

A solid state marginal oscillator for NMR detection

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Abstract. There exist numerous designs to study continuous wave NMR. Described is a marginal oscillator circuit composed of two JFETs that reliably detects NMR. The circuit is very sensitive, operates at low RF levels, and has a good signal to noise ratio for proton NMR at room temperature. The circuit is made from commonly available components and may prove useful in studying NMR at low temperatures.

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Introduction

NMR (Nuclear Magnetic Resonance) is an important tool to probe the properties of matter. The discovery of NMR came from the advances in quantum mechanics in the 1920s. In 1927, Pauli predicted the quantum spin of electrons which led to the detection of nuclear magnetic moments in 1933. Then, in 1937, I.I. Rabi predicted and observed nuclear magnetic resonance. And in 1946, Purcell and Bloch simultaneously observed NMR in bulk materials and would later go on to win the Nobel Prize in Physics for the discovery. The 1960s and 1970s gave rise to numerous NMR spectrometers and myriad new techniques to detect NMR. Currently, NMR is the principle behind MRI machines, and it is also indispensable for physicists and chemists studying the properties of matter [1-2].

NMR arises from the inherent spin property of fundamental particles. As a result of this spin, every electron, proton, and neutron has a magnetic moment associated with it. For electrons the magnetic moment associated with the spin angular momentum $\hbar S$ is:

$$\mu_s = ge\hbar S/2m_e, \quad (1)$$

where g is the Landé splitting factor, e is the charge of an electron, m_e is the mass of an electron, and $e/2m_e$ is called the electron gyromagnetic ratio. We ignore the magnetic moment associated with the orbiting angular momentum because it tends to cancel in molecules. In the case of the nucleus, a magnetic moment, μ_I , results from a total spin angular momentum of coupled nucleons $\hbar I$:

$$\mu_I = g_I e\hbar I/2m_p, \quad (2)$$

where g_I is a dimensionless constant, I is spin quantum number and an integral or half integral number depending on the nucleus, and m_p is the mass of a proton [2]. Further description of NMR can be described with both classical and quantum mechanics.

We will first describe the quantum mechanical approach to NMR. When placed in a static magnetic field, the magnetic moment vectors will precess about the axis parallel to the magnetic field. Then, the nuclear spin angular momentum vectors can exist in distinct quantum states with distinct energy levels illustrated in Fig. 1. The value of the vector component parallel to the internal field, \mathbf{B} , is $m\hbar$, where m ranges from $-I$ to $+I$.

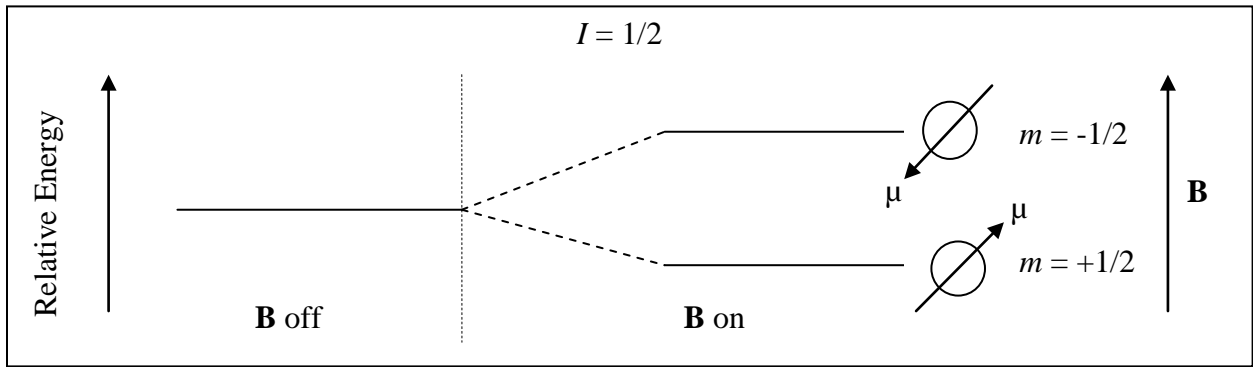


Figure 1. Energy level splitting for nuclear spin $I = \frac{1}{2}$ in magnetic field \mathbf{B} with magnetic moment μ .

Since the energy of a magnetic moment is $-\boldsymbol{\mu} \cdot \mathbf{B}$, the energy of the m th state is given by:

$$E_m = -\gamma m \hbar B, \quad (3)$$

where γ is $g_I e / 2m_p$ and called the nuclear gyromagnetic ratio. Therefore, the energy difference between two adjacent states is

$$\Delta E = \hbar \gamma B, \quad (4)$$

and radiation of angular frequency

$$\omega = \gamma B \quad (5)$$

will induce a transition between energy levels (and therefore spin states). These transitions form the basis of NMR in a quantum mechanical description [2-3].

From a classical viewpoint, one can view NMR as harmonically oscillating nuclei. It is still true that the magnetic moment vectors of the nuclei precess about the magnetic field. Now,

it will also be useful to define the magnetization vector \mathbf{M} as the total magnetic moment per unit volume; \mathbf{M} allows us to treat an assembly of nuclear spins. The magnetization vector will precess at some angle around the axis of the magnetic field at an angular frequency referred to as the Larmor frequency, which is dependent upon the strength of the magnetic field and the specific nucleus. If a weak, oscillating, transverse magnetic field of angular frequency $\omega = \gamma B$ as described in Eq. (5) impinges upon the nucleus, the nucleus will resonate at this frequency which is the same as the Larmor frequency. Then, the magnetization vector will relax to its equilibrium state after the disturbance of the transverse magnetic field much like a damped harmonic oscillator [2].

Currently, two methods are used to detect NMR. Pulsed NMR requires the use of short, strong pulses of RF radiation to hit the sample, and information is gathered by observing the samples response to the pulses. Pulsed NMR is most easily understood with the quantum mechanical view of NMR. My research focuses on the method that first observed NMR, the continuous wave (CW) method. CW NMR relies on an applied magnetic field along with constant, weak RF radiation and is easily understood with the classical description of NMR. In practice, one sweeps either the frequency of the radiation or the strength of the applied magnetic field through resonance in order to observe it. One advantage of CW NMR is that the very low level radiation will only minimally disturb low temperature systems.

Detection of CW NMR relies on the precessing magnetization inducing a voltage in the coil wrapped around the sample. To calculate the magnitude of the CW signal, we turn to the dynamic magnetic susceptibility χ . χ is defined as the ratio of the magnetization and the applied transverse field. Therefore, χ depends on the angular frequency of the field. When a coil is wound around a sample with some dynamic susceptibility, the inductance is enhanced as

$$L = L_o (1 + \eta\chi), \quad (6)$$

where η is the filling factor of the sample. $\chi(\omega)$ is complex so that it can be written as

$$\chi = \chi' + i\chi'' \quad (7)$$

Plugging Eqs. (6) – (7) into the equation for the complex impedance of an inductor, we obtain

$$Z = -i\omega L_o(1 + \eta\chi') + \omega L_o\eta\chi'' + r. \quad (8)$$

The imaginary part of the susceptibility causes a change in the real part of the impedance of the inductor. Effectively, the sample adds further resistance

$$\Delta r = \omega L_o\eta\chi'' \quad (9)$$

to the inductor. As the quality factor Q of the coil is defined as

$$Q = \omega L/r, \quad (10)$$

the resistance introduced by the sample at resonance changes the Q of the coil. When the coil is placed in parallel with a capacitor and resonated, the combination acts as resistor of resistance R given by

$$R = Q\omega L. \quad (11)$$

Therefore, a change in Q will lead to a change in R which leads to a change in the voltage of the coil given by

$$\frac{\Delta V}{V} = \frac{\Delta Q}{Q} = -Q\eta\chi'' + \epsilon\chi'. \quad (12)$$

However, ϵ is so small we can ignore the last term and easily calculate the signal voltage for CW NMR [2].

My research focused on the design, fabrication, and testing of a CW NMR detector. A marginal oscillator served as the means of detection. A marginal oscillator is a circuit that oscillates with very small amplitude so that any extremely small energy absorption causes a large variation in the amplitude of oscillation [4]. The increased resistance in the circuit due to the

increased Q will lead to higher energy dissipation in the sample coil and therefore detection. The detector design incorporates very low levels of RF radiation, good signal to noise characteristics, good sensitivity, and construction from commonly available electronic components that could easily translate to a printed circuit board. Furthermore, the detector was tested and troubleshot using a small 300G electromagnet to test ESR and a magnet capable of over 10kG to test NMR.

The Detector

The marginal oscillator, shown in Fig. 2, consists of two junction field effect transistors (JFETs). We chose to use JFETs as opposed to other transistors based on the success of others [5] and their unique characteristics. We chose MPF102 JFETs for their high input impedance,

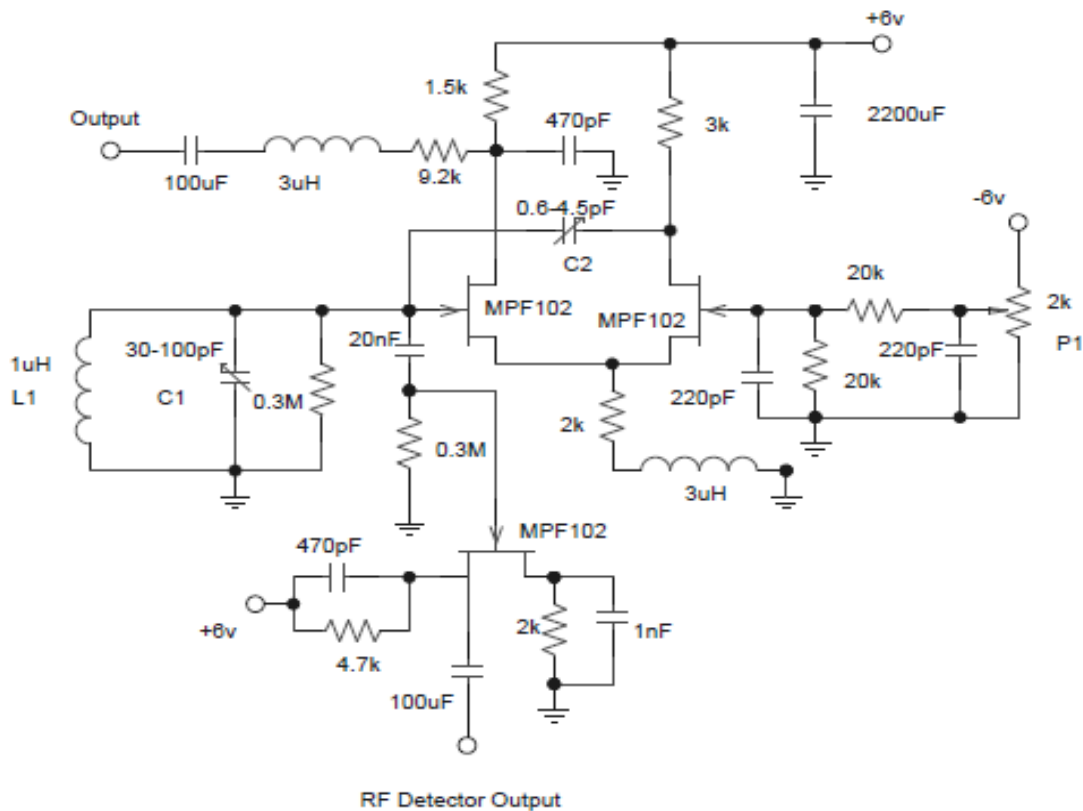


Figure 2. Detailed electrical diagram of the marginal oscillator circuit.

very good signal to noise ratio, and high availability. C2 is a very small variable capacitor to adjust the amount of feedback the marginal oscillator provides to the RLC system. P1 is a potentiometer that acts to vary the negative voltage on the gate of the second transistor to make the circuit as marginal as possible. The signal is sent from either output to a 1000X amplifier and then viewed on a digital oscilloscope. Two outputs determine the best method for viewing the signal.

In order to minimize electrical noise, we used a high quality power supply. In addition, the circuit has a 2200uF electrolytic capacitor to ground in order to reduce any noise from the power supply. Also, an aluminum box houses the circuit to shield it from extraneous fields. I soldered all the components onto a solid sheet of copper to provide an excellent ground plane required for the low RF levels. Moreover, I placed the housing on a large sheet of copper forming a ground plane connection between the magnet and the circuit.

The detection of the NMR signal depends on the RLC tank circuit. The high quality coil L1 that is wrapped around a sample serves to radiate RF energy to the sample at the resonant frequency of the RLC circuit. The RLC circuit consists of L1, the variable capacitor C1, the 0.3M resistor in parallel, and the inductance and capacitance of a small length of coaxial cable connecting L1 to the aluminum housing. C1 tunes the circuit to the desired resonant frequency. The marginal oscillator also operates at this resonant frequency. The marginal oscillator detects the NMR signal due to its high sensitivity to the energy absorption in L1.

Testing ESR

I first tested the circuit using electron spin resonance (ESR) which is very similar to NMR but relies on the spins of free electrons instead of the nucleus. Since electrons have much less mass than a nucleus, ESR up to 100MHz requires small magnets with fields up to ~300G. A

detailed view of ESR requires gigahertz frequencies and much higher (~10T) magnetic fields. My setup consisted of a magnet capable of 300G, a variac and transformer in series with the power supply to the magnet, a 1000X amplifier, a high quality power supply, a digital oscilloscope, a large sheet of copper, and the circuit itself. The variac served to oscillate the magnetic field at 60Hz to produce a static image on the oscilloscope when triggered at 60Hz. I used a sample of 2,2-Diphenyl-1-Picrylhydrazyl (DPPH) at room temperature in testing as it is often used as a standard for ESR [6]. I placed the sample in the magnet, and the magnetic field was swept through the resonance by increasing the current of the magnet's power supply. The setup was critical in testing and changing components to achieve the best signal. The results of ESR at 50 MHz are shown in Figure 3. This result is what was viewed directly on the oscilloscope with no time averaging or other manipulation. It displays the excellent signal to noise ratio achieved with the marginal oscillator.

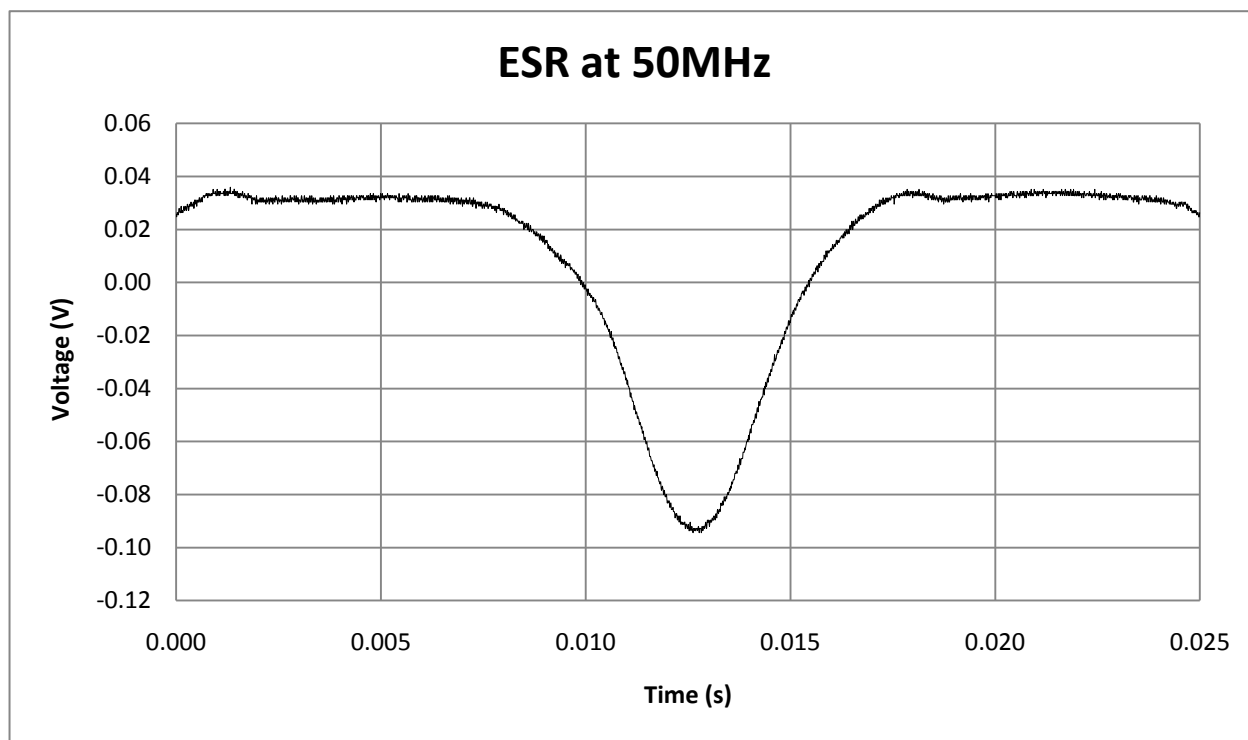


Figure 3. ESR of DPPH at 50MHz. Clear absorption dip.

Testing NMR

I tested the detection of NMR using the marginal oscillator in a similar manner to ESR. Glycerin was used as a sample for its numerous protons that could be observed with NMR. I used the same equipment as I did for ESR testing, but instead of modulating the field by placing a transformer in series with the magnet, I used a Helmholtz coil-like apparatus to produce an oscillating magnetic field in the center operating at 60Hz. I placed the apparatus with the sample and coil wrapped around the sample in the center of a large electromagnet. I wound the sample coil and adjusted C1 to resonant at 20MHz. NMR was detected at a field strength around 4700G. Results are shown in Figure 4.

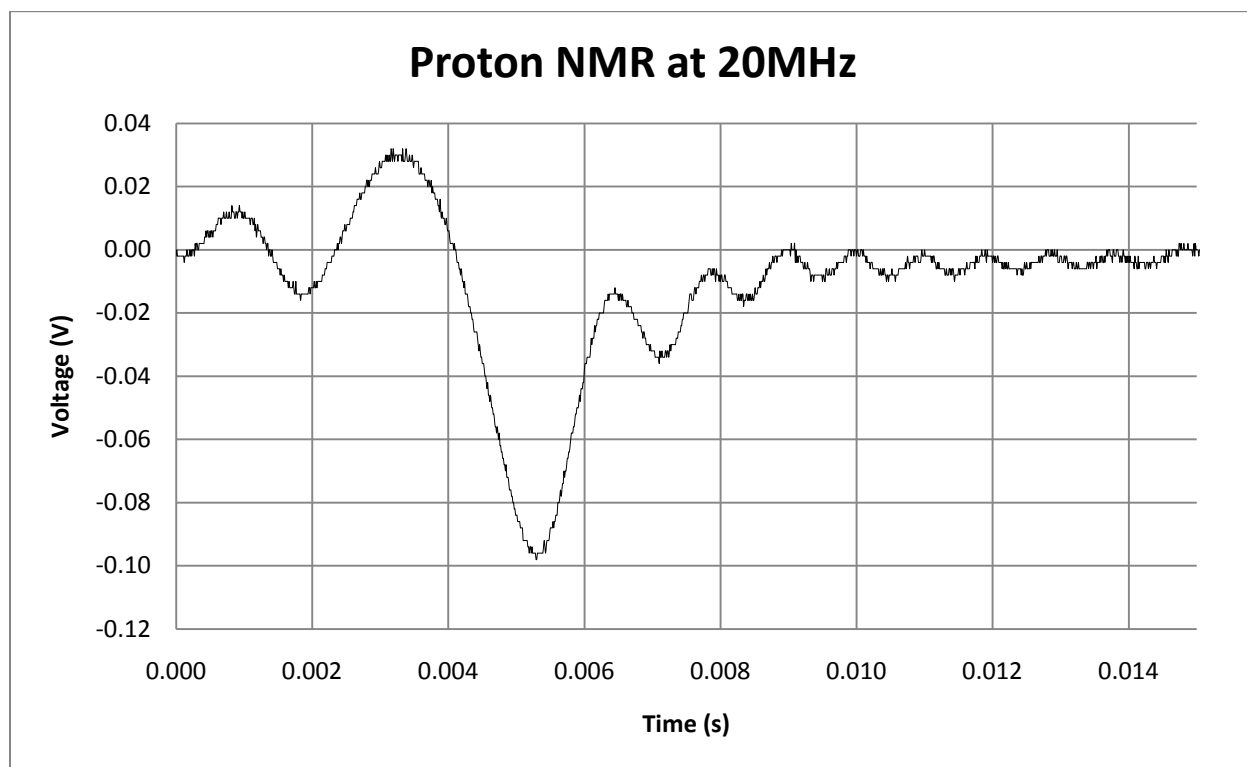


Figure 4. Proton NMR of Glycerin at 20MHz. Note wiggles and pre-wiggles.

The signal displays the characteristic wiggles of the proton relaxing to the ground state similar to a harmonic oscillator. The noise in the signal is less than 5mV, while the signal is 128mV. Therefore, the power signal to noise ratio is 655 or 28dB. According to the geometric and magnetic properties of the coil and sample, I calculated the signal amplitude to be roughly 20 μ V. Given that the noise introduced by the amplifier electronics can be ignored [2], I calculated the noise of the coil assembly to be 0.45 μ V. Therefore, the most ideal power signal to noise ratio is 1936 or 32dB. The extra noise as compared to Fig. 3 may be a result of the instability of the larger magnet. Still, the achieved signal to noise ratio is very good at room temperature.

Conclusion

The marginal oscillator circuit presented in Fig. 2 worked well to detect proton NMR. It can be used for ESR; however, a system capable of gigahertz frequencies would be more suitable. High quality, low noise components were essential in presenting the best possible signal. This circuit design would be suitable for studying CW proton NMR at room temperatures. Due to losses and extra capacitance in coaxial cable, the current design did not work well for cable length of 15ft. To improve the system in the future, a method for using the apparatus in strong (>10T) magnets should prove useful. If the challenges of the cable length to the sample coil can be overcome, the system may be able to detect NMR for other materials such as silver when placed in a stronger magnet. Also, the system may work well at low temperatures due to the low noise components, but that requires further research. If the circuit operates well in strong magnets and at low temperatures it could be very useful for use in the Microkelvin Laboratory at UF which will soon have a 20T magnet. Making the marginal oscillator an

integrated circuit is another improvement for the future as well. The circuit performs well as a marginal oscillator for CW proton NMR, but improvements can be made for more applications.

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