

ELECTRONIC PROBE SIMULATOR

A small electronic probe simulator has been designed for the **PLM-5** Pulsed Platinum NMR Thermometer. The simulator is intended to serve for the following purposes:

- PLM-5 hardware and software development
- Production testing of **PLM-5** electronics units
- It replaces the cooled probe in a PLM-5 tutorial
- It allows the user to check the operation of the PLM-5 electronics without a probe
- It allows the user to develop and test his/her own PC software without a cooled probe

The **PRS-1** simulator is a small box powered from mains. It is connected to the **PLM-5** preamplifier using a short 50 ohm coaxial cable. No other connections are needed. The simulator imitates the behaviour of a Platinum sample in most respects.

The operation and circuitry of the **PRS-1** is described below in detail with the help of the circuit schematic. Precise knowledge about its construction and behaviour is the key to understand what one can - and cannot - expect

this "toy" to do. The reader may also find it interesting to see how relatively low-cost analog electronics is used to simulate a complicated physical phenomenon.

The following text begins with a discussion about a real probe unit and setup for Pulsed Platinum NMR Thermometry. The theory of Platinum thermometry is handled only superficially and all but accurately. The purpose is to give the reader at least some idea of what happens in the Platinum Probe so that he/she is able to follow the next sections that explain how these phenomena are implemented by the circuitry.

THE PROBE AND A SIMPLIFIED THEORY

A real probe consists of a platinum sample inside a "horizontal" signal coil, which in turn is located inside a homogeneous "vertical" steady magnetic field. The sample is either a bundle of several hundred very thin insulated Platinum wires or a small amount (usually less than a gram) of fine and pure Platinum powder. The spin magnetic moments of the nuclei become quantized in a non-zero magnetic field, each having a quantum number

of either +1/2 or -1/2. It is customary to say that the spins are either aligned or opposed to the magnetic field.

The magnetic field tries to put the system in order by aligning all the spins, whereas temperature tries to introduce disorder by mixing this alignment. If the field is negligible, or if the temperature is infinite, half of the myriad spins are aligned and half are opposed. This is the maximum possible disorder for two states. If the field were infinitely high or if the temperature were zero, all spins would be aligned. This would represent a perfect order in the spin system.

In practice, the situation is always between these two extremes. The important quantity for us is the relative difference between nuclei having aligned and opposed spins. This difference, multiplied by the field generated by one single nucleus and by the number of the nuclei in the probe is the static magnetisation, later called **M0**. The **Curie Law** states that **M0** is inversely proportional to the absolute temperature.

Measurement of M0

This static magnetisation is measured as follows: An AC magnetic field, which is perpendicular to the steady DC field, is applied to the Pt sample for a short time (transmitter burst, or TX burst). The frequency of the AC field must be the Larmor precession frequency of the spin magnetic moments of the Pt nuclei (this frequency, in turn, depends on the magnitude of the steady DC field). The short burst feeds energy into the spin system, and this energy makes the spins precess more or less in phase. The coherence of the precession makes it detectable in the macroscopic scale: The signal coil, which was previously used for sending the TX burst, is now used to pick up induction that is generated by the alternating magnetic field, which in turn is generated by a large number of coherently precessing nuclear magnetic moments.

The size of the signal that is received depends on several factors: **First**, naturally, the bigger is the sample the more there are nuclei and the higher is therefore the signal. **Second**, the more energy is fed to the spin system, the higher is the signal. The transmitter burst can be varied in both length and amplitude, but there is a maximum signal strength that can be achieved this way. After that, the signal starts to diminish but after a minimum it starts to grow again, in a cyclic way. **Third**, the signal size depends on the static magnetisation. Nuclei with aligned and opposite spins precess in 180 degree phase shift resulting in a zero macroscopic net field. If the two available quantum states were equally occupied, no net effect could be seen (=infinite temperature). The fact

that the occupations differ in a magnetic field makes a net effect possible.

Thus, keeping all other factors unchanged, the signal strength gives us a thermometer that works according to the Curie Law, i.e. the signal amplitude is inversely proportional to the temperature. The constant of proportionality, which is later called **C**, depends on many factors that are not known precisely. Therefore, it must be measured at some temperature, which is determined using another thermometer. Because the Curie mode has to be calibrated in order to be useful, it is called a "secondary thermometer", and it can only be used to extrapolate temperatures, starting from the calibration temperature.

Unfortunately, the signal from the nuclei does not last long. In the microscopic scale, the nuclei experience slightly different and varying magnetic fields, which makes their Larmor frequencies slightly different. The coherence of their motion, and hence also the detectable signal, is gradually lost. This happens exponentially at a rate called **T2**, the spin-spin relaxation time constant. This time constant is about 1 millisecond for a very successful Platinum sample, but usually it is only a few hundred microseconds.

Because of its origin and waveform, the decaying signal is called "FID", Free Induction Decay signal. Fig 1 shows the shape of an electronically simulated "FID" signal. In the Curie mode, the PLM-5 tracks the changes in the FID signal amplitude, compares the present value with a value stored at the calibration temperature, and calculates the present temperature.

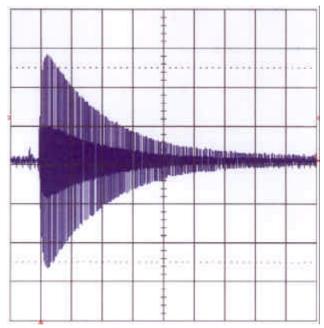


Fig. 1: A Free Induction Decay (FID) signal, produced by the PRS-1 simulator



Spin-Lattice Relaxation

In addition to making precessions coherent, the transmitter burst has also another effect: it feeds energy into the spin system, making the difference between aligned and opposed spins smaller. In other words, the spin system is heated by the TX burst. After the transmission, the spin system will have a temperature which is higher than the temperature of the atomic lattice of the sample. It is the latter quantity that we usually mean when we talk about the temperature of the material. If we measure the static magnetisation again soon after the first transmitter burst, we would get a lower value than previously.

The spin system is not, however, totally independent of the lattice. There are interactions that transfer energy between them, and therefore the heated spin system starts to cool down toward the lattice. Again, this cooling is exponential with a time constant called **T1**, the "Spin-Lattice Relaxation Time Constant". According to the **Korringa relation**, this time constant is inversely proportional to the lattice temperature, and the constant of proportionality is called **K**, the Korringa constant.

Unlike C, the Korringa constant depends on few things only, mainly on the sample material and unfortunately, but to a much lesser extent, also on some other factors. For Platinum, T1 is about 30 msK (milliseconds * Kelvins). Once measured, it can be expected to remain rather unchanged for long times and between measurements. T1 is therefore an "almost" primary thermometer which needs calibration, but only seldom.

The **PLM-5** can be used to measure **T1**. This mode starts by measuring the static magnetisation **M0** of the sample, which is assumed to be in equilibrium. Then, a long transmitter burst is applied to the sample for heating up the spin system significantly (NMR people say that the magnetisation vector of the sample is tipped by 90 degrees). Soon after this "90 degree burst" the magnetisation M1 is measured using a second transmitter burst, which is now much shorter. We do not want to heat the spins for the second time, as this would disturb the exponential recovery that we are trying to measure. The reading is very small, because the spin system has had little time to recover toward its equilibrium state **M0**. After a delay comparable with the expected **T1**, we measure the third magnetisation M2. Based on the two points (M1,M2) taken from the exponential recovery curve plus one point representing the final value M0, we can calculate **T1**. Note that the **M0** reading is not taken after tens of T1 time constants, which would make the instrument very slow, but just before the recovery measurement. We only have to assume that a sufficient time has passed since the previous measurement.

The usual practice is to keep the TX burst as short as possible in order to reduce nonidealities in the measurement. Unfortunately, the smaller we make the TX burst the worse becomes the signal-to-noise ratio. If we want to improve the S/N ratio by increasing the TX burst length, we must include its spin heating effect in the calculation of T1. In order to do so, this effect must be measured, and this is one of the PLM-5 operating modes. The magnetisation is measured two times, first time from an equilibrium system and second time soon after a variable TX burst. The ratio of the two measurement shows, how much the extra TX burst had heated the spin system. The NMR people say that the TX burst tips the magnetisation vector. The ratio M1/M0 is the cosine of the tipping angle Theta.

THE PRS-1 SIMULATOR

The **PRS-1** consists of the following main sections:

- A tuned LC tank circuit, corresponding to the signal coil and capacitors of a real probe
- A voltage-controlled oscillator whose frequency is qualitatively dependent on input current ("magnet current"). This corresponds to the fact that the NMR frequency of the sample depends on the strength of the magnetic field.
- Circuit for generating an exponentially decaying voltage. The decay time constant is equivalent to **T2** and is about 1 millisecond.
- Circuit for determining the starting level of the above mentioned decaying voltage. This starting level corresponds to static magnetisation M0, and therefore it was made dependent on BOTH the position of the "Temperature" potentiometer AND the magnitude of the input current ("magnet current").
- A mixer that multiplies the exponential decay voltage by the oscillator waveform. This symmetric square-wave signal, modulated by the exponentially decaying voltage, corresponds to the FID signal that the signal coil will pick up.
- Circuits for rectifying and stretching the PLM-5 transmitter burst in order to yield the required logic signals.
- Circuit for making the starting point of the **T2** decay voltage also dependent on the length of the transmitter burst. This corresponds to the fact that the **FID** amplitude depends on the TX burst length.
- Circuit for reducing magnetisation M0 by a factor that depends on the transmitter pulse



length. This corresponds to the spin heating effect of the TX burst.

Only one major aspect is not simulated: The **amplitude** of the TX burst has no effect on the **FID** signal. It has to be sufficient in order to generate the logic signals.

The **PLM-5** Current Supply (CS-10) is connected to the front panel banana sockets of the **PRS-1**. Accidental inversed polarity is indicated by a red light. The current shall be less than 5 Amperes. Excess current will saturate circuits and it will overheat the shunt resistor R28. A red light warns about a high current.

The voltage drop across R28 is amplified and then it drives the voltage-controlled oscillator U4. A typical NMR frequency of 250kHz is achieved when the current is 3.6...3.8 Amperes (the f(V) dependence of the 74HC4046 is far from accurate). U4 oscillates all the time, but the square-wave is not fed into the tank circuit as long as no T2 voltage exists. One could think that all the spins precess at $f_{\rm O}$, but the precessions are incoherent.

The signal used for driving U4, "Magfield", further controls a current source that consists of U10B, Q6, U10A and Q5. The output current delivered by Q5 reaches its maximum of 4 uA when the magnet current is 5A. If this current were used as such to charge the capacitor C13, charging would be linear and the final voltage would be the saturation voltage of the current source.

But if we add a resistor R in parallel with C13, then the final voltage would be I*R and hence dependent on the magnet current. The charging time constant would be R*C13. By making R inversely dependent on some controlling device called "temperature", we would have an **M0** that depends on 1/**T** and a spin-lattice recovery rate that also depends on 1/T. We hope to be able to simulate about 10mK temperature with the PRS-1, which means a **T1** of as long as 3 seconds. Therefore, the resistor in parallel with C13 must be adjustable downwards from 1Mohm. Only 1-turn carbon potentiometers may be obtained for such a high resistance, but they are inconveniently rough for our purpose. The solution was to use an active resistor which is controlled by a 20kohm 10-turn potentiometer. This active resistor consists of U1A, U1B, R36, R17, R37, R34, R35 and the potentiometer which is connected to J1 (1=hi, 2=wiper, 3=lo).

An equation for this circuit is derived in the end of this text. The "LO" temperature impedance becomes 1Mohm, whereas "HI" temperature impedance is limited not to go below 2kOhms in order to prevent the circuit from becoming unstable. Because of the limiter, the behaviour deviates slightly from 1/T. The "Temperature"

knob has no scale - the purpose is to discourage using the simulator for any quantitative measurements.

Note that if we charge C13 via a fixed resistor, we can implement **M0** dependence on the NMR field, but the **T1** would be fixed. An active floating resistor, on the other hand, might be difficult to design....

It is now time to assume that the **PLM-5** preamplifier supplies a transmitter burst. A typical value for such a burst is about 20Vpp, f=250kHz, and its duration e.g. 10*4us = 40us. The burst is received by the tank circuit consisting of L2 and C6+C7. Transistors Q2 and Q3 have two functions: they buffer the TX burst so that it can be used to drive the transformer L1. After the TX burst, the base-emitter diodes isolate the tank circuit from the transformer load. The transformer steps up the TX burst before it is full-wave rectified by diodes D2..6. The rectified voltage is forced to stay below appr. 5V by diodes D4 and D7. The time constant of the rectified TX burst (now called "TX pulse") is determined by R3*C2. It must be long enough to keep the ripple acceptable (the voltage shall not fall below the CMOS treshold level), but short enough to turn off the TX pulse very soon after the burst has ended.

The magnetisation voltage **M0** across C13 has been connected to C8 via the X-switch of U3. This switch is normally in the X0-position. So C8 also has the voltage **M0**. After buffering (U10D), this voltage is fed to the Z-switch. This switch has so far been in the Z0-position, but during the TX pulse it goes into Z1-position. Then the **M0** voltage charges 10nF capacitor C14 via 10kOhm resistor R21 during the TX pulse. It is the voltage across C14 that is used for the exponentially decaying "**T2** signal". What is the voltage level after the TX burst depends now on the **M0** voltage (which in turn depends on "temperature" and "magnet current") and on the TX burst length. This dependence does not have the same cyclic nature that is exhibited by a real probe, but for short TX pulses the behaviour is sufficiently similar.

After the TX pulse, the Z-switch of U3 returns back to Z0-position, so that R23 starts to discharge C14. The discharging time constant (100kOhms*1nF=1ms) is equivalent to the spin-spin relaxation time constant **T2** of a real probe.

PRS-1

Electronic Pt Probe Simulator for the PLM-5

The "T2 signal" is buffered and inverted. The two opposite decaying voltages are fed to the analog switch U2, which is controlled by the VC0 frequency. The resulting product of these signals is a symmetrical squarewave that decays exponentially with time constant T2 (Fig 2). This signal is then attenuated and injected into the tank circuit. The LC-circuit removes the sharp edges of the square wave and makes it look more sinusoidal. This "FID signal", ranging from tens of microvolts to some millivolts, is then amplified and measured by the PLM-5 (Fig 1).

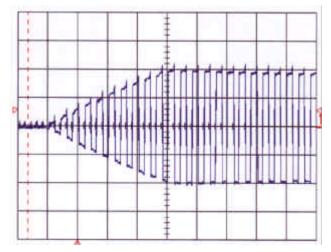


Fig. 2: The square-wave FID signal before injection into the tank circuit.

As previously discussed, a TX burst heats the spin system, which means that its magnetisation is reduced. This was implemented in the simulator as follows. A second logic signal is derived from the TX pulse, and this second signal has a much longer turn-off time which keeps the logic level at 1 during several **T2** time constants. R1*C1 is 10ms which fulfils this requirement.

C8, which was coupled to C13 before the TX burst, is disconnected by the new pulse called "Latchgate", so that C8 will maintain its charge as long as Latchgate is true, regardless of what we do with C13. In order to simulate the heating effect, we have to discharge C13 by a charge which depends on both the original M0 voltage and the length of the TX burst. A gateable discharge pump serves for this purpose. U10C and emitter follower Q4 invert the original M0 voltage. During the TX burst, the collector of Q1 is brought near to -M0, so that current will be drawn from C13 via trimmer P1, which is used to adjust the discharge rate. The discharge is not linear, neither does this "spin heating" behave in a cyclic way like in the real probe. But it operates correctly in the following respects: 1) If M0 is originally zero,

there will be no discharging at all and 2) for short TX bursts, the discharging effect is roughly proportional to burst length and original **M0** voltage. P1 is adjusted so that a 200 us TX burst (50 cycles at 250 kHz) totally destroys the magnetisation (tips the magnetisation vector by 90 degrees). Because of the long turn-off time constant of the Latchgate signal, C8 remains isolated from C13 well beyond the time needed to measure the **FID** signal.

This arrangement looks rather complicated, but it implements in a beautiful way the behaviour of the real Pt sample: the signal amplitude depends on the magnetisation before the TX burst and the heating is realized only afterwards.

SOME TYPICAL OPERATING MODES WITH THE PLM-5

(The following text may change as the **PLM-5** software development proceeds)

Tune the probe capacitance for operation at a fixed NMR frequency

In the **PLM-5** probe tuning mode, the magnetic field is zero. Repeated long TX bursts are injected to the probe via a high-ohmic resistor. The AC amplitude across the signal coil is monitored by the **PLM-5**. The amplitude is maximised by using the trial-and-error method in setting the tuning voltage.

If varicap tuning is not used, one should find a suitable combination of fixed capacitors and solder them permanently across the preamplifier input. As the magnet current is zero, also the **M0** voltage and VCO frequency are almost zero and U2 will not feed any significant AC signal that could disturb this measurement. The "probe" is now aligned with the desired TX frequency, whereas the correct "magnet current" remains unknown.

Find the transmitter frequency that suits to a nontunable probe

In the probe tuning mode, vary the synthesizer frequency. Display the input signal and use trial-and-error method to find the frequency that results in the maximum amplitude. Keep the magnet current at zero. The TX frequency is now aligned with the probe of fixed tuning, whereas the correct "magnet current" still remains unknown.

Find the "magnet current" that complies with the previously tuned PLM-5+probe

In the Curie mode, make automatically repeated measurements and monitor the **M0** amplitude as display graph 1 and the current as graph 2. Find the optimum current value by sweeping the CS-10 output from target 1 to target 2. Using the cursor, determine the current that gave the maximum **M0**. Note that here the Curie measurement can be repeated in close succession, because the heating effect does not shift the optimum. It is, however, important that the repeat intervals are even. You shall not rely on firing the TX bursts manually.

Tune the PLM-5 for a probe using a fixed or trapped NMR field

The **PLM-5** may be used under circumstances where the magnetic field cannot be adjusted, and so the precession frequency is fixed although it may be unknown. When excercising with the simulator, open the top cover and measure the VCO frequency from TP6. Adjust then the CS-10 output current for any assumed NMR frequency.

The **PLM-5** alignment consists now of tuning both the tank circuit capacitance and the transmitter frequency. You can make this in the Curie mode. Maximise the **FID** signal iteratively by adjusting either the tuning voltage or transmit frequency in turn for maximum amplitude until no further change improves the response.

Determine the tipping angle Theta

The Theta setup mode of the **PLM-5** uses three TX bursts: two with a fixed length for measuring the magnetisation and one with a variable length for tipping the magnetisation vector. This method is almost similar to the Korringa mode, except that the delay between the initial **M0** measurement and the 90 degree pulse is quite long and that the **M2** point is not used for anything.

As shown in Fig. 3, the first thing to do is to measure the static magnetisation when the spins are at an equilibrium temperature with the lattice. After the M0 measurement, the PLM-5 waits for e.g. 20*T1 time constants (or just long enough!). Then a variable TX burst is fired and very soon after it a second measurement for M1 is made. The hardware permits a minimum time separation of 1 ms, but one has to use at least 10-20ms in order to let the spin-spin interaction to fully destroy the precession coherence. If the second burst length is zero, the two measurements shall give identical results. Record the ratios of the results for all interesting angles, or even better, plot a curve.

The **FID** amplitudes do not change with the length of the variable TX burst so that you can easily extend this method to find also the burst length that produces a 90

degree tipping angle. Do not try, however, to obtain a zero **FID** signal but be satisfied with an angle of 80-85 degrees. Otherwise there is a danger that the spins are tipped by more than 90 degrees. Then the magnetisation will recover through zero, and the **PLM-5** will calculate a wrong **T1** time constant.

You should wait 10-20 **T1** time constants before making a new measurement. With a real probe you must plot separate curves for each transmitter amplitude that you plan to use. In the case of the simulator, however, you cannot vary the TX amplitude as it has no effect on the "heating effect".

Although tedious, the tipping angle must be measured because of two reasons: The Korringa mode works the better the closer the 90-degree burst is to its optimum value. Second, if you must use a long TX burst in order to improve the S/N ratio at a high temperature, T1 can be calculated accurately from the Korringa mode results only if the tipping angle is known. Very high precision is not needed, an estimate is better than nothing.

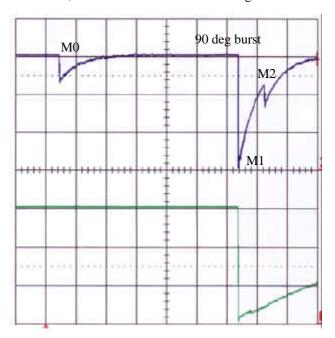


Fig. 3: Three-point method for determining the tipping angle Theta. Here tipping is about 90 degrees.

Ordinary measurements

The **Curie mode** measurement is very simple: a TX burst is fired and the amplitude of the resulting **FID** signal is measured.

The **Korringa mode** is more complicated and very similar to the previous tipping angle measurement:

Magnetisation **M0** is measured when the spin system is assumed to be in equilibrium (**Fig. 4**). Then a long TX burst is fired in order to heat up the spin system as near to infinity as is practically possible (the magnetisation vector is tipped by almost 90 degrees). As soon as the precession coherence has disappeared completely, the magnetisation **M1** is measured.

In **Fig. 4** this time delay is 200 ms. As seen from the figure, the magnetisation has not yet recovered significantly. The **M1** measurement can be better seen from the lower, zoomed trace. The tipping effect seems small because the magnetisation is still near to zero.

After a delay comparable with the expected **T1**, magnetisation **M2** is determined. **T1** is then calculated from the three results. If a large tipping angle must be used, then at least an approximation on the tipping angle must be included in the calculation.

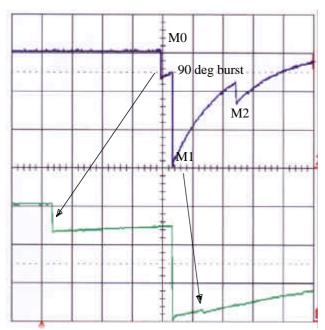
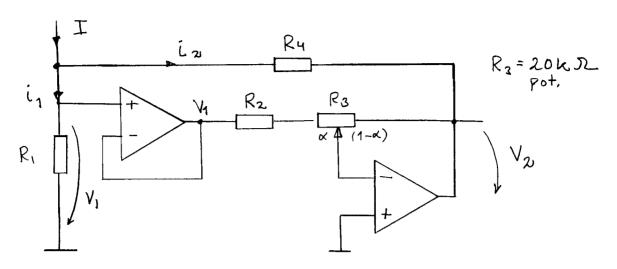


Fig. 4: T1 measurement in the Korringa mode



$$I = i_1 + i_2 = \frac{V_1}{R_1} + \frac{(V_1 - V_2)}{R_4}$$

$$V_2 = -V_1. \quad \frac{(1 - \alpha)R_3}{R_2 + \alpha R_3}$$

$$I = V_1 \left[\frac{1}{R_1} + \frac{1}{R_4} \left(1 - \frac{(1 - \alpha)R_3}{R_2 + \alpha R_3} \right) \right]$$

$$Z = \frac{R_1 R_4}{R_4 + R_1 \left(1 + \frac{(1 - \alpha)R_3}{R_2 + \alpha R_3} \right)} \left(= \frac{V_1}{I} \right)$$

Hax when $\alpha = 1$. Require $2 = 1M\Sigma$. Select $R_i = R_Y = 2M\Sigma$. $Z_{max} = \frac{R_1R_Y}{R_1R_Y} = \frac{4(M\Sigma)^2}{4M\Sigma} = 1M\Sigma$ ("Lo Temperature")

