Detector for Nuclear Quadrupole Resonance Spectroscopy

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Abstract— Nuclear quadrupole resonant spectroscopy is method similar to nuclear magnetic resonant spectroscopy also called zero field NMR [1, 2]. The response signal magnitude is very low and it is immersed in to the noise. There can be used some methods to harvest signal from noise it can be matched receiver [3] or averaging. This authors describe detector for Nuclear quadrupole resonant spectroscopy based on statistic methods and probability of distribution, that allow to measure repetitive signals below noise level. The paper presents the mathematical model and practical solution of the detector, and problems such as the dynamic range and signal distortion based on the signal-to-noise ratio are also analyzed in the given context. If the time of signal occurrence is known, the repetitive signal below the noise level can be harvested out of noise by averaging because of the wanted signal is correlated therefor highlighted by averaging contrast to the noise which is not correlated so it is supressed by averaging. The same principle we can use in domain of digital signal. So the input signal can be converted to the digital representation. There is an comparator with a triggering level immersed in the noise so the comparator is flipping continuously and the probability of output values is affected by input signal. The output digital signal can be processed by FPGA.

1. INTRODUCTION

One of the most significant obstacles in the usage of Nuclear quadrupole resonance spectroscopy is the magnitude of the response signal. This signal is very low and immersed in noise. Thus, increased demands are put not only on the shielding or the quality of the detector but also on the measurement time because of the signal immersion in noise. Out of the methods mentioned in the abstract, only averaging is suitable for spectroscopy. in this context, there then arises the need of a minimal amount of measurements. Generally, the result of the averaging process improves with the growing number of measurement repetitions; at the same time, however, the measurement time becomes longer. The second method outlined herein consists in that a matched reciever can be used to detect the presence of specific substances.

2. MATHEMATICAL MODEL

According to the well-known equation for the averaging of repetitive signals under the noise level, a signal can be harvested out of noise. Noise is not correlated, and thus it is suppressed by averaging; conversely, a signal is correlated and therefore highlighted by averaging (1).

We need to know where the signal begins. Due to known waveform of the excitation pulses and the time of the excitation start, it is not difficult to determine beginning of the response signal.

$$x_{avg}(t) = \frac{1}{n} \sum_{i=1}^{n} (x_i(t)) \tag{1}$$

Generally, we have to use a fast analogue-to-digital converter, which is a rather expensive device. The same principle can be used in the domain of digital signals; thus, we can convert an input signal to the digital form. This procedure is facilitated by a comparator, whose trigger level is immersed in the noise. This means that the comparator flips continuously, and consequently there is digital noise at the output of the comparator.

The probability of output values for a comparator without an input signal (only white noise is present at the input) is, at any time, the same for both output values (in our case, 1 and −1 due to signal centering) (2).

$$\begin{aligned} p(1) &= 0.5 \\ p(-1) &= 0.5 \end{aligned} \tag{2}$$

However, in the case of an input signal $f(t)$, the probability of output values is affected by this signal (3).

$$\begin{aligned} p(1) &= x = 0.5 + kf(t) \\ p(0) &= 1 - x = 0.5 - kf(t) \end{aligned} \tag{3}$$

The magnitude of the signal is proportional to the splitting of the probability of the comparator's output values. But due to the limitation, the proportionality is non-linear and depends on the signal-to-noise ratio. The digital averaging can be described by (4).

$$x_{avg}(t) = \sum_{i=1}^{n} (2 * p(1(f_i(t))) - 1) = \sum_{i=1}^{n} p(1(f_i(t))) - p(-1(f_i(t))) \tag{4}$$

As shown in Fig. 1, the dependence on the SNR markedly influences the sensitivity and linearity of the detector. Signals with a high SNR are easily noticable, but the linearity is not good. The signals immersed deep in noise (signals with a low SNR) exhibit good linearity, but their sensitivity is inferior.

The problem of this mathematical model and also of the circuit analysed below is overdrive. If the signal magnitude is higher than the noise magnitude, then the probability of the occurrence of symbols +1 or −1 is close to zero for one of the symbols and close to one for the other.

The averaged output signal is led to the FFT procesor and converted from the time domain to the freguency domain, where we can observe the occurrence of the searched substance (Fig. 2). From the characteristics of the digital NQR detector for different SNRs, the dynamic ratio can be determined. The lowest limit of the detector dynamic ratio is given by sensitivity of the detector;

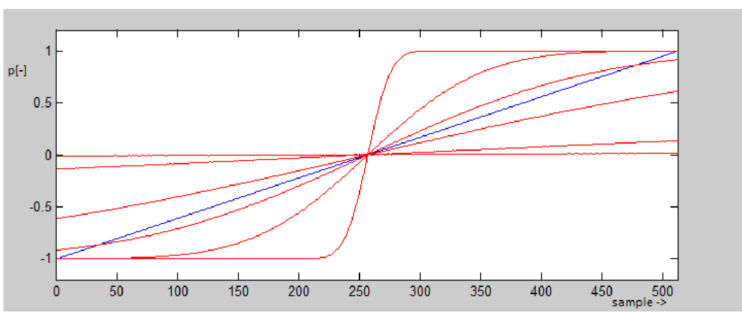

Figure 1: The averaging of 10^7 an input signal with with different SNR levels. The blue line represents the original signal and also the output of analog averaging (regardless of the signal-to-noise ratio). The red curves indicate the results of digital averaging. The steepest curve stands for SNR 20 dB; the gradually flattening one is for 6 dB, 0 dB, −6 dB, −20 dB; and the flattest line represents −40 dB.

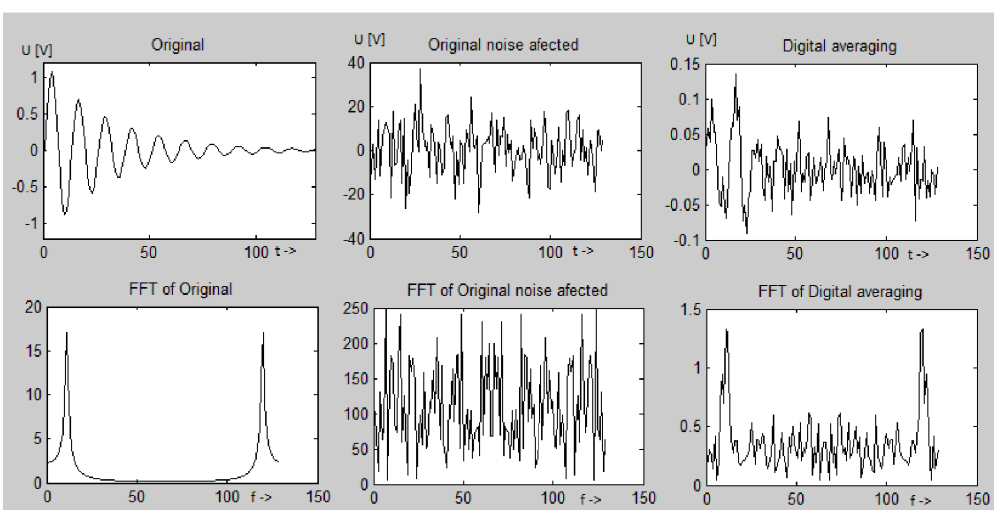

Figure 2: Example of noise-affected and averaged signal. The 1st row is for the signal in the time domain; the 2nd row represents the signal in the spectrum. SNR = −30 dB, 10000 averaging.

the highest limit is then determined by linearity of the output signal. Due to the non-linearities caused by high SNR, the higher harmonic frequencies are produced. These higher freguencies can be detected as foreign substances which, in fact, are not present.

3. PRACTICAL REALISATION

The system for NQR spectroscopy (Fig. 3) consists of an excitation circuit (a radio frequency generator, an amplifier, and a probe). The probe is used both as a part of the excitation circuit and as a component of detector. Furthermore, this probe constitutes an LC resonant circuit (the examined substance is placed into the coil) connected to the excitation circuit and the detector via decoupling circuits. The decoupling circuits protect the detector from damage caused by a high level of the signal from the excitation circuit. The detector is described in more detail within references [4, 5]. In general terms, it is followed by an FPGA for signal processing (averaging and the FFT). The whole spectroscope is regulated by a microcontroller (which can also be implemented in the FPGA) or a PC.

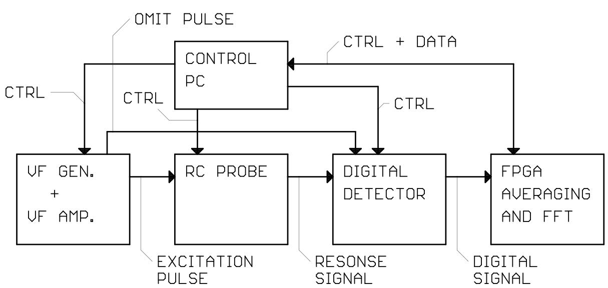

Figure 3: Block scheme *o* NQR spectroscope.

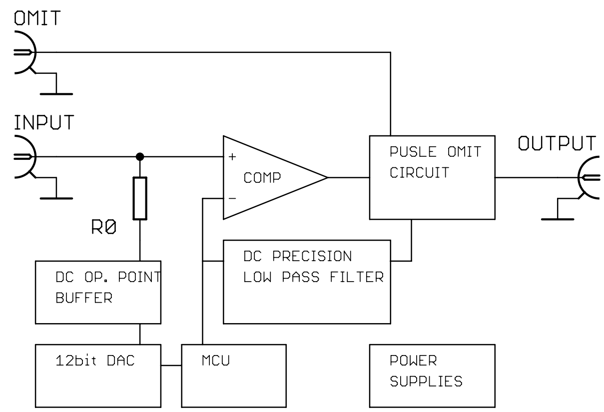

Figure 4: Block scheme NQR detector.

The fabricated digital NQR detector comprises the high speed comparator [6–8] with low-pass feedback circuits designed to pass the DC component of the signal without corruption. The filter can be realised as passive (an RC ladder network) or active; the active variant then utilises DC precision filters (Fig. 5). In both these cases, howeever, it is necessary to use foil condensators with low leakage currents.

Another part of the detector is a DC operating point circuit implemented as a 12-bit DA convertor regulated by a microcontroller (Fig. 6).

The digital part of the cicruit is implemented as an FPGA. The FPGA contains averaging and FFT or averaging and matched recievers. The second solution can be used to search for pre-specified substances (for example, 35Cl or 14N). Thanks to the matched reciever implemented in the FPGA, a large amount of substances can be retrieved.

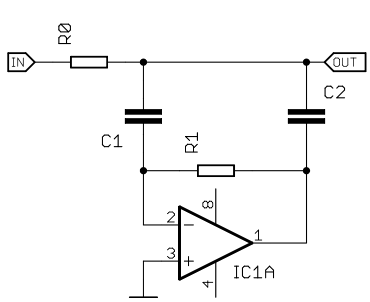

Figure 5: DC precision low-pass filter.

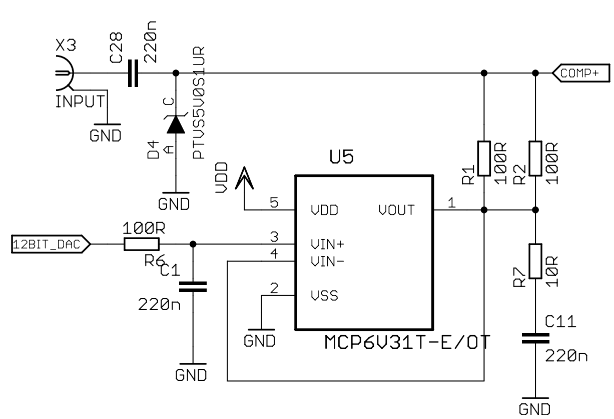

Figure 6: Implementation of the circuit for the DC operating point setting.

4. CONCLUSION

A mathematical model has been developed and tested in MATLAB. Based on this model, the proposed detector was created and measured; the measurement showed the necessity to limit the signal bandwidth by a low-pass filter for better sensitivity. Due to the significant number of measuring cycles required for clear results, the method of averaging detection became rather time-consuming; in this context, the most problematic aspect definitely consists in the presence of the relaxation time. Importantly, as the measurement of one sample can last several minutes, the commercial applicability of averaging-based NQR spectroscopy is limited to a great extent; commercial users would then probably prefer averaging marged with matched recieving. A matched reciever can be easily implemented in an FPGA.

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