PHY 4210-01 Senior Lab
Lab P2: Electron Spin Resonance

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March 28, 2019

Abstract

Electron spin resonance allows the structure of paramagnetic materials (such as diphenyl-picryl-hydrazyl or DPPH) to be investigated, as they have a nonzero momentum. The ratio of the magnetic moment and angular momentum is the gyromagnetic ratio of spin, g_s. Such a value for the electron was determined by applying various resonance frequencies and recording the magnetic field produced via Helmholtz coil, and determined to be $g_s = 1.49 \pm 0.13$. A resonance curve was produced by plotting voltage amplitude against the frequency seen from a resonance circuit box. The line width of the resonance signal was then calculated to be $0.49mT$.

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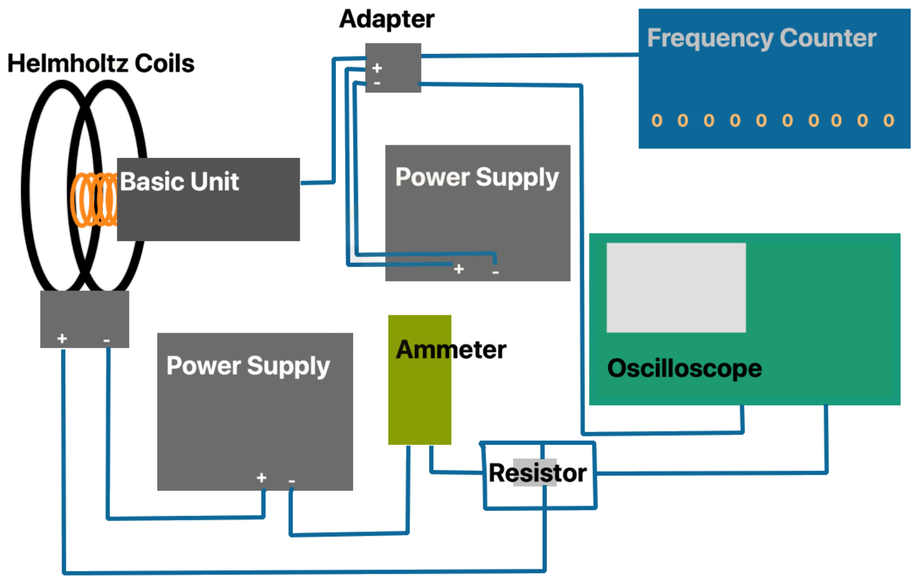

Figure 1: Schematic of equipment used in experiment

1 Data Analysis

1.1 Frequency Dependence of Resonance Field

Voltage was compared to frequency to obtain a graphical relationship for the frequency dependence of the resonance field. Such a relationship is shown below in figure 2. The amplitude of the voltage was obtained by measuring the peak-to-peak voltage from the oscilloscope and dividing it in half. The peak in the data distribution graphed in figure 2 is the resonance frequency for the field. This value occurs at a voltage of 1.01 V and a frequency of $4.18 * 10^7$ Hz. It is important to note that the electron spin resonance device divides the frequency by a factor of a thousand, which is reflected in the measurements taken with the Hewlett-Packard frequency counter. Thus the measurements needed to be corrected before analysis is carried out, i.e. the counter's frequency are multiplied by one thousand.

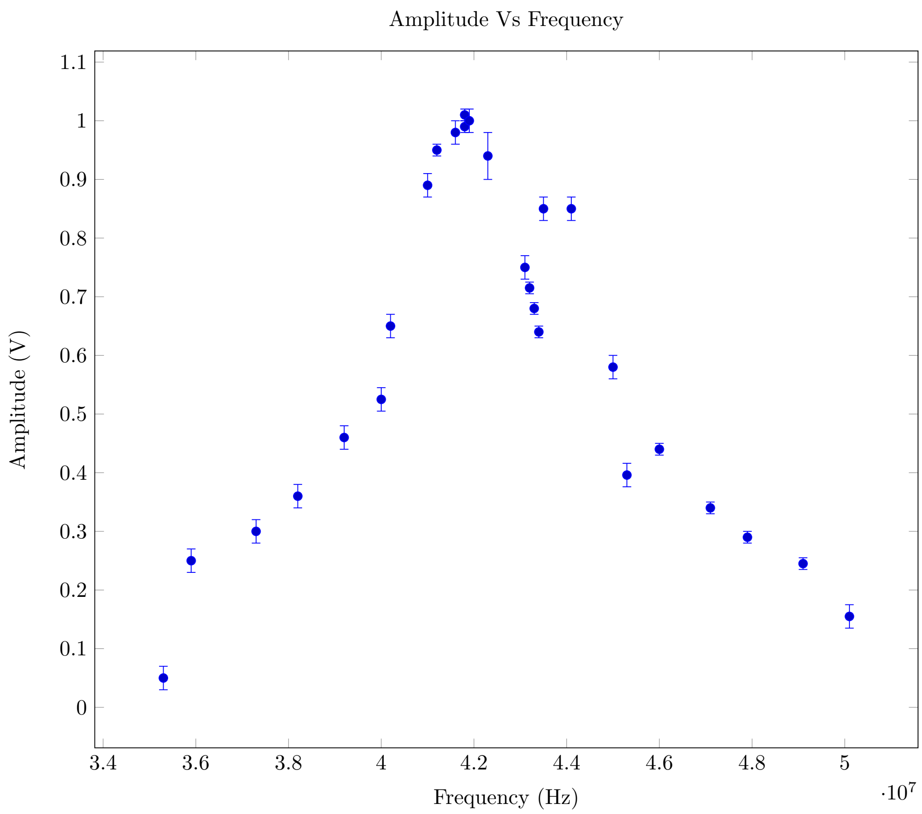

Figure 2: Voltage amplitude versus frequency: a graphic representation of the frequency dependence of the resonance field.

1.2 Experimental Value of Gyromagnetic Ratio

The gyromagnetic ratio is calculated using equation 1, where ν is the frequency, h is Planck's constant, μ_B is the Bohr magneton, and B_0 is the magnetic field strength.

$$g_s = \frac{h \times \nu}{\mu_B \times B_0} \tag{1}$$

The magnetic field used in calculating equation 1 must be calculated as well. It is determined from the measured current using equation 2, where $\mu_0 = 4\pi \times 10^{-7} \frac{Vs}{Am}$, the number of turns is $n = 320$, and the radius of the coils is $r = 6.8cm$.

$$B_0 = \mu_0 \left(\frac{4}{5}\right)^{3/2} \times \frac{n}{r} \times I \tag{2}$$

Rather than measuring the current directly, the current is calculated by measuring the voltage drop across a resistor, of which the resistance is also measured. This calculation is shown below in equation.

$$I = \frac{V}{R} \tag{3}$$

By substituting equation 3 into equation 2, and then substituting equation 2 into equation 1, we arrive at an expression for the gyromagnetic ratio in terms of known constants and measured quantities. This final expression is shown in equation 4.

$$g_s = \frac{h \times \nu}{\mu_B \times \left(\mu_0 \left(\frac{4}{5}\right)^{3/2} \times \frac{n}{r} \times \frac{V}{R}\right)} \tag{4}$$

1.3 Propagating Uncertainty in Gyromagnetic Ratio

The error in the experimental value of the gyromagnetic ratio is determined by propagating uncertainty in equation 4. There are no uncertainties associated with fundamental constants such as h, μ_B, and μ_0. It is assumed that the number of coil turns, n, also has no associated uncertainty because it was reported in the manual as such. The uncertainty in the radius is constant for all measurements, but the frequency, voltage, and resistance will differ for each measurement. Equation 5 shows this error propagation.

$$\delta g_s = g_s \times \sqrt{\left(\frac{\delta\nu}{\nu}\right)^2 + \left(\frac{\delta r}{r}\right)^2 + \left(\frac{\delta V}{V}\right)^2 + \left(\frac{\delta R}{R}\right)^2} \tag{5}$$

An example calculation for the value of g_s and its propagated uncertainty is shown below for a measurement taken with the large coil:

$$\begin{aligned} g_s &= \frac{6.626 \times 10^{-34} \times \left(3 \times 10^7\right)}{\mu_B \times \left(4\pi \times 10^{-7} \left(\frac{4}{5}\right)^{3/2} \times \frac{320}{0.068} \times \frac{0.44}{1.7}\right)} \\ &= 1.93 \end{aligned}$$

Again, the associated uncertainty is as follows:

$$\begin{aligned} \delta g_s &= g_s \times \sqrt{\left(\frac{1.00 \times 10^4\text{Hz}}{3.00 \times 10^7\text{Hz}}\right)^2 + \left(\frac{0.5\text{cm}}{6.7\text{cm}}\right)^2 + \left(\frac{0.1\text{V}}{2\text{V}}\right)^2 + \left(\frac{0.1\Omega}{1.7\Omega}\right)^2} \\ &= 1.93 \times \sqrt{(3.3 \times 10^{-4})^2 + (0.006)^2 + (0.05)^2 + (0.06)^2} \\ &= .15 \end{aligned}$$

We can calculate the discrepancy between the experimental and theoretical values as follows. Recall the theoretical value of g_s for DPPH is 2.0036, which is approximated as 2.00 due to the limited precision of the experimental value.

$$\begin{aligned}\Delta g_s &= |g_{s_{exp}} - g_{s_{theo}}| \\ &= |1.93 - 2.00| \\ &= 0.074\end{aligned}$$

Evidently, this difference Δg_s is less than 1σ, which is taken to be $\delta g_s = 0.15$.

1.4 Rejection of Data

During the data-taking process for the "big coil", a measurement at a particular frequency produced an experimental g_s value that seemed anomalous; most measurements fall between 1 and 4, but this measurement is around 13. Chauvenet's criterion will be used to determine if this datum should be discarded.

If one assumes this measurement to be valid, the resultant average and standard deviation are 2.59 ± 2.91 (quite an atrocity). The measurement in question, 13.08, differs from the average by 4.49σ. If a Gaussian distribution is assumed for the g_s values, the probability of obtaining a measurement that differs from the mean by this quantity is determined as follows:

$$\begin{aligned}Prob(\text{outside } 4.49\sigma) &= 1 - Prob(\text{within } 4.49\sigma) \\ &= 1 - .9999994 \\ &= 0\end{aligned}$$

Since the probability of a measurement being withing 4.49σ is so high, the probability of this measurement being outside this interval is effectively zero. Therefore, we can discard the anomalous datum with extremely high confidence.

1.5 Determining Line Width of Resonance Signal

The quantity δB_0 is representative of an absorption line, and is obtained when the energy is measured at a fixed frequency as function of the magnetic field. The line width δB_0 is used as an expression of the uncertainty in the energy of the transition. This is best represented by the equation $\delta E = g \times \mu_0 \times \delta B_0$. Using the uncertainty principle a relation is then found for δB_0.

$$\delta B_0 = \frac{\hbar}{2 \times g_J \times \mu_B \times T},$$

where T is the lifetime of the level and g_J is the Landé factor.

Experimentally δB_0 can be determined by equation 6, where δI is represented as $\frac{\delta U}{U_{mod}} \times I_{mod} \times 2\sqrt{2}$.

$$\delta B_0 = B \times \left(\frac{\delta I}{I_{mod}}\right) \tag{6}$$

This first requires an intermittent calculation of δI as follows:

$$\begin{aligned}\delta I &= \frac{\delta U}{U_{mod}} \times I_{mod} \times 2\sqrt{2} \\ &= \frac{0.55}{2} \times 0.156 \times 2\sqrt{2} \\ &= 0.121\end{aligned}$$

Substituting into equation 6 yields the following calculation:

$$\begin{aligned}\delta B_0 &= B \times \left(\frac{\delta I}{I_{mod}}\right) \\ &= 6.23 \times 10^{-4} \times \left(\frac{0.121}{0.156}\right) \\ &= 4.85 \times 10^{-4} T \\ &= 0.49 mT\end{aligned}$$

2 Results: Discrepancies and Uncertainties

2.1 Discrepancy in Gyromagnetic Ratio

The discrepancy between the experimental and theoretical values of G for each of the coils can be calculated with $\Delta g_s = |g_{s_t} - g_{s_e}|$, where g_{s_t} is the theoretical value of g_s and g_{s_e} is the experimental value. The discrepancy in the value of g_s for the small coil is:

$$\begin{aligned}\Delta g_{s_{\text{small}}} =& |(2.00) - (1.44)| \\ =& 0.56\end{aligned}$$

Since the standard deviation of the calculated values is $\sigma_{g_s,\text{small}} = 0.393$, the experimental value of g_s is

$$\frac{\Delta g_{s_{\text{small}}}}{\sigma_{g_s,\text{small}}} = \frac{0.56}{0.393} = 1.42\sigma$$

from the theoretical value of $g_s = 2.00$.

The discrepancies for the medium and big coils were calculated in the same manner, and the results are detailed in table 2.1. The results from the three coils are then used to calculate a true average value of g_s. The uncertainty in this value is the standard deviation of the mean, computed from all the data points across all the coils.

Table 2.1: The discrepancies between the theoretical and experimental values for g_s for the small, medium, and big coils as well as the average value of g_s.

Coil	Theoretical g_s	Experimental g_s	Δg_s	Standard Deviation (σ)	$\sigma \Delta g_s$
Small	2.00	1.44	0.56	0.39	1.4 σ
Medium	2.00	1.16	0.84	0.13	6.7 σ
Big	2.00	1.89	0.11	0.83	0.13 σ
Average	2.00	1.37	0.63	0.47	1.3 σ

2.2 Discrepancy in Line Width

The line width itself is representative of an error in the energy, as discussed above. Therefore, an uncertainty will not be calculated in the line width, as it is already a calculation involving uncertainties of constituent quantities. However, the experimental value can be compared to an acceptable range given by literature sources. The experimental line width was determined to be $\delta B_0 = 0.49mT$. The range given for theoretical line width was [0.15,0.81] mT, thus the experimental value is within the acceptable range.

3 Sources of Error

An ideal Helmholtz coil has a separation distance equal to its coil radii. The width of the "basic unit" module, which holds the coil samples, was larger than the radius of the coil. Thus the separation distance was limited to this width, and was larger than the coil radius. This restriction of the experimental set-up results in a magnetic field systematically lower than that indicated by calculations, as a true Helmholtz coil is designed with such a separation distance in order to maximize constructive interference of the constituent coils' fields. Any deviation from this set-up will result in a weaker field. Furthermore, because the magnetic field is systematically lower than the prediction, the calculated g_s is systematically higher that calculations predits, since the two quantities are inversely proportional.

Both the Helmholtz coil and the 1 $M\Omega$ resistor began heating up throughout the course of the experiment. The heating of the equipment causes energy loss in the system as the thermal energy transfers from the system to the surrounding region. This means that less energy is translated into the magnetic field, and since this quantity is directly proportional to the calculation of g_s, the value for g_s will be systematically lower than predicted. As the resistor heats up, its resistivity and thus resistance increases, however this effect was mitigated in the calculations by repeatedly measuring the resistance of the resistor, before every trial, and using each resistance for its respective calculation of g_s.

4 Conclusion

Within the experiment, the value of g_s was calculated for small, medium, and big coils, and these values were used to determine an average g_s value. The g_s value for the small coil was calculated to be $1.44 \pm 65 \times 10^{-3}$ with a discrepancy from the theoretical value of 1.4σ. The g_s value of the medium coil is $1.16 \pm 18 \times 10^{-3}$ with a discrepancy of 6.7σ, and the g_s value of the big coil is $1.89 \pm 210 \times 10^{-3}$ with a discrepancy of 0.13σ. The average g_s value is 1.37 ± 0.05 with a discrepancy of 1.3σ. Additionally, the resonant frequency of DPPH was determined graphically from Figure 2 to be 41 MHz.

5 Appendices

5.1 Appendix A: Data

5.2 Appendix B: Source Code