- Fourier-transform techniques are extraordinarily convenient, since they give a frequency-domain view of the signal with a high information content. Here you'll want a way to

acquire a time record for about 1 or 2 seconds, and you'll want to use a 'uniform window' optimized for a one-time signal like your free-precession signal. You'll get a 'Fourier power spectrum', perhaps on a decibel (logarithmic) vertical scale, and you'll see how superbly the signal peak stands above the noise floor. You'll want a way to locate the center of this peak on the frequency scale, perhaps to 1 Hz accuracy. Appendix 4 discusses the lineshape, and linewidth, you can expect in the frequency domain.

- Numerical fitting techniques offer the highest precision, but perhaps the slowest turn-around time, for frequency measurements. Here you'll again want to acquire a time record of the free-precession signal, for a duration of order 1 s, and then perform a least-squares fit to a function of the form

  $$f(t) = A + B \exp(-t/T) \cos(2\pi Ft + P) ,$$

  where A represents an offset, B an amplitude, T a time-scale for exponential decay, F the frequency you're after, and P a phase shift. With the proper least-squares technique, you can even extract an experimental uncertainty ∂F for your measured frequency, and this can be very small indeed.

Whatever technique you use for measurement of the precession frequency, it's convenient if it works using the pre-amplifier output signal (so there's one less tuning knob that you need to keep set), and if it works in near-real-time (so you have a result before you take the next data point).

II.B.1. Small variations of coil current, and linear models

What data can you acquire? You can start by measuring the precession frequency for zero current in the Helmholtz coils, and then for a small (<10 mA) current in them, to establish that you can make a difference, and to find what is the *sign* of the frequency change you can create. (Below, I call a current positive if it *raises* the precession frequency.) You will want to be able to use currents of <u>both</u> signs, so you might build a reversing switch for the current connections to the Helmholtz coils. *Especially* if you are using a constant-current power supply for the coils, you should remember to flip the current-direction switch **only** when the current has been dialed down to zero.

Q15. Why this requirement?

If you plot precession frequency as a function of coil current, you will start to see a linear variation emerge, but just as it becomes interesting, your signal will begin to disappear. Why? Because you'll have moved the signal out of the tuning range to which you've adjusted the sample coil. So as you change the precession frequency of the spins, you'll need to follow it with tuning adjustments to keep it up to familiar strength. Rather than do this by tedious guesswork-tuning at each new coil current, you can invest some effort in understanding the sample-coil tuning so that you can predict what tuning settings will be required for planned coil-current settings. Appendix 5 discusses this simple model.

Q16. How big a change in the field strength would be required to move the precession frequency by ±400 Hz (about what is needed to cover the 1.6 - 2.5 kHz tuning range of the sample coil)? What range of Helmholtz-coil currents would be needed to cover this range of field strength?

If you model the net magnetic field's magnitude, as a function of current, by

$$B(I) = B_0 + k\,I$$

and if you model the precession frequency as depending only on this magnitude,

$$f(I) = c_p\,B(I) = c_p\,(B_0 + k\,I) = c_p\,B_0 + (c_p\,k)\,I\ ,$$

then you can make a plot using I as independent, and f as dependent, variable.

Q17. What sort of plot does your theory predict this will be? What combinations of parameters can you deduce from the plot? What sort of precision are you getting for f-values? and what sort of precision does this yield for measured parameters in your model? What uncertainty can you assign to your measured parameters? Which of them can be compared with accepted values?

Q18. What can you find out about 'proton precession magnetometry', and what are some of its aplications?

II.B.2. Larger variations, and quadratic models

You may have found that the fit to the above linear model is imperfect; or you may have found a value for the proton gyromagnetic constant with a systematic error. You may also have found that even with locally optimized tuning, the signal strength, and the signal *duration*, drop off as you create larger fields with the Helmholtz coil. This is *not* because the Helmholtz coils create field inhomogeneities of their own; rather, it can be a symptom of misalignment of the Helmholtz coils' axis relative to the ambient magnetic field. Because the Helmholtz-coils' and the ambient fields are not collinear, they do not add as scalars. The resultant field will change in both magnitude and *direction* in space as you vary the current. Then the gradient corrections may fail to be optimal for the field as it varies in direction. Happily the frequency data themselves contain the diagnostic you need, as a slightly more complicated model will now reveal.

Suppose that the ambient field vector and the Helmholtz-coil field axis are separated in angle by θ, so that the ambient field has component $B_0 \cos\theta$ along the Helmholtz-coil axis, and another component $B_0 \sin\theta$ perpendicular to that axis.

Q19. What then is the component of total field along the Helmholtz coils' axis? What is the component of total field perpendicular to this axis? What is the magnitude of the resultant vector field? What is the prediction for the square of the field? How is the square of the precession frequency predicted to depend on Helmholtz-coil current I? What plot does this prediction motivate, and what parameters can you extract from what fit to this plot?

After your modelling and fitting have yielded parameters, you will be able to deduce a value for $\cos\theta$ and hence the misalignment-angle θ itself. [Unfortunately you won't know the sign of θ, nor whether the misalignment is in azimuth or altitude, but you could try changes by $\pm\theta$, in altitude and azimuth, and see what improves the alignment.]

If you can measure frequencies to 1 part in 2000, you could hope to determine all three coefficients to this order of precision. If you can deduce $\cos\theta$ to similar accuracy, you can detect misalignments of less than 2° by this method, and potentially correct them. More importantly, by this more careful modelling you can *segregate away* the misalignment error into a term separate from the other coefficients. Also (though you might not be able to estimate the coil constant k to this high a precision) you should be able to deduce, from your best estimate of

k and its uncertainty, a value for the proton's gyromagnetic constant c_p with its implied uncertainty, all *without* reference to 'book values'.

There's yet more that you can do with your model for frequency-squared vs. coil current.

Q20. Plot your model's prediction over the full range of ±3 A of coil current, and find the *two* regions in which it predicts frequencies in the range 1600 to 2500 Hz. Let your model predict that (non-zero) current at which the precession frequency ought to have the same value that it has at zero current.

Now if you tune up the sample coil and the gradients to see the optimal signal at zero current, then you should be able to get a new data point, at or near the same frequency, for this predicted (sign and) value of coil current. What you're looking for is the case of the Helmholtz coils providing a field of magnitude double, and direction opposed to, the ambient field; if all is well, you should see a free-precession signal and thereby get another data point to help constrain the parameters in your model. Taking data systematically around this new value of current is a searching test of your alignment and gradient corrections, and it's possible that the duration of the free precession signal will not be ideal. But if you can get new points in this range, then your entire set of data points will that much more tightly constrain the parameters of the model, and hence the coefficients you deduce from it.

The quality of your data, and the fit to it, can be so high that a special technique is needed to see if there are any imperfections. You have a list of *measured* frequency values as a function of current, and a model whose square-root will give *modelled* frequency values as a function of current. The differences between data and model are called *residuals*, and you should form the list of residuals, and plot them as a function of current. This is a good place to look for any systematic (unmodelled) deviations between data and theory. It is also a great place to learn empirically about the scatter in the data: the root-mean-square (rms) average of the residuals is a good measure of the typical degree of misfit between data and model.

Finally, you may reflect about this use of the Helmholtz coils to 'turn the field around', ie. to reverse the direction of **B** compared to the original ambient field. The prediction is that protons will then be precessing in the opposite direction or sense, compared to your original data set. There is no *direct* way to detect this opposite direction of precession,

Q21. Why not?

but you might think creatively about how you would go about determining the *sense* of rotation for a given species of nucleus. This will teach you how the *signs*, as well as the magnitudes, of nuclear moments are measured.

II.C. NMR of other nuclei

This section of the manual assumes that you have understood how to align the Gradient/Field Coil System, set the gradient adjustments, and use the Helmholtz coils, to be able to follow proton free-precession signals over some part of the 1600-2500 Hz tuning range of the EFNMR apparatus. With this capability in hand, we now take up the possibility of detecting the free-precession signals of nuclei other than protons; the use of the Helmholtz coils will extend this capability to some other nuclear species.

Not many nuclear species are "NMR-active" in the sense of being detectable by NMR techniques; the fundamental requirement is that the nucleus in question have a non-zero and preferably large nuclear magnetic moment. But most stable nuclei have an even number of both protons and neutrons (think of ^{12}C and ^{16}O), and such nuclei have *zero* nuclear spin and hence no magnetic moment at all. So the candidates for NMR need to have an odd number of either protons or neutrons. They need to be stable nuclei, and have large isotopic abundance, and be available at adequate density in a liquid environment. This list of stipulations narrows the field markedly, and the further 'customer requirement' of nuclei of chemical interest or biological abundance cuts the list down to quite a small number of nuclei. We'll discuss the cases of ^{19}F, ^{31}P, and ^{2}H =D below.

II.C.1. ^{19}F, Fluorine

Fluorine may or may not be of any great chemical or biological interest to you, but it is certainly the next-easiest nucleus to detect (after protons) and a good introduction to the experimental issues involved in detecting other nuclei by NMR methods. You might first use as samples some perfluorinated liquids (available from TeachSpin) to provide adequate numbers of fluorine nuclei within the available sample volume. The polyether compounds in the liquids have the approximate empirical chemical formula $(C_3F_6O)_n$ and an approximate density of 1.65 g/cm^3, which is enough to show you that (happily mono-isotopic) ^{19}F is the only NMR-active nucleus present to any extent, and also sufficient for you to compute the number of fluorine nuclei present.

Q22. At this density, how many grams of C_3F_6O would fit in your 125-cm^3 sample bottle? How many moles of C_3F_6O does this represent? How many moles of fluorine would this give you for a sample? What would polymerization of C_3F_6O to $(C_3F_6O)_n$ do to this number?

Q23. And by contrast, how many grams of H_2O will fit in your 125-cm^3 sample bottle? How many moles of H_2O does this represent? How many moles of protons-in-hydrogen would this give you for a sample?

Finally, ^{19}F has a nucleus approximately describable as a 'closed shell plus valence proton', so its magnetic moment is similar to that of a proton -- just about 6% smaller.

So if you are getting good proton free-precession signals in the earth's field, you can merely tune the sample coil to resonate with an expected frequency 6% smaller than that for protons, and you should be able to capture fluorine free-precession signals straightaway. [See Appendix 5 for a discussion of a systematic way to accomplish sample-coil tuning.] You should not expect that the magnetization timescale T_1, or the decay timescale T_2, will be the same as for protons in water; you might want to measure T_1 very approximately, so as to know what polarization time to use hereafter.

Once you have seen any fluorine signal at all, you should be able to obtain, from the gyromagnetic constant c_p for protons, a new gyromagnetic constant c_F for fluorine. You should also be able to predict where a lot more fluorine data could be taken, since you can now exercise the Helmholtz coils and arrange to see fluorine signals over the full tuning range of frequencies. Given your approximate value of c_F, you can predict where in frequency fluorine signals should appear for any given value of Helmholtz-coil current; and given your tuning model for the

sample coil, you can predict ahead of time how you'll have to tune up the coil for optimal signals. Hence you should systematically and rapidly be able to acquire data over a large part, or over two branches, of your frequency vs. coil-current model for fluorine. Such data can very tightly constrain the combination of parameters c_F k, as proton data will similarly constrain c_p k. Taking the ratio of these can give c_F / c_p with *very* high precision, *not* limited by the absolute accuracy with which you can estimate the coil constant k.

II.C.2. ^{31}P, Phosphorus

If you are inclined to try other nuclei, you might look over the appropriate nuclear tables systematically to find species of large isotopic abundance, non-zero nuclear spin, and adequately large nuclear magnetic moment, just to see how your choices are limited. A sample definitely worth trying is ^{31}P (in the form of neat 86% H_3PO_4, phosphoric acid -- not to be spilled!). This sample incidentally contains plenty of protons, so you will see proton signals at the expected frequencies (though with T_2 times quite different than for pure water), but the sample ought also to give free-precession signals of the new nucleus under the appropriate conditions. You may circumvent a major search effort by taking as given the phosphorus-to-proton ratio ratio $c_P/c_p \approx 0.40 \pm 0.01$.

You will have noticed that even fluorine samples give precession signals of smaller amplitude than you get from protons in water, and now it's time to be a bit quantitative about the expected signal size for new species. Rather than try to predict absolute signal amplitudes (which would require all sorts of details about sample-coil geometry and tuning, amplifier gains and the like) we will concentrate only on *relative* signal sizes, since proton signal sizes are easily measured empirically. The first factor in signal size is merely the number of nuclei present, so you can start by estimating the number of protons-in-hydrogen in the 125-cm^3 samples of water that you've been using, and then by estimating the numbers of ^{19}F or ^{31}P that you can fit into the same sample space given the chemical forms you're using. The second factor in signal size has to do with the initial magnetization that is produced by the polarizing current in the sample coil; we'll assume that the coil carries the same (perhaps 3 A) current for both species in turn, and that the polarizing current is in both cases left on for $\geq 3\ T_1$ so as fully to magnetize the nuclei in question (and how do you know what T_1 will be, for a nucleus as yet undetected, in some novel chemical environment? Here's the romance of the discovery process!). Then the prediction for saturation magnetization is

$$M_\infty = N \left(\frac{I+1}{I}\right) \frac{\mu^2}{3k_B T} B_p$$

where N is the number density of the nuclei in question, I is the nuclear spin (so I Π is the nuclear angular momentum), μ is the magnetic moment, B_p is the polarizing field used, and $k_B T$ reminds you that nuclear polarization is a competition between the polarizing field's effort at orientation and the thermal effects of disorientation. This standard result is more easily used if we note that the gyromagnetic ratio γ (= 2π c in our notation) is defined to be the ratio between magnetic moment and angular momentum, so that $2\pi\ c = \mu/(I\ \Pi)$. Putting all these things together, we find that the saturation magnetization is predicted to vary as

$$M_\infty \propto N\ I\ (I + 1)\ c^2$$

with the other variables assumed to be the same for two species being compared.

Now the initial magnetization is *not* the only thing which affects the signal size, since it's the magnetization's precession which induces the emf picked up by the coil. Rather than contemplate the effects of differing precession frequencies, we imagine that we compare species made to precess at the same frequency, as with (protons in the ambient field) and (fluorine in a Helmholtz-coil-assisted field chosen to produce that same frequency). Then there are no new factors involving precession frequency, coil quality factor, or amplifier response, and the calculation above ought to give predictions for the relative amplitude of (initial) free-precession decay signals.

Q24. What does this model predict for the ratio of signal sizes, comparing ^{19}F to ^{1}H in the samples you used? How does this compare to what you observed?

Q25. What does this model predict for the ratio of signal sizes, comparing ^{31}P to ^{1}H in the samples you will be using? How does the predicted signal size for ^{31}P compare with the noise level in the signal you are detecting?

You've learned how rapidly the apparently enormous signal-to-noise ratio for protons gets eaten up by less favorable experimental circumstances for other nuclei. Because of the unfavorable signal-to-noise ratio in time-domain detection, it will very likely be necessary for you to use a frequency-domain technique for you to find that peak attributable to ^{31}P in the spectrum of the detected signal.

II.C.3. Deuterons (^{2}H) in heavy water

Finally, you may have heard about the widespread use of ^{13}C-NMR, especially by organic chemists. This would be a lovely target nucleus for earth's-field NMR study, except for the mere 1.1% natural abundance of ^{13}C in terrestrial carbon. Isotopically-enriched carbon is certainly available, but the prospect of filling a 125-cm^3 sample bottle with such material sounds very expensive. Nevertheless, the idea of isotopically enriched samples need not be entirely abandoned, since there is one isotope available in enriched form in huge quantities and (relatively) modest cost. This is ^{2}H, deuterium, or heavy hydrogen, whose natural abundance is a pitiful 0.016%, but which is available in 99% (or even 99.9%) isotopic purity as heavy water, D_2O. It takes about 150 g of heavy water to fill a standard sample container, and since the material is both expensive and hygroscopic, you must to keep the container sealed (and stored!) properly. But you will be able to see ^{2}H free-precession signals, even though the deuteron-to-proton ratio $c_D/c_p \approx 0.15$; you might confirm that (at fields chosen to give equal precession frequencies) the ^{2}H signals are predicted to be about 16-fold smaller for heavy (as compared to light) water. Then you'll need to create a model for expected frequency as a function of Helmholtz-coil current, and also set your sample-coil tuning appropriately, before you can search for these small signals. The use of Fourier-transform detection techniques is almost certainly a prerequisite for finding small signals at imperfectly known frequencies, but the payoff is considerable. The measurement of the gyromagnetic constant for deuterons in heavy water is enough to fix the magnetic moment of the deuteron, and you should be able to measure this with sufficient precision to show that it is *not* equal to the sum of the proton and the neutron magnetic moments. See Appendix 6 for the details of this calculation.

II.D. Studying the spin-spin relaxation time, T_2

This section of the manual assumes that you have completed the gradient-cancellation algorithm

of section I.C, but it does not require that you use the Helmholtz coils. The assumption is that you have succeeded in getting long-lasting free-precession signals for protons in water, and the goal of this section is to teach you something about what controls and affects the 'spin-spin relaxation time' T_2.

Recall that the establishment of nuclear polarization during the polarizing interval is governed by an exponential approach to equilibrium magnetization, and described by a 'spin-lattice relaxation time' T_1. By contrast, free-precession signals obtained after the polarization time are empirically observed to decay approximately exponentially, with a time constant conventionally labelled T_2^*. Here T_2^* is so labelled since magnetic-field inhomogeneities certainly affect the decay of free-precession signals, and hence it's not easy to be assured that the 'true' relaxation rate T_2 is being measured even in the best-adjusted fields. Nevertheless there is merit in studying the T_2^*-values you can obtain, since you can easily extract clues about what affects this quantity.

The assumption is that polarized protons represent a sample with precessing angular momentum, and that truly free precession would have this angular momentum precess in direction but not change in magnitude. Because of the conservation of angular momentum, protons will lose angular momentum only to other species or objects that can exert a torque on them. The external magnetic field is one such 'object', but it merely creates precession; loss of angular momentum must be to other objects that can exert a torque on protons' magnetic moments. These objects themselves need to have magnetic moments, and in the case of water (and so many other molecules) lacking *electronic* magnetic moments, these can only be other protons. Hence the name 'spin-spin relaxation'.

[One other source of relaxation in water is the presence of dissolved oxygen, O_2, since this molecule possesses a sizeable magnetic moment. If you have access to de-oxygenation facilities, or dissolved-oxygen measurement capability, you might compare distilled water before and after a de-oxygenation treatment to see if you can increase the relaxation times.]

But if we blame proton-proton interactions for the intrinsic T_2 for pure water, we can still expect the T_2 times to vary in the presence of other species than water. We might expect that dissolved molecules or ions will change the T_2 time, depending on whether they have magnetic moments, and depending on their concentration. So there is a rich field of study available to you, if you care to mix up samples and measure T_2^* times obtained. Do remember to make intercomparisons with your pure-water standard, to make comparison to that part of T_2^* due merely to magnetic-field inhomogeneities.

You might start with preparing solutions of strengths 0.0001 M, 0.001 M, 0.01 M, and 0.1 M of common salt (NaCl) and sugar (sucrose, $C_{12}H_{22}O_{11}$) to gain some practice both with sample preparation and with extraction of T_2^* times. You might note that sugar contains protons, which themselves might contribute to NMR signals; you might note that dissolved salt yields the ions Na^+ and Cl^-, both of which have closed electron shells and hence lack electron magnetic moment. Then prepare some solutions of (say) $CuSO_4$ in the concentration range of 0.0001 M - 0.0030 M, and you'll see that something is drastically affecting the T_2 times. You might plot the relaxation rate $r \equiv 1/T_2^*$ as a function of concentration of the dissolved ion Cu^{++}, and you might look up 'paramagnetic ions' to understand what is going on. And supposing that magnetic

interactions between protons and copper ions are the cause of what you're seeing, you might wonder if these interactions have their consequences on the T_1 times as well.

There are many other studies that can be conducted, for which T_1 or T_2 is the relevant dependent variable, and for which the independent variable is up to your imagination. There is an expected dependence of these quantities on the viscosity of the liquid sample involved, and you might think of using hydrocarbon oils in a series of varying viscosity to study these. Or you might let the viscosity vary with temperature, starting a study with a bottle of hot oil and watching the effects as it cools and grows more viscous. Or you might consider water again, and wonder about *solid* water (ie. ice -- but don't fill a sample bottle quite full before you freeze it!). Or you might prepare a gelatine sample in hot water, and watch by NMR to see what happens as it gels. If you mix up a batch of epoxy adhesive, you can watch the progress of a chemical reaction by NMR (but you'll never get the sample back out of the bottle). If you have or use a water filter, you might use NMR to test its efficiency at removing paramagnetic ions from its throughput. What about water molecules in the environment of a zeolite crystal? or the water in a banana? or the 'water of hydration' in a crystal? Your study is limited only by your creativity.

II.E. Pulsed-gradient spin echoes

The celebrated phenomenon of the 'spin echo' can be detected using the EFNMR Gradient/Field Coil System. Your first studies will require only a protons-in-water sample, in the ambient field, but with gradient cancellation completed after the fashion of section I.C. above. A spin echo is a phenomenon best detected in the time (not the frequency) domain, but in this apparatus it can also be detected directly by ear, in real time, so the echo is much more literal than figurative.

Here's how you can imagine setting up one kind of 'spin echo'. Suppose you have optimized all three gradient cancellations, so that a sample of polarized protons produces a free-precession signal detectable (and audible) for a few seconds of time. Now if one of the gradients, say the x-gradient of field strength, is deliberately mis-adjusted, say by 1 μT/m, then you have seen that the free-precession signal dies away in a much shorter time -- about 0.2 s, according to the model of Appendix 1. The question is, why has the signal decayed away? Is it because the magnetic moments are lost? No, says the existence of the spin-echo phenomenon: the loss of signal is in part *reversible*, and the decayed signal can be *resuscitated*, by the variation of a gradient adjustment in time.

To consider the example above, suppose the x-gradient setting is 1 μT/m too high at and after $t = 0$, the start of free precession. The signal rapidly dies away, and has practically vanished by $t \approx 0.3$ s. Now suppose that later still, at $t = 0.5$ s, the x-gradient is suddenly re-adjusted, not to the ideal value, but to *another* wrong value, this time 1 μT/m too *low*. The signal will not magically re-appear right at $t = 0.5$ s; but if this new gradient is maintained for $t \geq 0.5$ s, then the signal will re-appear(!) around $t = 1.0$ s.

This remarkable prediction is worth testing out experimentally before you work out the details of the mechanism. You'll need to have worked out the gradient adjustments, so that you can get a long-lasting free-precession signal. Now for the first time you are about to exercise the capabilities of the 'x-gradient step change' part of the EFNMR Gradient/Field Coils controller

box. Arrange to measure the x-gradient coil current by monitoring the x-gradient shunt voltage at the appropriate current-monitor outputs on the controller's front panel. You will see a voltage appropriate to the current required to cancel the x-gradient in the ambient field; record that voltage. Now find the 3-position step-change toggle switch, and move it from its uppermost 'off' position to the middle '- step' (say that as "minus step") position. Note that the switch will stay in that position, and that the current-monitor output will read a lower voltage; record this voltage too. Finally, push down and hold the toggle switch to its lowest '+ step' (say "plus step") position, and note that you get a third reading of the voltage at the x-gradient-coil current monitor. Note that the toggle switch allows you to generate displacements of equal size, negative and positive, relative to that x-gradient setting which cancels the ambient x-gradient.

Now get an optimized free-precession signal with the toggle switch in its ordinary uppermost (= off) position. Next, for comparison, see what a difference you get if you put the toggle switch to its middle (= - step) position, and then initiate a polarization time and the subsequent free-precession time. You should see on a 'scope, and hear on the speaker, the signal dying away in a much shorter time. (And no surprise: you're deliberately operating with a incorrectly-adjusted x-gradient.) Now repeat that signal acquisition, but this time with your fingers on the toggle switch. Have the toggle switch, as before, in the middle (= - step) position, but this time, wait for the audible end of the free-precession signal, and then push down and hold the toggle switch to its bottom (= + step) position. You should hear by ear, and see on the 'scope, the effect of this change in the gradient; what you've heard and seen is called a 'pulsed gradient spin echo', since you achieved it by suddenly changing the gradient from one value to another.

It is well worth trying a few more attempts at this hands-on switching, to understand the time relationships involved. You can hear the beginning of the free-precession signal, and you can *choose* how long to wait before switching to the opposite sign of gradient offset. You can see what happens if you only hold the toggle switch down momentarily (as opposed to holding it down for the full duration of the echo). You can even try getting the 'echo of an echo' by releasing the toggle switch after the first echo, and letting it return to the middle (= original, - step) position.

After you've enjoyed this hands-on, ear-detected introduction to the spin-echo phenomenon, you may want to automate and regularize the process. Here you'll want to send the 'trigger out' signal of the EFNMR controller, not only to the 'scope that you've been using, but also to the 'trigger in' connector on the EFNMR Gradient/Field Coils controller. Now the trigger pulse which arrives at the beginning of the free-precession signal will execute the start of the 'step delay' function (adjustable on the front panel over the 0 - 3 second range) and at the end of this set interval will execute the switch to the 'plus step' condition automatically (and reproducibly).

To see the time relationships involved, you might use your 'scope to display, in addition to the free-precession signal, a signal from the x-gradient coil-current monitor. You can acquire one trace with the gradient-step capability off, and a subsequent one with the x-gradient set to the 'minus step', but automatically switching to the 'plus step' after your chosen delay time. Make a sketch of the x-gradient strength vs. time, and the x-gradient *error* vs. time, appropriate to these signal acquisitions, and you'll have the timing diagram needed for understanding the theory below.

What is going on with the protons? Assume that you start with all the gradients exactly canceled, so all the protons experience the same field, and all precess at the same frequency, staying in phase for the whole duration (several T_2's) of the free-precession signal. Now consider what happens in the 'minus step' condition, which applies from $t = 0$ to $t = T_{delay}$. There is now a (negative) gradient present, so protons at larger x-values experience a smaller field, and those at smaller x-values experience a larger field. The result is *differing* proton precession frequencies for differing locations in the sample; protons at negative x-values get *ahead* of the others in their precession. When phase differences between protons at opposite ends of the sample reach 180°, the signal is diminished by dephasing; not much later, the signal is virtually gone, due to more complete dephasing. But the protons and their magnetic moments are not gone, and the signal can be resuscitated by arranging for the 're-phasing' of the protons. A step reversal of the gradient error is all that's required to do this; if for $t \geq T_{delay}$, the x-gradient error is *opposite* to what is was before, we now have the case that protons at larger x-values experience a larger field, and those at smaller x-values experience a smaller field. Once again the protons will precess at different rates; but now those protons at larger x-values, which were *behind* in phase at $t = T_{delay}$, will precess at a faster rate, and catch up with those protons at smaller x-values, which were ahead in phase at $t = T_{delay}$. When $t = 2 \cdot T_{delay}$, this catch-up process should be complete, and *all* the protons will (temporarily) be in phase again. At this time, the full sample will be precessing in phase, giving as large a signal as if all the protons had been in phase for the full duration of the experiment.

Q26. What does this model predict for the time of occurence of the echo? What does it predict will happen if the size of the 'minus' and 'plus' steps is changed (there's a rear-panel adjustment for this step size, and again the front-panel x-gradient current-monitor output will tell you what step size you're selecting)? How can you get the 'echo of an echo', according to this model? What would happen if, right at the peak of the echo, you were to switch the gradient errors off altogether?

There are plenty of applications for these pulsed-gradient spin echoes. The first of these is a highly sensitive method for the optimal settings of the y- and z-gradients: arrange to see a triggered spin echo at (say) $t = 1$ s, and now watch the strength of the echo as a function of the y- or z-gradient setting. Only if the y- and z-gradients are set perfectly will the echo be at maximal strength. For that matter, only if the x-gradient is set perfectly will the echo be at maximal strength. The prediction is that the echo will (temporarily) reach the full strength of the ideal free-precession signal, limited only by $\exp(-t/T_2)$ relaxation.

Another more important application has to do with an implicit assumption in the explanation above. For the rephasing to work out perfectly, it is crucial that a given proton be at, and stay at, the *same* x-location for both the '- step' and the '+ step' parts of the time evolution. If a given proton is moving during the precession time, then it can acquire a phase gain during the interval $0 < t < T_{delay}$ which is *not* compensated by the phase loss acquired for $t > T_{delay}$. You can actually observe this effect; you might want to set to a rather large value of gradient-step size, confirm that you can get a spin echo, and then try again with a not quite full, freshly shaken-up(!) bottle of water in which the protons will be in motion during the whole free-precession time. (Less mundane proton motions can be detected in high-field NMR apparatus, including the motion of protons due to convection or even to mere passive molecular diffusion.)

II.F. Magnetic-resonance imaging

This section of the manual describes the use of the EFNMR Gradient/Field Coil System to demonstrate the glamorous technique of (one-dimensional) magnetic resonance imaging, and thereby to illustrate the physical basis of all MRI technologies. In this section, we'll assume a proton sample, operated in the ambient field, with the gradients corrected according to the algorithm of section I.C. You will want the gradient-step function of II.E. turned back off, and you will finally have a chance to use the 'segmented sample container' that's available from TeachSpin. Finally, this section definitely requires that you be able to detect free-precession signals and view them in the frequency domain; it is very useful to have a shot-by-shot view of the Fourier transform of each free-precession signal, in addition to the oscilloscope view of the time-domain signal you've used thus far.

The basis of all magnetic imaging is the use of deliberate, tailored, non-zero gradients of magnetic field across a sample. In your TeachSpin apparatus, we'll suppose that you know how to cancel out all gradients in the ambient field, and that you now deliberately depart from a net x-gradient of zero to (say) an x-gradient of 4 μT/m.

Q27. Work out the significance of this: how different does this make the field for protons not at the origin, but at x = +3 cm? How different does this make the precession frequency for these protons, compared to those at the origin?

Now suppose there are thin 'slabs' of proton-containing water, one centered at x = 0 and another at x = 3 cm. Both slabs' worth of protons can be polarized by the same polarizing current, and both will then precess in the local field. But in the presence of a deliberate gradient, protons in the two slabs will precess at distinct frequencies (as in the example above). Both slabs of protons will induce emfs in the sample coil, so the signal emerging will be a superposition of two distinct frequencies. This makes for a complicated waveform in the time domain, but a beautifully simple result in the frequency domain: there should be one peak at f_0, for protons at x = 0, and another peak at $f_0 + \Delta f$, generated by the protons in the slab at x = 3 cm. In fact the distribution of protons in x-space has been mapped into a distribution of signal strength in f-space.

This calculation illustrates a few technical requirements as well. The tuned sample coil has a Q of order 70 near f = 2000 Hz, so its pick-up efficiency drops to half-strength at locations $f = [1 \pm 1/(2Q)]$ 2000 Hz, or at 2000 Hz ± 15 Hz. Hence we would like protons at the ends of the sample container to be mapped to frequency-space locations no more than about ±10 Hz away from protons at the origin. This puts an upper limit on the size of the gradient that can be used. There's a lower limit as well, if proton signals from different slabs are to be resolved in frequency. If free-precession signals decay with $T_2^* \approx 1$ s, then even protons at one single x-value will show up in a signal peak with width of order 0.5 Hz (and to attain this resolution will require a signal-acquisition time of 1-2 s minimum duration); so a gradient has to be chosen which will map a chosen separation in space to a separation in frequency of $\geq$ 1 Hz. But within these limits, the size of the gradient chosen is arbitrary, so the 'scale factor' of the x-to-f mapping is under your control.

The reality of all this theory is very easily illustrated using the TeachSpin segmented sample

container. This consists of seven compartments, each of x-extent about 7.8 mm, separated by partitions of x-extent about 3.2 mm (and a total length of container of 78.6 mm).

Q28. Compute the volume, in cm^3, of each sample compartment.

Water is best added to a cell by injecting it using the syringe-needle device accompanying the cell; water is best removed from a cell by inverting the container (access holes down) and blowing air into the cell with the syringe (thereby displacing the water out through the access hole -- execute this operation over a sink).

Now you might want to start by filling cells #1 and 2 with water, and leaving the others empty. If you place the sample container symmetrically inside the sample volume of the EFNMR apparatus, you have a sample of water roughly filling the x-interval {- 36.6 to -17.9 mm}. Practice acquiring a free-precession signal from this sample of water, first with the gradients optimized; be sure you can view this signal in the frequency domain, with resolution of order 1 Hz. Now if you change the x-gradient from optimal by amount ±4 μT/m, you should see this signal get displaced in frequency space.

Q29. By how far, in frequency space, do you expect it to be displaced?

To confirm that you're really sensitive to the water-sample's position, you can remove the sample container and re-install it turned end-for-end, so that the water is now in the place where formerly empty cells #6 and 7 were located. Now the signal should be displaced in frequency by Δf, but in the *other direction*. This will give you a way to understand the sign of the gradient you have added, and the sign of the linear mapping between x-space and f-space.

With this all understood, you may fill any cells you wish, with whatever volume of water you wish (the syringe will let you deliver a metered amount of water), and thus create a chosen distribution of protons in x-space. Find the conditions that give you the best view of the resulting free-precession signal in frequency space; you may want to display the Fourier power spectrum on a *linear* rather than logarithmic scale. You should be able to see an *image* of your chosen proton distribution, obtained by one-dimensional MRI technology!

To get another look at the power of Fourier transformations, look instead at the time-domain view of the precession signal on your 'scope. You'll see what looks like a weak signal, lasting only a short time, followed by mere noise; but that signal is the superposition of the emfs induced by the protons in the separate cells, and it contains (in encoded form) all the information that goes into the Fourier transform. Then the transformation into frequency space *decodes* that information, and what comes out is recognizable as a depiction of proton distribution in space.

There are lots of other 'images' you can get out of this form of MRI. Your image thus far depicts proton abundance, so image contrast depicts differing densities of protons. But you can imagine medical contexts in which proton density in space is boringly uniform, and there's the need instead to depict some other property of protons. How about an image which depicts not proton abundance, but proton T_1 time? You could *fill* all seven cells of your sample container, but using water with differing concentrations of some paramagnetic ion, so that they varied from short to long T_1 times. Then the use of long polarization times would fully polarize protons in all the cells, and give an 'image' without contrast, whereas the use of an intermediate polarization time would differentially polarize the protons, so now the resulting image should display contrast.

The data acquisition rate of this MRI device is rather low, and the signal-to-noise ratio is only adequate, but in principle this device could give the data required for obtaining three-dimensional images.

Q30. How could you distinguish two sub-samples of protons, having the same x-coordinates, but different y-coordinates? How could one distinguish two sub-samples of protons, having the same x- and y-coordinates, but different z-coordinates? What can you look up about fully three-dimensional MRI which confirms your creative ideas, and perhaps extends them?

Appendix 0. The gyromagnetic ratios: values and notation

This appendix establishes some notation, and gives some 'best values', for proton precession frequencies.

We introduce first the gyromagnetic ratio γ, defined classically as the ratio between a system's magnetic moment μ and its angular momentum L:

$$\gamma \equiv \frac{\mu}{L}.$$

The definition is extended into quantum mechanics by taking for both μ and L their maximum projections along any axis, and applied to nuclei whose angular momentum is given in terms of their spin I by

$$L = I \Pi .$$

Now the precession of an angular momentum vector is described by

$$\frac{d\mathbf{L}}{dt} = \boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B} = \gamma \mathbf{L} \times \mathbf{B}$$

which is an equation of motion for **L** which conserves both the magnitude of **L** and its projection on the axis defined by **B**. But **L** does change with time, by precessing about **B** at (angular) frequency

$$\omega = \gamma B.$$

According to the latest (2005) results found at http://physics.nist.gov/cuu/Constants/index.html, the gyromagnetic ratio for free and isolated protons is given by

$$\gamma_p = 2.675\ 222\ 05(23) \times 10^8\ s^{-1}\ T^{-1}$$

where the (23) expresses the uncertainty in the last digits, which amounts to 0.086 part per million (ppm) uncertainty. But NMR users don't work with free and isolated protons, instead using protons inside atoms or molecules. Such protons experience *less* than the full external field B, and hence precess at a slightly lower rate, on account of the 'diamagnetic shielding' created by the molecular environment. The gyromagnetic ratio for protons in water molecules in a spherical sample at 25 °C is called the 'shielded gyromagnetic ratio' and is given by

$$\gamma_p' = 2.675\ 153\ 33(23) \times 10^8\ s^{-1}\ T^{-1}.$$

Note that there's a difference of nearly 26 ppm between the two values; the variations in diamagnetic shielding for different sites in various molecules accounts for a large part of the usefulness of NMR to chemists.

In this experimental manual, we will use only ordinary (not angular) frequencies, and because $f = \omega/2\pi$, we will find most useful the combination

$$\frac{\gamma_p'}{2\pi} = 42.576\ 3875(37)\ \text{Hz}/\mu\text{T};$$

we choose to call this the 'gyromagnetic constant', labelling it c_p for explicit reference to protons.

Appendix 1. Gradients and their consequences

This appendix works out at varying levels of detail the consequences, and the character, of magnetic-field gradients in NMR.

First, a very approximate consequence of gradients. In the presence of a gradient of strength g, two points separated in space by distance S will have field differing in magnitude by

$$\Delta B = g\, S$$

and protons at these two sites will differ in precession frequency by

$$\Delta f = c_p\, \Delta B = c_p\, g\, S.$$

In a time T for which $\Delta f \cdot T = 1$, protons at two such sites will be a full cycle out of phase, so surely there will be observable consequences in a time

$$T \approx 1/(c_p\, g\, S).$$

Q31. For typical values $c_p = 43$ Hz/μT, $g = 3$ μT/m, and S = 6 cm = 0.06 m, find what dephasing timescale this model predicts.

Next, a more detailed treatment of gradients' consequences. We might model the sample in the TeachSpin apparatus as a circular cylinder of length L = 7 cm and diameter 2R = 5 cm, and then compute the detailed consequences of having protons distributed through a range of field strengths, and having precession frequencies distributed through a range of frequency values.

For a field whose magnitude has only an x-gradient, we can write

$$B = B(x) = B_0 + g\, x\,, \text{ so } f = f(x) = c_p\, B(x) = f_0 + c_p\, g\, x.$$

Now if we form phasors exp[-i 2π f(x) t], and include the whole sample by integrating over x from -L/2 to +L/2, we get the resultant phasor at time t, and find that its real part can be written

$$V(t) \approx \cos(2\pi\, f_0\, t)\, \frac{\sin(\pi\, c_p\, g\, L\, t)}{(\pi\, c_p\, g\, L\, t)},$$

which displays oscillations at the central frequency f_0, but multiplied by a time-dependent envelope function of the form sin(q)/q. This envelope function falls to half its initial value at q = 1.895, and to zero at q = 3.142; it allows us to define a half-amplitude point at time

$$t_{1/2} = \frac{1.895}{\pi}\, \frac{1}{c_p\, g\, L}.$$

For a field whose magnitude has only an y- or z-gradient, we can write (say)

$$B = B(y) = B_0 + g\, y\,, \text{ so } f = f(y) = c_p\, B(y) = f_0 + c_p\, g\, y.$$

Again we form phasors exp[-i 2π f(y) t], and integrate over y from -R to +R, but this time weighting them according to $(R^2 - y^2)^{1/2}$ to describe a circular cross section, thereby getting a much less familiar integral. Nevertheless, the resultant phasor at time t has a real part

$$V(t) \approx \cos(2\pi\, f_0\, t)\, \frac{J_1(2\pi\, c_p\, g\, R\, t)}{(2\pi\, c_p\, g\, R\, t)},$$

where $J_1(q)$ is the first-order Bessel function of the first kind. In this case $J_1(q)/q$ forms the envelope function; it falls to half its initial value at q = 2.215, and to zero at q = 3.832. This allows us to define a half-amplitude point at

$$t_{1/2} = \frac{2.215}{\pi}\, \frac{1}{c_p\, g\, 2R}.$$

Both detailed results support the generic form first introduced above.

Finally, a discussion of just what, and how many, gradients a magnetic field can have. The generic vector field $\mathbf{V}(x,y,z)$ in three dimensions has *nine* first-order gradients, from the list $\partial V_x/\partial x$, $\partial V_y/\partial y$, . . . $\partial V_z/\partial z$. But the magnetic field satisfies Maxwell's equations, which impose divergence and curl conditions on the first-order spatial derivatives, leaving only *five* independent gradients.

If the z-axis is aligned with **B** at the origin, and the gradients are small enough over the region of interest, we can define the field as

$$\mathbf{B}(x,y,z) = B_0\,\mathbf{z} + \mathbf{B}_1(x,y,z)$$

where the constant B_0 gives the field's magnitude at the origin, and where the function $\mathbf{B}_1$ vanishes at the origin and can be taken to be of first-order smallness near the origin. Since NMR precession frequencies depend only on the *magnitude* of **B**, we desire only that the magnitude, or equivalently the magnitude-squared, of the field be independent of position to first order. That magnitude-squared is given by

$$B^2(x,y,z) = \mathbf{B}\cdot\mathbf{B} = B_0^2 + 2\,B_0\,\mathbf{z}\cdot\mathbf{B}_1\,(x,y,z) + \text{smaller terms},$$

and because of the dot product, we now see that only the z-component of the $\mathbf{B}_1$ function matters. Taking the square root to first order, we get

$$B(\delta x, \delta y, \delta z) = B_0 + \delta B = B_0 + (\partial B_{1z}/\partial x)\,\delta x + (\partial B_{1z}/\partial y)\,\delta y + (\partial B_{1z}/\partial z)\,\delta$$

which shows that only *three* first-order gradients need to be corrected to make the magnitude of the field spatially uniform.

Appendix 2. Deliberate additions to the gradients

This appendix discusses the deliberate addition of magnetic-field gradients in the sample's vicinity, for instance by positioning a permanent magnet at some distance from the apparatus.

We will consider a permanent magnet as a point magnetic dipole $\boldsymbol{\mu}$, and we'll consider only the simplest case in which the magnet is placed lying in the z = 0 plane, and with its dipole axis aligned along the z-axis, of the EFNMR coordinate system. Then the NMR sample lies in the 'equatorial plane' of the permanent magnet, and if their separation is R, the field at the sample due to the magnet is given by

$$\mathbf{B} = -\frac{\mu_0}{4\pi}\frac{\boldsymbol{\mu}}{R^3} .$$

Here $\mu_0/4\pi \equiv 0.1$ μT·m/A in SI units. For reference, we note that the permanent magnet's moment is given by the product of the material's saturation magnetization M and the magnet's volume V; for a NdFeB magnet in the form of a cylinder of diameter and length 1.27 cm, the value of μ might be

$$\mu = M\,V = (1.06 \times 10^6\ \mathrm{A/m}) (1.6 \times 10^{-6}\ \mathrm{m^3}) = 1.7\ \mathrm{A\ m^2},$$

so that at a distance of R = 1m, this magnet will produce a field of strength 0.17 μT.

Q32. Confirm this calculation, and compute the frequency shift this would create for proton precession frequencies.

Of equal relevance is the *gradient* that this magnet would produce. Suppose that the permanent magnet is located on the x-axis, still oriented with its moment along z; then it will create a field with (-)z-direction at the sample, but this z-directed field will have a gradient in x, just because the magnet is closer to one end of the sample than the other. The magnitude of that gradient follows from the R^{-3} dependence given above, which yields

$$\partial B_z/\partial R = (\mu_0/4\pi)\,(3\mu/R^4) .$$

Q33. Show this gradient would be 0.51 μT/m for the magnet in question at distance of R = 1 m, and compute the dephasing timescale its presence would yield.

So one can imagine a systematic experiment, placing such a magnet at a point along the x-axis, always oriented along the z-direction, but varying in distance R from the sample. For each value of R, one could determine first the gradient-correction needed for an optimal free-precession signal, and next the frequency of that signal. The first of these would contain the information about the *gradient* that the magnet is contributing, while the second of these would contain the information about the *field* that the magnet is contributing. Their distinct R^{-4} and R^{-3} dependences ought to be distinguishable in a plot vs. R-value; and since the measured quantities are in absolute units, the magnetic moment of the magnet could in fact be deduced in two independent ways.

Appendix 3. The Helmholtz coils' geometry

The Helmholtz coil pair in the EFNMR Gradient/Field Coil System is designed and manufactured in terms of an archaic but perfectly well-defined length unit, the inch: 1 inch ≡ 25.4 mm. The design data given here will enable you to compute your best estimate of the 'coil constant' k, which gives the field generated at the center of the coils per unit current in the wires. Recall that there are 30 turns in each of the two coils, and that the same current I flows in each and every turn, because of a series connection of the coils.

The coils are wound on wooden forms designed to have a center-to-center separation along the z-axis of 11.95 inches; you may measure the actual separation yourself, and check to see if it's uniform around the circumference. The coils are wound in three layers, each of ten turns, starting at the bottom of a groove in the wooden frame having nominal diameter 23.69 inches. The #20 AWG copper wire used has a diameter of 0.035 inches, and the successive layers are separated by a layer of Kapton tape of nominal thickness 0.002 inches. Thus the outer sides of the outermost turns are expected to define a diameter of 23.91 inches; this number you may also check by direct measurement (on both coils, and at several places around the circumference).

With these measurements completed, you have all that's needed to locate each of the 30 turns on each coil both in radius away from the z-axis and in position along the z-axis. Now find or derive a result, depending on the Biot-Savart Law, for the field generated on the axis of a co-axial pair of coils, each of radius a, located at $z = +b$ and $-b$. This field will be a function of z, and you'll first want to evaluate it at $z = 0$.

A first model of the coils assumes that all 30 turns in each coil may be conflated to a single turn, carrying a current of 30I, taken to have the 'average position' of the separate turns. Evaluate the coil constant in this model, and see if you get $k \approx 90\ \mu T/A$. You might also evaluate the predicted on-axis field as a function of z, to see the degree of uniformity that can be expected in the relevant range of $|z| \leq 2.5$ cm. (The variation in field strength for points *off* the z-axis is much harder to compute, but you may be assured that variations off-axis are no worse than the ones you've just seen for on-axis locations.)

A more complicated model of the coils locates all 30 turns, in each coil, at their actual locations, and assigns separate a_j and b_j values to each of 30 superimposed coil pairs. Then the field at the center, or the field as a function of z, is also the superposition of the results for the 30 two-turn coil pairs. You should get a result very similar to, but perhaps more reliable than, your result above.

The hardest part of your modelling task might be to estimate, or justify, an uncertainty ∂k for your coil constant k; the uncertainty will depend mostly on the degree to which you can be sure where the coils' turns are located in space. The payoff of an honest calculation of $k \pm \partial k$ is a first-principles measurement of the proton's gyromagnetic constant, together with its uncertainty.

Appendix 4. The Fourier transform of a decaying sinusoid

This appendix works out the detailed analytic form of the Fourier transform to be expected for the ideal free-precession signal, and extracts from it a relationship between the T_2 decay time of the signal and the linewidth of the computed transform.

We suppose that the real voltage signal emerging from the EFNMR controller box can be written

$$V(t) = V_0\, e^{-q\,t} \cos \omega_0 t$$

where $q = 1/T_2$ describes the rate of exponential decay. Here $\omega_0 = 2\pi f_0$ gives the central frequency of the signal; but since the signal's duration is only of order a few T_2, we might expect (from an 'uncertainty principle' sort of argument) a frequency 'uncertainty' of order $\Delta f = 1/T_2$. The calculation below is intended to make this argument both clear and precise.

To perform the Fourier transform mathematically (as data-processing equipment might perform it in the experiment) we first realize that this signal exists only for $t \geq 0$, and then generalize it to the complex wave,

$$V_{complex}(t) = V_0\, e^{-q\,t} \exp(i\,\omega_0\, t) \quad \text{for } t \geq 0 .$$

Then the Fourier transform,

$$\tilde{V}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} V(t)\, e^{-i\,\omega\,t}\, dt$$

can be computed analytically, with result

$$\tilde{V}(\omega) = \frac{V_0}{\sqrt{2\pi}} \frac{q + i(\omega_0 - \omega)}{q^2 + (\omega_0 - \omega)^2} .$$

This complex function is likely to be displayed via its magnitude and phase; alternatively, its absolute square gives the Fourier power spectrum,

$$|\tilde{V}(\omega)|^2 = \frac{{V_0}^2}{2\,\pi} \frac{1}{q^2 + (\omega_0 - \omega)^2} .$$

This is a Lorentzian function, centered at frequency $\omega = \omega_0$, and falling to half its peak value at $\omega = \omega_0 \pm q$. Hence its full width (in angular frequency) at half maximum is $\Delta\omega = 2q$, so its FWHM in ordinary frequency is $\Delta f = 2q/(2\pi)$. In instrumental practice, this width is best found by locating two points on the sides of the Lorentzian peak which are 3 dB (a factor of two) down in power, or equivalently two points down by a factor of $1/\sqrt{2} \approx 0.707$ in indicated rms voltage.

If this Δf gives the width in frequency, we can choose a variety of measures for the duration-in-time of the time-domain signal. Our decay rate q is connected to the standard T_2 time-scale via $q = 1/T_2$; in turn T_2 is operationally available as the time during which the signal V(t) decays to 1/e of its initial amplitude. Even easier to read off a 'scope is $t_{1/2}$, the time during which the signal V(t) decays exponentially to half of its initial amplitude; this is given by $t_{1/2} = (\ln 2)/q$.

So we now have both factors for a "frequency-time uncertainly product", giving

$$\Delta f \cdot t_{1/2} = \frac{2q}{2\pi} \cdot \frac{\ln 2}{q} = \frac{\ln 2}{\pi} \approx 0.2206 .$$

Sure enough, the product is independent of the decay rate, and shows the correlation between long decay times and narrow spectral lines. The product is also of order 1, but is now precisely

specified, provided that the two 'uncertainties' are also precisely defined as they were above.

It follows that if a free-precession signal with a decay time of $T_2 = 1.0$ s is observed, this will have $t_{1/2} = 0.69$ s and the Fourier transform of this signal ought to have a full width (at half-maximum-power points) of

$$\Delta f = \frac{.2206}{t_{1/2}} = \frac{.2206}{0.69\ \text{s}} = 0.32\ \text{Hz}$$

It is actually important *not* to call this the 'uncertainty in frequency', however; what this Δf really gives is the linewidth of the Lorentzian peak observed. The actual experimental uncertainty in the frequency location of the *center* of this peak is likely to be smaller than Δf; if there are no other sources of frequency uncertainty, the uncertainty in the estimated location of line center, ∂f_0, might be as small as the above Δf divided by the signal-to-noise ratio of the data.

Appendix 5. Systematically tuning the sample coil

Using the EFNMR Gradient/Field Coil System, you'll want to be 'frequency-agile', since you'll be able to change the current in your Helmholtz coils and thereby move your NMR signals around in frequency. For NMR signals at any one fixed frequency, it's easy enough to tune the resonance of the sample coil to match the NMR frequency, but for data-taking over a range of frequencies, it's a good idea to be able to tune the coil systematically rather than by trial and error. This appendix describes how that systematic tuning might be achieved.

For purposes of tuning, the sample coil may be thought of as a fixed inductance L. The emf induced in this coil is magnified by placing a capacitance C_{total} in parallel with L; here C_{total} is all contained in the controller box, but it's made up of three parts:

$$C_{total} = C_{fixed} + N \cdot 5.0\ nF + n \cdot 0.50\ nF \ ,$$

where C_{fixed} is a fixed capacitance, and where N and n are integers in the range 0-15, corresponding to the settings of the coarse, and the fine, tuning switches. Each clockwise 'click' of either switch adds another increment of capacitance to the total, and those increments are (nominally) 5.0 nF and 0.50 nF for the coarse and fine adjustments respectively. Finally, the complete LC-system resonates at (angular) frequency

$$\omega_{res} = \frac{1}{\sqrt{L\,C_{total}}} \ .$$

Q34. Convert this result to ordinary frequency $f_{res} = \omega_{res}/2\pi$, and rearrange to give $1/f_{res}^2$. Show that a plot of dependent variable $1/f_{res}^2$ as a function of independent variable 10N + n ought to give a straight line, and see what parameters you can compute from its coefficients.

Here's a method for detemining the resonant frequencies f_{res}; it can be used *without* the need to generate actual NMR signals. Instead, it uses as a source a signal generator, capable of giving a (steady) sine-wave output in the 1-3 kHz range. It's best if the generator has a 'sync' output, since that can be used to trigger an oscilloscope and also to run a digital frequency meter. The only device that you need to build is a small circular coil, of perhaps 10 turns and 1-cm radius, hand-wound with copper wire. The idea is to tape that coil into place, perhaps onto one of the wooden beams supporting the Helmholtz coils in the EFNMR Field Coil apparatus, in such a position that ac signals in the little coil will couple some flux, and therefore induce some emf, in the sample coil. When you have such a coil in place, send an attenuated sine-wave from the generator to the coil, and use the 'scope to look at the output of the pre-amp in the EFNMR controller; the signal generator is going to be producing a (steady-state) surrogate for the signal which would otherwise be generated by precessing nuclear moments.

Once you can detect such a signal at the preamp output, set the generator to a fixed frequency of (say) 2000 Hz, and tune up the LC system (ie. vary the coarse- and fine-adjust switch settings) to maximize the output of the preamp. [To simulate the proper *scale* of the signals, adjust the amplitude of the generator output until the pre-amp output is about 200 mV peak-to-peak.] Now you can record N and n, the settings (in the 0-15 'clicks' range) of the switches which make the LC-circuit resonant at this frequency value.

To take data systematically, it's easiest to set N and n to fixed values, and then vary the generator

frequency f until resonance is achieved; once a resonant value f_{res} is thereby found, you have another datum in the form of a combination of {N & n, f_{res} } which can contribute to the data set. It is not required that you try all $16^2 = 256$ combinations of N and n, since the model above can fix all the unknowns using only a subset of these possibilities. Now plot the data in the form that is predicted to give a linear fit, and from the coefficients of a best-fit line, determine the values of L and C_{fixed}. (You should find values on the order of $L \approx 70$ mH and $C_{fixed} \approx 50$ nF.) That fully determines the model, which can then be turned around to give

$$10\,N + n = \frac{1}{4\pi^2\, L\, (0.5\text{ nF})\, f_{res}^2} - \frac{C_{fixed}}{0.5\text{ nF}}$$

You might use this expression as follows: suppose that you are back to doing NMR, and you are varying the Helmholtz coil current; and that you are graphing, as you go along, the NMR precession frequency f as a function of this current. Suppose your plot suggests that the next point you want to take is near f = 1700 Hz; the plot will tell you about what current will be needed, and the equation above, given best-fit values of L and C_{fixed}, and a chosen value of f = 1700 Hz, will tell you what number is needed for the integer 10 N + n. That will tell you how to set the tuning switches. For example, if the formula tells you that 10 N + n needs to be 132, you could set N = 13 and n = 2 (or N = 12 and n = 12) and you'd have the sample-coil system all set to be resonant to the 1700-Hz signal you expect to get from your next NMR datum.

A model like this can materially speed the process of data-taking, since it avoids the tedious tuning-by-guess that is otherwise required at each new value of Helmholtz-coil current. It also illustrates the important lesson that not only natural phenomena, but also scientific apparatus, can and should be modelled mathematically by the proficient physicist.

Finally, while you have a signal generator in place to excite emf in the sample coil, you might also monitor the output of the main or 'tuned' amplifier of the EFNMR controller, to determine the setting required on its ten-turn tuning knob to get its gain to peak at any particular target frequency. There may not be a simple model relating this setting to the tuned-amplifier passband frequency, but a plot of your data will give you a graphical version of a 'look-up table', so that you can set this tuning knob to the proper value for data-taking at some target frequency.

Appendix 6. Understanding the deuteron magnetic moment

This appendix illustrates the conversion between gyromagnetic constants and nuclear magnetic moments, introduces the 'nuclear magneton' as a scale for nuclear magnetic moments, and addresses the glamorous question of predicting the deuteron magnetic moment by 'additivity'.

This conversion starts from the classical calculation of the angular momentum and magnetic moment expected to exist for any rotating rigid body in which charge and mass are spatially distributed in the same way. If the total charge is Q and the total mass is M, then the result is

$$\gamma = \frac{\mu}{L} = \frac{Q}{2M} .$$

If such a model is applied to a spin-1/2 proton, with magnetic moment μ_p and mass m_p, we get the expectation

$$\mu_p \text{ ?=? } (e/2m_p)\, L = (e/2m_p)\, \Pi/2 = e\, \Pi/(4m_p).$$

If the proton were a "Dirac particle", we'd expect a proton magnetic moment larger than this by a famous factor of 2, allowing the prediction

$$\mu_p \text{ ?=? } e\, \Pi/(2m_p) ;$$

this combination of fundamental constants is in fact called the 'nuclear magneton' μ_N, and it gives a natural unit in terms of which to measure nuclear magnetic moments. Imagine the surprise when the proton magnetic moment was in fact measured, and found to have a value, in units of nuclear magnetons, more like *three* than one!

Your NMR data already give a value for the proton magnetic moment, since we've written the gyromagnetic ratio as

$$\gamma = \frac{\mu_p}{L} = 2\,\pi\, c_p \quad ;$$

accepting that the angular momentun for protons is $L = \Pi/2$, we get

$$\mu_p = 2\,\pi\, c_p\, L = 2\,\pi\, c_p\, \Pi/2 = \pi\, \Pi\, c_p.$$

You can now evaluate μ_p from your data, and $\mu_N \equiv e\, \Pi/(2m_p)$ from accepted values, and see for yourself that μ_p/μ_N is emphatically not one. The ratio that you do get is called "the proton magnetic moment in nuclear magnetons".

If you have obtained any free-precession signals at all from heavy water, you have the data to determine the gyromagnetic constant c_d for deuterons. Accepting that deuterons are spin-1 nuclei, you can by a similar procedure compute μ_d from your data, and then the ratio μ_d/μ_N, which is called "the deuteron magnetic moment in nuclear magnetons".

Finally you can look up (though alas, not easily measure) the neutron magnetic moment in nuclear magnetons. Now, see if the deuteron magnetic moment is equal to the sum of the proton and neutron magnetic moments. Here you'll need to pay attention to your uncertainty estimates to decide whether you too are entitled to be surprised.