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VIRTUAL INSTRUMENT – THE NMR MAGNETOMETER

Gregor Geršak, Janez Humar, Dušan Fefer

Faculty of Electrical Engineering, University of Ljubljana, Ljubljana, Slovenia

Abstract − In this paper a Nuclear Magnetic Resonance magnetometer (NMR) in a form of a LabVIEW Virtual instrument (VI) is proposed. The heart of the magnetometer remains the marginal oscillator with a proton sample. The magnetic resonance signal and all other auxiliary signals are generated and controlled by a set-up composed of a digital counter (for resonance frequency measuring), a VXI system (for the modulation signal generation and for the sampling of the oscillator output), a programmable DC voltage source (for oscillator frequency control) and a personal computer controlling the measurement. The virtual magnetometer was built and preliminary test measurements were done. The measuring results of the determination of a field-coil coil-constant showed that the virtual NMR magnetometer's readings were comparable to the classic NMR magnetometer's within 5×10^{-4}.

Keywords: virtual instrument, NMR magnetometer, VXI.

1. INTRODUCTION

Nuclear magnetic resonance (NMR) based magnetometers, especially magnetometers based on the proton gyromagnetic ratio γ_p' as recommended by the Committee on Data for Science and Technology (CODATA) represent the highest level of the metrological pyramid for the DC magnetic flux densities [1, 2]. In the field of the precision DC magnetic flux density measurements these magnetometers have the highest measuring accuracy, thus representing the most accurate standards for realising the physical quantity of the magnetic flux density [3].

Accurate NMR measurements using a classical proton magnetometer in a magnetic dynamic environment, where there are a lot of extraneous magnetic fields and other electromagnetic disturbances, can be sometimes quite difficult. Especially in the case, where the laboratory is situated in a larger building, which is hosting also other electrical engineering laboratories (as in our case at the University of Ljubljana). We decided on improving the stability of the instrument by substituting different (hardware) modules of the magnetometer with signal acquisition and processing by means of a personal computer.

2. DESCRIPTION OF THE MEASURING SET-UP

The measuring set-up consists of an oscillator module, a digital counter measuring the NMR frequency, a VXI-1500 system generating the modulation magnetic field and sampling the oscillator module output, a parallel port controlled DC voltage source for tuning the resonance circuit and a personal computer controlling the measurement.

A simple LC resonance circuit consists of a detector coil wounded around the NMR sample and a voltage controlled capacitor (varicap diode) for sweeping the oscillator frequency (Fig. 1). When the resonance circuit is tuned to the proton precession frequency, the resonance frequency determines the measured magnetic flux density. The oscillator frequency control enables the frequency sweep when searching for an unknown resonance frequency. The amplifier and the feedback loop ensure the stable oscillation and high sensitivity of the circuit to provide an optimum signal-to-noise ratio (SNR) [3, 4]. For observing the differentiated absorption line of the NMR sample the oscillator low frequency output (LF) is used (Fig. 1). An amplitude demodulator, an operational amplifier and a bandpass filter with the centre frequency equal to the modulation field are added for this purpose[4].

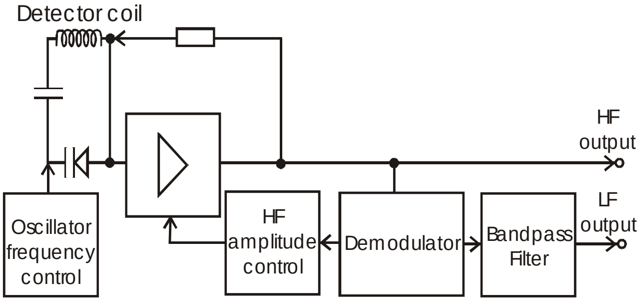


Fig.1. Block diagram of the oscillator module

The protons of the aqueous solution of the paramagnetic copper sulphate represented the NMR sample. The salt was added to ensure the absorption line half-width of 2 μT and thus shorter relaxation times. In case of the protons the 2 μT corresponds to about 80 Hz. Further on, the signals of the same frequency were used also for the modulation field frequency and with it for the generating of the oscillator module low frequency output.

When the sample is put in a magnetic field to be measured, the magnetic dipoles start to presses in a certain direction. When the oscillator frequency equals to the nuclear magnetic resonance frequency of the protons in the sample an absorption of a certain amount of energy from the oscillator resonance circuit occurs.

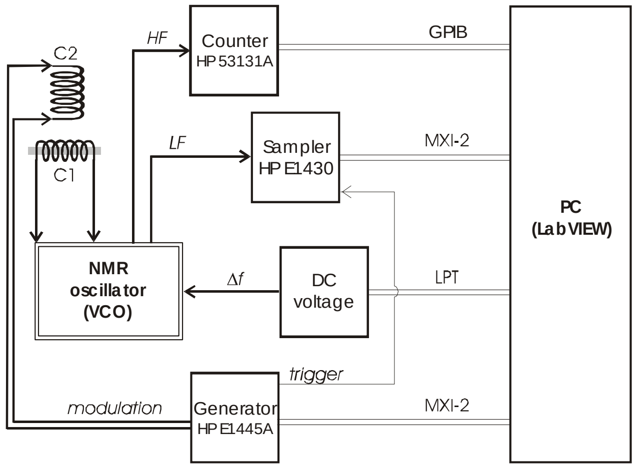


Fig. 2. Block diagram of the measuring set-up. *HF* and *LF* – high and low frequency oscillator module output, Δ*f* – oscillator frequency control, C1 – detector coil with the NMR sample, C2 – modulation coil, LPT, GPIB and MXI-2 – data buses.

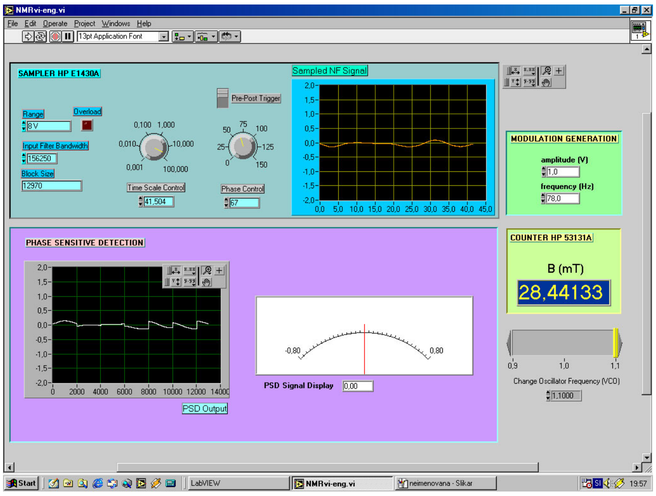
The NMR frequency is proportional to the magnetic flux density via the gyromagnetic ratio of the proton. Thus the measurement of the unknown flux density is translated to the frequency measurement [5, 6].

When using the oscillator module the magnetic flux density is calculated from the oscillator HF output, whereas the occurrence of the resonance is detected by observing the oscillator LF output.

The amplitude of the magnetic flux density was calculated from the HF output multiplied by the gyromagnetic ratio of the proton [1]. A 225 MHz digital counter HP 53131A (by Hewlett Packard) was used for the frequency measurement (Fig. 2). The counter was connected to the personal computer via a GPIB bus (by National Instruments). Prior to frequency measurement all additional processes of the counter, such as math and statistics functions, as well as the instrument's display were turned off in order to ensure maximal data acquisition speed and maximal data transfer rate via GPIB.

The oscillator LF output was sampled by a VXI system ADC module HP E1430A (by Hewlett Packard). Acquiring of the LF signal was triggered by an additional VXI module HP E1445A (by Hewlett Packard, 13 bit DAC, generates arbitrary signals of maximal sampling frequency of 40 MSa/s). The generator was used for generating the sine modulation current, which powered the coil producing the modulation field for the NMR frequency determination. The generator's Marker Out square output was used as a trigger for the sampling module HP E1430A. The trigger can be time delayed (pre-post trigger option). Thus a phase lock of the LF oscillator output and the square-generator trigger signal could be done. This way the analog part of the phase sensitive detection (phase sensitive device - PSD) was built. All the further signal processing was done in the LabVIEW environment.

The sampling module HP E1430 is a 23 bit sigma-delta ADC with a maximal sampling signal frequency of 10 MSa/s and 8 MB FIFO memory. The continuous mode of successive block sampling was used to acquire the low frequency signal of the oscillator used for the detection of the NMR occurrence in the sample.



Range 8 V

Input Filter Bandwidth 156250

Block Size 12970

Time Scale Control 41,504

Phase Control 67

amplitude (V) 1,0

frequency (Hz) 78,0

B (mT) 28,44133

PSD Signal Display 0,00

Change Oscillator Frequency (VCO) 1,1000

Fig. 3. The front panel of the virtual NMR magnetometer. The upper part represents the sampler and pre/post triggering control for the phase detection process. In the lower part the phase sensitive detection is graphically presented, also to enable easier phase shifting. On the right side the amplitude and frequency of the modulation filed can be set. A numerical display shows the measured flux density in mT. Under the flux density the oscillator frequency control bar is visible.

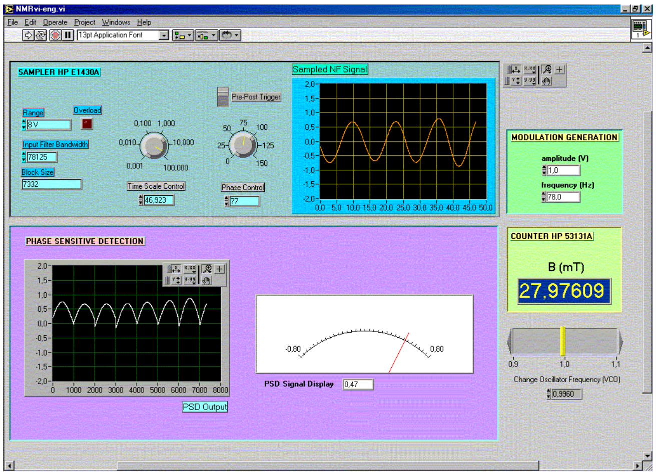
Both VXI modules were connected to the personal computer (VXI-PCI8000 card) via the MXI-2 bus.

The DC voltage generator was used for controlling the oscillator frequency. The generator was a 16-bit DA converter, controlled by a personal computer via the parallel port. A stable zenner diode source was used as a reference for the DA converter. Amplified output of the DAC was a stable DC voltage with amplitude from 0 to 7 V. A LabVIEW Virtual instrument controlled the voltage source.

After the acquiring of the LF and HF signals, the data transferred to the personal computer could be processed. Multiplying of the LF signal and the squared modulation signal and averaging the product performed a simple phase sensitive detection. The PSD output signal was used for the resonance frequency detection.

By manual sweeping of the oscillator frequency both extremes were found and stored (Fig. 2). In this first version of the virtual NMR magnetometer the resonance discriminator was not realized and the automatic locking to the maximum of the absorption line was not available. Instead, the resonance frequency was calculated as the mean value between both extremes of the differentiated absorption line of the sample. The minimum and the maximum of the PSD signal could be observed on the front panel display of the virtual NMR magnetometer (Fig. 4). The Fig. 3 the shows the conditions when the oscillator frequency was far from the resonance, hence only noise could be seen on both graphical displays. On the Fig. 4 we can observe the conditions in the extreme.

To evaluate the measurements of the built virtual NMR magnetometer a comparison with the classic proton magnetometer (by the Physikalisch-Technische Bundesanstalt, Lab. 2.23) was made. We decided on a comparison measurement using both the magnetometers in determining the coil-constant of a field coil. The results are shown in the Table I.



Range 8V
Input Filter Bandwidth 78125
Block Size 7332
Time Scale Control 46,923
Phase Control 77
amplitude (V) 1,0
frequency (Hz) 78,0
B (mT) 27,97609
PSD Signal Display 0,47
Change Oscillator Frequency (VCO) 0,9960

Fig. 4. Front panel of the virtual NMR magnetometer during the measurement, at the moment when the PSD signal reached one of the maximum values (the measured flux density B = 27,97609 mT).

3. CONCLUSIONS

The comparison was done in a multilayer Helmholtz type air-cored coil (circular, 40 cm in diameter, 800 turns of round Φ2 mm copper wire). The coil was powered by a DC current source HP 6554A (60 V, 9 A, by Hewlett Packard). The current was measured directly by using a digital multimeter HP 34401A (by Hewlett Packard). A series of measurements were done to calculate the repeatability of measurements. During the time of the measurements (10 min) the coil temperature raised by 1 °C.

The measurement uncertainty of the classic proton magnetometer was calculated by our standard procedure by adding the contributions of type B uncertainties (uncertainty of the gyromagnetic ratio, sample susceptibility uncertainty due to the cylindrical shape of the sample, uncertainty due to the chemical shift caused by the paramagnetic ions in the sample and uncertainty of the magnetometers time-base calibration) and type A uncertainties (uncertainty due to the zero crossing detection and uncertainty of the magnetometers internal digital counter).

Using the calculated uncertainty of the proton magnetometer and the difference between both measurements the worst-case error of the virtual NMR magnetometer was determined. Preliminary measurements were done in the field range from 10 to 30 mT.

The results from Table I show that the built virtual NMR magnetometer is comparable to the common low field proton magnetometer within the order of 5×10^{-4}.

TABLE I. Comparison of the two NMR magnetometer measurements of a Helmholtz coil coil-constant (*vi*NMR - Virtual NMR magnetometer, NMR - proton magnetometer, K – the coil-constant in mT/A, U - extended uncertainty of the measurement (k = 2), Δ_{Krel} – relative deviation between the constants).

Magnetometer	**Coil-constant** $\boldsymbol{K \pm U}$	$\Delta_{\mathbf{Krel}}$
***vi*NMR**	5,1731 mT/A ± 0,0026 mT/A 5,1731 $(1 \pm 5 \times 10^{-4})$ mT/A	5×10^{-4}
NMR	5,1745 mT/A ± 0,0006 mT/A 5,1745 $(1 \pm 1 \times 1{,}2 \times 10^{-4})$ mT/A	

The virtual NMR magnetometer enables the operator more flexibility when conducting measurements in an environment where NMR measurements could be handicapped by different disturbing signals and extraneous fields. The complex of both VXI modules enables also an easy alteration of the modulation field amplitude and frequency, phase shift of both PSD input signals and changes of the sampling time. This can be very helpful when optimising a measurement with a very poor SNR resonance signals.

The operator can choose between different alterations. The modulation field amplitude and modulation field frequency can be optimised according to the half line-width of the sample to improve the SNR. The HF frequency measurement time can be set according to operator’s needs (faster or more accurate measurements). When measuring with a common magnetometer, where together with the oscillator module also the time-base module, the digital counter, the resonance discriminator, the frequency sweep, the modulation generator and the power supply are built-in in the same housing, one can often notice some interference through ground connections and other influence of neighbouring modules. Because the virtual NMR magnetometer consists only of an oscillator and the power supply, there is less possibility of that. On the other hand, the acquiring of the viNMR signal and processing of the sampled signal is in case of an unstable oscillation very difficult.

In the future, we plan to add a Virtual sub-instrument for complete automatic resonance frequency search by means of a software resonance discriminator. Thus it would be possible to automatically lock the oscillator frequency to a certain flux density. The latter is very useful for the field homogeneity measurement of coils or magnetic flux density control. We intend to add also a FFT signal processing and develop some alternative algorithms for the resonance frequency searching and determining.

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AUTHORS: Gregor Geršak, Janez Humar, Dušan Fefer, Faculty of Electrical Engineering, University of Ljubljana, Tržaška 25, 1000 Ljubljana, Slovenia, tel. +386 14768409, fax. +386 14768214, gregor.gersak@fe.uni-lj.si, janez.humar@fe.uni-lj.si, dusan.fefer@fe.uni-lj.si.