Spin Resonance and the Proton g Factor

George R. Welch
2 February, 2018

1 Introduction

The purpose of this laboratory is to understand spin resonance, both nuclear and electronic, and to measure the g-factor of the electron and proton. You will learn about the gyromagnetic ratio of a charged spinning body, and learn how the g-factor relates to gyromagnetic ratio.

Homogeneous classical bodies have a g-factor of 1. Relativistic quantum theory (the Dirac equation) predicts that charged spin-1/2 particles have a g-factor of 2. (For electrons, the actual value differs only slightly from 2 due to quantum electrodynamical effects.) When the gyromagnetic ratio of the proton was first measured and its g-factor was found to differ substantially from 2 (it is more like 5.5) this was stunning proof that the proton was a composite particle, not an elementary particle like the electron.

You will make measurements using a Tel-Atomic, Inc. CWS 12-50 cw NMR/ESR spectrometer.

Reference:

- Advanced cw NMR/ESR System, Tel-Atomic, Inc.
  `http://www.telatomic.com/spin_resonance/CW_NMR_ESR.html`

2 Gyromagnetic Ratio and Larmor precession — classical story

2.1 A spinning collection of charge has a magnetic moment

Consider a solid (rigid) body with charge Q and mass M, rotating with angular velocity ω about some axis. For generality, suppose the mass and the charge are not necessarily distributed the same way, so denote the charge distribution by $\rho_q(\vec{r})$, and mass distribution by $\rho_m(\vec{r})$,

The volume element dV shown in Fig. 1 has charge $dq = \rho_q dV$ and sits a distance $r_\perp$ from the rotation axis. We can consider that little charge constituting a differential current loop about the axis. This "loop" produces a magnetic field, which we can integrate over the distribution. The current will be the charge dq divided by one rotational period: $dI = \omega dq/(2\pi)$. The magnetic moment will equal the product of this current and the cross-sectional area:

$$d\mu = dI \cdot A$$

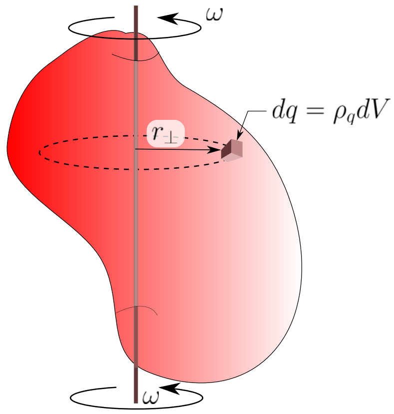

Figure 1: A solid rigid body of charge Q and mass M rotating with angular velocity ω about some axis. We consider a differential element $dQ = \rho_q dV$ which rotates a distance $r_\perp$ from the axis.

$$= \left(\frac{\omega dq}{2\pi}\right)\left(\pi r_\perp^2\right)$$
$$= \frac{\omega}{2}\rho_q r_\perp^2\, dV$$

And so, the magnetic moment is given by

$$\mu = \frac{\omega}{2}\int_V \rho_q r_\perp^2 dV \tag{1}$$

2.2 Gyromagnetic ratio

We recall that the angular momentum $\vec{S}$ of a spinning rigid body is

$$S = I\omega = \omega \int_v \rho_m r_\perp^2 dV \tag{2}$$

Comparing this with Eq. (1) we see that the magnetic moment is proportional to the angular momentum

$$\vec{\mu} = \gamma \vec{S} \tag{3}$$

The proportionality constant γ is called the **gyromagnetic ratio** for the particular spinning object. The units of γ are angular-frequency divided by magnetic field, or radians per second per Tesla. Typically we measure real frequencies in the laboratory rather than angular-frequency, so it is customary to quote values for $\gamma/(2\pi)$ in Hz per Tesla (or MHz per Gauss, or something like that).

This factor of 2π is important, and is a common source of errors in calculations. **Do not blow it.**

2.3 g-factor

The gyromagnetic ratio γ defined by Eq. (3) parameterizes how much magnetic field the object has for a given angular momentum. It is useful to find a dimensionless number which parameterizes the same thing.

Let us first consider the special case when the charge distribution of this spinning object has the same functional form as the mass distribution, that is, when the mass and charge are distributed the same way:

$$\rho_q = \frac{Q}{M}\rho_m \tag{4}$$

In this case, combining Eqs. (1) and (2) gives

$$\mu = \frac{1}{2}\frac{Q}{M}S \tag{5}$$

which gives

$$\gamma = \frac{1}{2}\frac{Q}{M} \tag{6}$$

Now, the mass and charge do not necessarily have the same distribution, so it is convenient to factor this quantity out of the gyromagnetic ratio and to write, in general

$$\gamma = g\,\frac{Q}{2M} \tag{7}$$

where g is a dimensionless constant called simply the **g-factor** for this spinning object. For the case above where the charge and mass have the same distribution, $g = 1$.

Exercise for students: Calculate the g-factor for a uniform solid sphere of mass M, with charge Q uniformly distributed about its surface. If you cannot do this, then you may not understand the above discussion. *Answer:* $g = 5/3$.

2.4 Larmor Presession

In order to see a common situation where the gyromagnetic ratio (or the g-factor) is an important parameter, consider a magnetic dipole $\vec{\mu}$ in a static magnetic field $\vec{B}$. The torque $\vec{\tau}$ on the dipole, the potential energy W, and the force $\vec{F}$ on the dipole are given by:

$$\begin{aligned} \vec{\tau} &= \vec{\mu} \times \vec{B} \\ W &= -\vec{\mu} \cdot \vec{B} \\ \vec{F} &= -\vec{\nabla} W = \vec{\nabla}(\vec{\mu} \cdot \vec{B}) \end{aligned} \tag{8}$$

We write the magnetic moment as proportional to the spin $\vec{\mu} = \gamma\vec{S}$ where γ is the gyromagnetic ratio. Let's consider a uniform magnetic field, so $\vec{F} = 0$ and then the equation of motion is

$$\vec{\tau} = \frac{d\vec{S}}{dt} = \frac{1}{\gamma}\frac{d\vec{\mu}}{dt} = \vec{\mu} \times \vec{B} \tag{9}$$

so

$$\frac{d\vec{S}}{dt} = -\gamma\vec{B} \times \vec{S} \tag{10}$$

which means that $\vec{\mu}$ precesses about $\vec{B}$ with a resonant frequency $\omega_0 = \gamma B$ or

$$\omega_0 = \gamma B = g\frac{Q}{2M}B \tag{11}$$

This important frequency ω_0 is called the Larmor frequency.

3 Quantum Mechanical Story

The Dirac equation predicts that a spin-1/2 particle of charge q and mass m will posses a magnetic moment

$$\vec{\mu} = \frac{q}{m}\vec{S}$$

which can can be written in analogy to Eq. (5) as

$$\vec{\mu}_S = g_S\frac{e}{2m}\vec{S} \tag{12}$$

where $g_S = -2$ and e is the magnitude of the electron charge. This prediction, that spin-1/2 particles will have a g-factor exactly equal to 2 is a key success of the Dirac equation and relativistic quantum mechanics.

In actuality, an isolated electron interacts with the ground state of the quantized electro-magnetic field and with its own field, which results in a quantum electrodynamic (QED) correction to the g factor. The current best result is

$$g = -2.0023193043622(15)\,.$$

This extremely precice value has enabled the testing of QED to unprecedented levels, and the development of the technology to make this possible enabled Hans Dehmelt to win the 1989 Nobel Prize in Physics.

In atoms, electrons have orbital angular momentum $\vec{L}$, and this orbital angular momentum produces a magnetic moment given by

$$\vec{\mu}_L = g_L\frac{e}{2m}\vec{L} \tag{13}$$

The value of g_L is exactly equal to one, by a quantum-mechanical argument analogous to the derivation of the classical gyromagnetic ratio.

When spin and orbital angular momentum couple to produce states of total angular momentum $\vec{J} = \vec{L} + \vec{S}$ the resulting magnetic moment is written as

$$\vec{\mu}_J = g_J\frac{e}{2m}\vec{J} \tag{14}$$

and in this case, g_J is called the "Landé g factor" after Alfred Landé. It is a straightforward exercise in quantum mechanical angular momentum theory to express g_J in terms of g_L, g_S, and the angular momentum quantum numbers J, L, and S.

3.1 Larmor Precession

We consider a quantum mechanical spin $\frac{1}{2}$ particle in a uniform magnetic field $\vec{B}$. We take the direction of the field to be the z-axis, so $\vec{B} = B\hat{z}$ and write

$$S_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle \tag{15}$$

where $|\pm\rangle$ are the eigenstates of S_z

We have seen that the classical potential energy of a magnetic moment in a magnetic field is is $W = -\vec{\mu}\cdot\vec{B} = \gamma B S_z$. So, we write the quantum mechanical Hamiltonian as

$$H = \gamma B S_z = \omega_0 S_z \ . \tag{16}$$

Thus we have the picture of two energy levels, with energies $\pm\hbar\omega_0/2$ shown in Fig. 2.

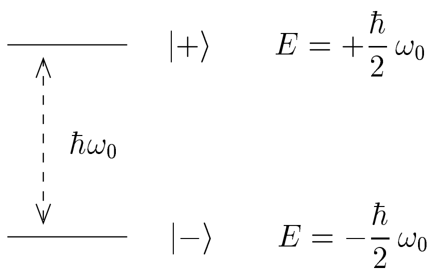

Figure 2: Spin $\frac{1}{2}$ in a magnetic field.

$$H|+\rangle = \frac{\hbar\omega_0}{2}|+\rangle \tag{17}$$

$$H|-\rangle = -\frac{\hbar\omega_0}{2}|-\rangle \tag{18}$$

It is straightforward to show that an oscillating magnetic field drives transitions between these two energy levels when the oscillating frequency is equal to the Larmor frequency ω_0 given in Eq. (11).

4 Measurement

The NMR apparatus allows you to place a sample in a strong magnetic field and radiate the sample with RF (radio-frequency) electromagnetic radiation that is generated by a programmable RF generator. If the sample contains spinning charges (that is, magnetic dipoles), then they will undergo Larmor precession as described above. If the RF frequency matches the Larmor precession frequency, this precession will be driven by the oscillating magnetic component of the RF field, and some the RF will be absorbed and scattered.

By detecting the strenth of the RF that is radiated by the generator, it is possible to detect the presence of the little spinning magnetic dipoles. Please note that this absorption signal is very weak, and difficult to detect. I. I. Rabi won the 1944 Nobel Prize in Physics for doing it. We have a lot of technology that Rabi did not have, so our life is easier.

4.1 scanning

The NMR apparatus can operate two ways. It can apply a strong *slowly varying* magnetic field, with a constant RF frequency, and let you look for the resonance when the magnetic field is right – or – it can apply a strong *constant* magnetic field, with a slowly varying RF frequency, and let you look for resonance when the RF frequency is right. In either case, the resonance you are looking for occurs when Eq. (11) is satisfied.

However, the frequency resolution of the programmable RF generator is low, so it is almost always desirable to **fix the RF frequency and scan the magnetic field.**

4.2 detection

Because the absorption resonance you are looking for is very weak, we use *phase sensitive detection* just as you learned in the lockin amplifier experiment. In addition to the strong slowly-varying magnetic field mentioned above, we apply a small sinusoidal oscillating field. By looking at the component of the signal at this oscillation frequency, **we obtain a derivitive signal** with high signal to noise.

5 Experiments

First you need to understand the use of the apparatus. You do not need to read the entire manual to get started. I recommend reading the following:

- Section 1, page 9, first couple of paragraphs.

- Section 8, pages 29-34.
- then skim quickly pages 35-40
- Section 9.1, page 41. Note the collection of samples on the table.
- Section 10.3, pages 53-54.
- Section 10.2.3, page 50.
- Section 10.5, pages 56-59.

After that, you should be able to use the machine.

5.1 proton g-factor

Start with the the NMR experiment, Section 10.2.3 above. Use the glycerin sample.

It is not straightforward to enable communication between the Tel-Atomic CWS12-50 spectrometer and its associate software. A technique that seems fairly reliable is to first exit the software. Next make sure the spectrometer is turned on and that the serial-USB adapter from the spectrometer is connected to the computer. Then start the software. Now, from the "Spectrometer" menu choose "Comm Port" and then "COM2". Note that it is COM2 and not COM1. (These are legacy terms from the days when PCs had RS232 serial ports.) Then from the Spectrometer menu, choose "Connect". This should enable communication between the software and the spectrometer. If it fails, try repeating it. If that fails, try turning off the spectrometer and repeating.

Here is some very important advice for getting good data. First, remember that you are trying to measure the precession frequency of tiny little spins (protons or electrons) in an applied magnetic field. Protons are much heavier than electrons, and you need a substantial magnetic field. You will be using radio-frequency detection in the vicinity of 13–15 MHz because this is a *fairly* quiet spectrum that is straightforward to detect.

It might make more sense to you to think of setting the magnetic field to some value (which causes the spins to precess) and then sweeping the RF-field until it matches the spin-precession frequency causing a resonance that can be detected. This would work, but experimentally it is not so easy. While it is easy to produce a precise RF oscillator, it is much easier to scan the current in a magnetic field than to scan the RF as described in Sec .4.1. So, we will do the experiement backward: we will fix the RF frequency and scan the magnetic field to find the resonance. Then we will increase the RF frequency and again find the magnetic field that produces a resonance. By repeating this over a range of RF frequencies, we can find the plot the magnetic field at each resonance versus the frequency used, and the slope will be **one over** the gyromagnetic ratio.

The magnetic field needed for proton spin resonance at these frequencies is several kilo-Gauss. (Remember that the Earth's magnetic field is approximately one-half Gauss.) The electromagnet on the table, like most electromagnets in this field range, exhibits hysteresis. This is important for you to understand. It means that if you set the current to some value and measure the magnetic field, then increase the current, then decrease it back to the starting value, the magnetic field *will not* be the same as your first measurement.

Nonetheless, you have the potential to make a very accurate measurement of the proton gyromagnetic ratio by plotting the resonance magnetic field for several different RF frequencies and measuring the slope. The intercept will not be zero because of the hysteresis in the magnet, but the slope can be very accurate.

For this to work well, it is important for you to take your magnetic field data sequentially. Do not find the resonance at low magnetic field, then high, then low again. Take smooth steps in magnetic field *only in one direction.*

First, you need to understand the software. Let's start on the lower left of the display with the block labeled "operating mode". Choose "NMR 1H". This means the hardware will be optimized for detecting protons.

Next, there is a block called "Detection". The field called B0 is the magnetic field at the center of the sweep. You cannot type a value into this field, but instead the buttons beside it move it up or down. The amount they move it up or down by is the amount beside it next to the word "by". The field called F is the radio-frequency that is applied, and it is changed the same way as B0. Below this are sliders for Gain and Phase. Gain is just the gain in the signal amplifier. Phase is the phase setting of the built-in lock-in amplifier. This will make much more sense after you have done the lock-in experiment.

Next. there is a block called "Modulation". You can choose between "Field Sweep" and "Frequency Sweep", but for all these experiments it should be set to Field Sweep for the reasons described above. The value determines the full scale sweep of the magnetic field. So, for example: if you set B0 to 3200 Gauss and Field Sweep to 10 Gauss, then the magnetic field swcan will go from 3195 Gauss to 3205 Gauss. Make sure you understand this!

The "2nd Mod Amplit" setting is very important. Refer to Sec 4.2. While the magnetic field is scanning (by the amount chosen above) a small dither is added to the magnetic field, and the lockin detector uses this to find the signal. Obviously the second modulation amplitude must be small compared to the field sweep, because it will broaden signals, and it should also be somewhat smaller than the signal linewidth. It takes a bit of iteration to find a good setting.

The Sweep Time is just the amount of time for one sweep. Start with this set to the minimum (30 seconds) but you may want to increase it later to get better signals.

A thing that makes this hard is that the instructions tell you to set the RF frequency to 14 MHz. But there is sometimes a lot of RF noise in our lab, making this frequency nearly unusable. We have found that turning the RF frequency down as low as it will go, to about 13 MHz works much better. However, you have to match the magnetic field to the RF frequency.

Here I will describe a method that I find works well. First, turn the magnetic field as low as it will go. (Should be 3073 Gauss.) Set the control to increase the field by 1 Gauss. Now, increase the magnetic field by about 10 Gauss (10 clicks) from whatever it was (so it should now be about 3083 Gauss). Set the RF frequency to about 13160 kHz, and set it's increment to 10 kHz. Set the Field Sweep to 15 Gauss, Second Modulation Amplitude to 1.5 Gauss, Gain to 100, and Phase to 0.

Now, perform a single scan. If you are incredibly lucky, you will see the resonance. If you win the lottery, it will look like the picture on page 50 of the manual, but more likely it will be very distored and that is okay. If you do not see the resonance, increase the frequency by 10 kHz and repeat. Keep doing this about 5 times. If you still don't find the resonance, move the frequency back to where you started, and repeat about 5 times, in 10 kHz decrements, down in frequency. If you still don't find the resonance, come find the instructor.

After you find the resonance, you want to optimize it, and get a feel for how the resonance field and frequency are related. To do this note the value of the magnetic field at the resonance and the frequency. Calculate the ratio, and use this to estimate what value to set the frequency so that the resonance appears about 1/4 of the way through a scan. Take a scan. Now repeat this until the resonance is about 1/4 of the way.

The reason you want to have the resonance this way is so that you do not have to wait the full 30 seconds for each scan to finish while you are adjusting things. It will go quicker if you can just abort the scan as soon as you see the resonance.

Now, adjust the "Gain" until the resonance is large, but the spectrometer is not complaining about saturation.

How wide is the resonance? Set the "2nd Mod Amplit" to a value that is less than about 1/4 of the full linewidth. You may have to readjust the gain, take a scan, and decrease the second modulation amplitude.

Now, you want to adjust the "Phase" setting. To do this note that when it is set perfectly the resonance will look like the picture on page 50 of the manual. You can change the phase in 1.5° increments, but it is difficult to see much change when you are close to the correct value. When the phase control is 90° from the correct value, the resonance will be minimized and will look very distorted from this picture, perhaps with multiple positive and negative excursions. I find that it is easier to adjust the phase to *minimize* the signal than to maximize it, because a minimum is easier to see. Then, when you feel like you have found the minimum, just add 90° to the phase setting (modulo 360) and you should have the maximum.

It does not matter if your phases is 180° off. That will just produce a picture that is the mirror image of the one shown on page 50. The resonance field is the field when the signal crosses zero at the center. To find this field, let a scan finish and a purple vertical line will appear on the display. You can drag this line to the center of the resonance and read the offset on the upper left of the display. The magnetic field at the resonance is just the B0 setting plus this offset.

You now have one data point! It is the resonance magnetic field and the RF frequency. Estimate your uncertainty in this magnetic field value.

The object is to find the resonance frequency for as many different values of the RF that you can, so that you can plot the resonance magnetic field versus the RF-freqnency.

To do this note again the ratio of the frequency to magnetic field. This ratio should be something like 3100 G/13.2 MHz = 0.23 G/MHz. Increase the frequency by 20 kHz. Now, increase the magnetic field by $20 \times 0.23 \approx 5$ G. Now do a scan. The resonance should be in about the same place. If not, use this to correct your ratio. Keep doing this until you have increased the radio frequency by about 100 kHz from your first data point. That is your second data point. Keep doing this until you have about 10 data points. I have actually gotten 18 data points this way myself, from a starting frequency of 13,160 kHz, in 100 kHz increments, up to 14,860 kHz.

Perform a 2-parameter fit to get the gyromagnetic ratio γ. Do not blow the factor of 2π. Convert the gyromagnetic ratio γ to the g-factor, and compare your result to the known g factor of the proton: 5.585694713(46).

5.2 electron g-factor

Next turn to section 10.3 of the manual (page 53). Do essentially the same thing as above, extracting the electron g-factor.

5.3 conclusion

Compare your value to the known value, and discuss why the g-factors of the electron and proton are different.

Be careful to state your uncertainties, and discuss systematic effects when you write up the lab.