

Automated NQR – Spectrometer

Michael IVANCHUK, Volodymyr BRAJLOVSKYJ
Department of the radio engineering and informative safety
Jurij Fed'kovych Chernivtsi national university
Chernivtsi, Ukraine, Kotsiubynsky str. 2, 58012
m.ivanchuk@chnu.edu.ua

Abstract—Improvement of an autodyne Nuclear quadruple resonance spectrometer is offered. The change of frequency of oscillatory LC circuit of the spectrometer is carried out in two ways: by varicap and variable capacitor. A processor module for the capacitor and varicap control is developed. The unit allows to scan and measure the level and frequency of the NQR-signal. The unit is controlled by the personal computer.

Index Term—Nuclear quadruple resonance, Analog-to-digital converter, Digital-to-analog converter, Microcontroller, Stepper motor.

I. INTRODUCTION

Nuclear quadruple resonance (NQR) is a resonance absorption of electromagnetic energy in crystals, caused by transitions between power levels, appearing as a result of interaction of kernels possessing an electric quadruple moment with the electric crystalline field. NQR is the special case of nuclear magnetic resonance (NMR) in crystals. The so-called “pure” NQR is observed in the absence of the permanent magnetic field [1]. In this papers we offer automated method of NQR-signal registration [2].

For the capacity change in the autodyne LC circuit an semiconductor varicap diode is usually used [3]. Such method has the substantial failing – with the change of varicap capacity its active conductivity changes considerably. As a result the LC circuit quality factor also changes and the base datum line deflects.

Use in the oscillatory LC circuit of a combined capacitor (parallel connection of the varicap and variable capacitor) allowed to decrease the drift of the datum line of NQR signal registration at the frequency change of autooscillations. Adjustment of the LC circuit operating frequency is realized by combined method: the rough setting is carried out by capacity of variable capacitor, and for exact setting varicap is used. Such method allows to decrease substantially the range of varicap quality factor (Q factor) change from the operating frequency.

II. AUTODYNE LC CIRCUIT WITH THE COMBINED CAPACITOR

Autodyne LC circuit used in a NQR spectrometer with the combined capacitor is represented in Fig. 1. The explored sample is placed in the inductance coil L1 [2]. Capacitors C1 and C2 are intended for reduction of the mutual influencing of characteristics and for the improvement of oscillatory LC circuit Q factor. Frequency scanning is executed by adjustment of general capacity C in the oscillatory LC circuit.

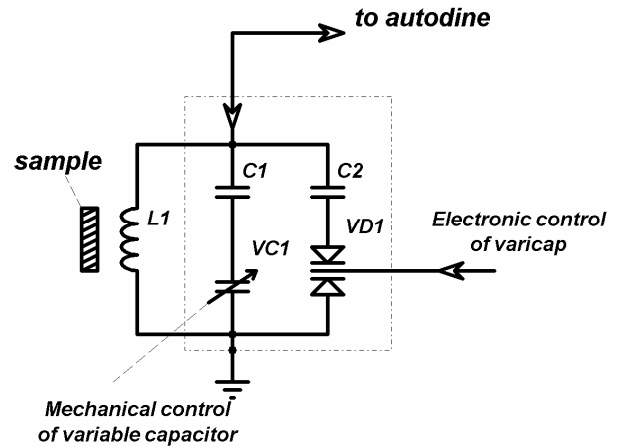


Figure. 1. Measuring LC circuit with the combined capacitor

Variation of the VC1 capacity is carried out mechanically by the stepper motor. Developed unit of data capture and control provides the motor control.

III. UNIT OF DATA CAPTURE AND CONTROL

For the autodyne NQR spectrometer control with combined capacity setting for frequency tuning a specialized control unit on the microcontroller (MC) basis is developed. The unit executes such functions as measurement of the operating frequency of the LC circuit, measurement of the level of NQR response signal, stepper motor control, which kinematics is related to variable capacitor. The varicap capacity adjustment is carried out by built-in DAC.

Block diagram of the NQR spectrometer on the basis of data capture and control unit is shown in Fig. 2.

The oscillations in the measuring LC circuit are supported by autodyne. High frequency (HF) signal amplitude in LC circuit is proportional to the NQR response signal. Synchronous detector (SD) demodulates this signal. The detected SD signal is processed by ADC.

HF signal from the LC circuit passes to the cymometer. The cymometer is realized as program for MC. Precision of cymometer is 1 Hz. Information about frequency is compared to the set value of frequency, and MC carries out the proper control.

Unit of stepper motor control (USMC) and voltage from DAC are used for setting of LC circuit frequency.

A variable capacitor sets frequency with step of 4000 Hz. At 420 steps it provides scanning range of 1,68 MHz.

The exact setting of frequency is realized by varicap supplied with 12-bit DAC. It provides precision of frequency adjustment on the level of 1 Hz.

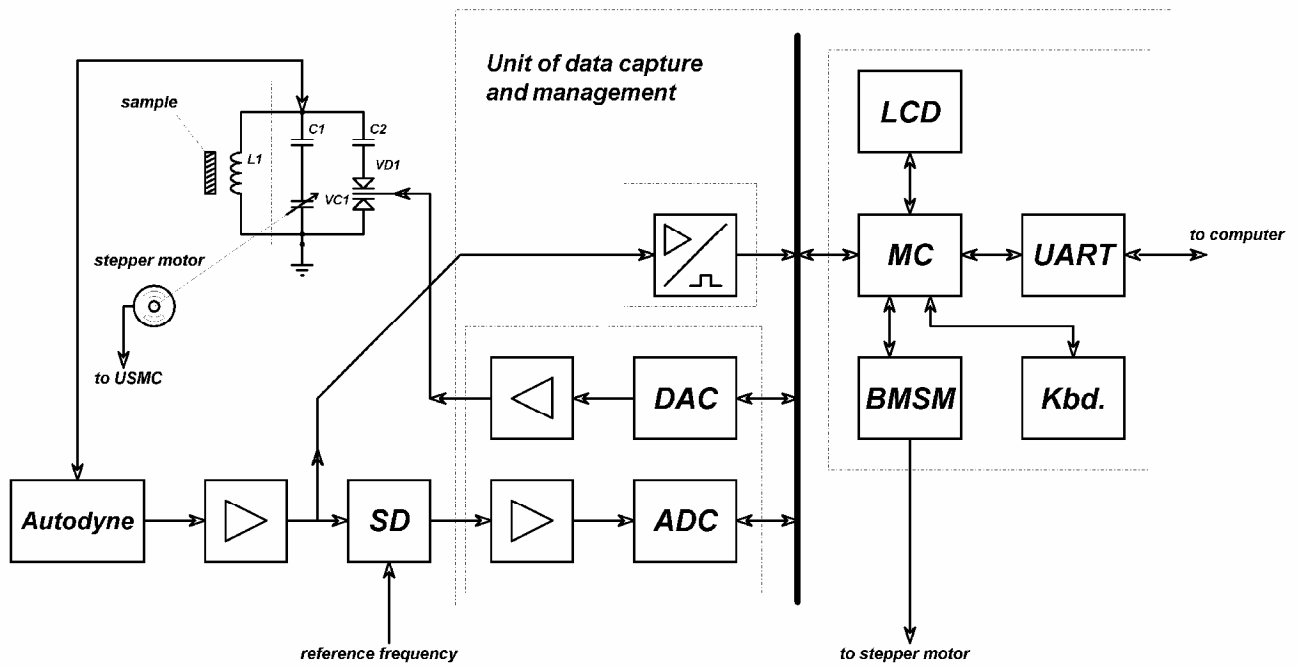


Figure 2. Block diagram of the NQR spectrometer on the basis of unit of data capture and control

Digital part of the unit of data capture and control is shown in Fig.3. Microcontroller PIC18F452 [4], is used as the basis of the control module. MC executes the control functions of all devices of the unit. For user dialog realization keyboard and display are used. As LCD is used 2x16 characters LCD AC162 with a build-in driver H44750. Matrix keyboard 3x4 provides user data input. The

conversational mode of operations is developed to allow a user to set the basic modes of operations with NQR spectrometer.

Connection with the computer on protocol RS-232 is carried out with the use of integrated circuit (IC) MAX232 [5].

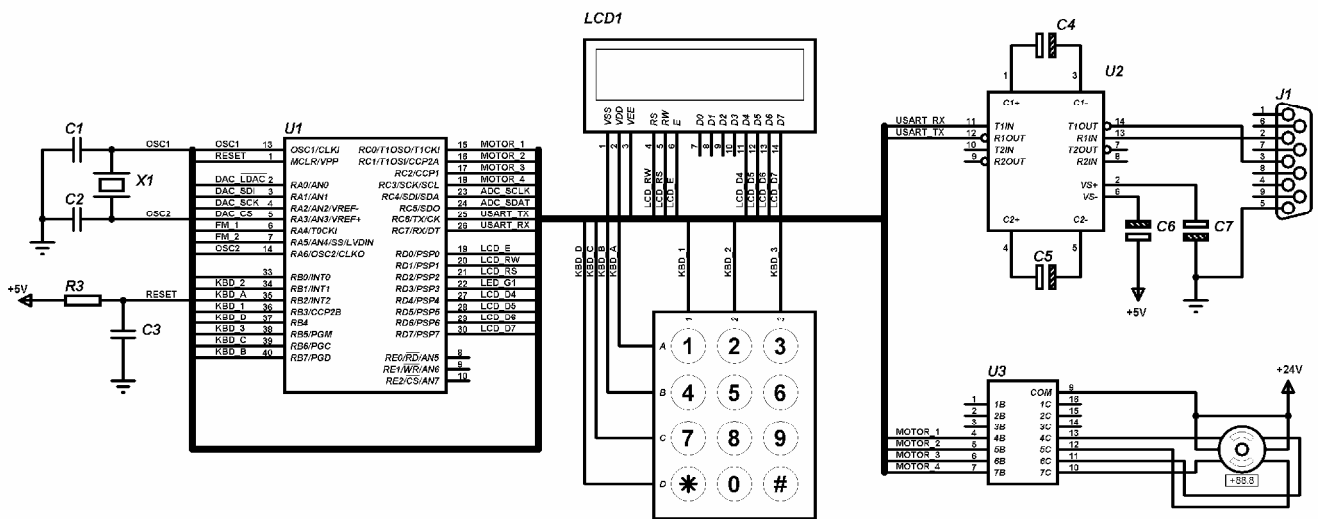


Figure 3. Schematic circuit diagram of digital part of the unit of data capture and control

ADC realized on the basis 16-Bit Sigma-Delta A/D Converter TC3400 with single polarity input. Input voltage range is a 0 .. 2,5 volt. An entrance signal have a range from -2,5 V to + 2,5 V. For realization transformation voltage ranges is used circuit on the precision operation amplifier AD8552 basis (Fig.4). Precision reference voltage source REF192 (+ 2,5 V) is a reference voltage generator for DAC MCP4921. Frequency exactness and stability of its support

on exactness DAC. For providing of maximally high-quality indexes as a reference voltage source of reference voltage DAC the integral precision supporting reference voltage source of type REF192 is used, that is intended for the use as of source of supporting tension a 8 - 12 bit ADCs or DAC [6]. He provides reference voltage 2,5 V with exactness $\pm 0,08 \%$. At the same time is used 10 - bit DAC provides exactness of Least Significant Bit (LSB) $\pm 0,097 \%$.

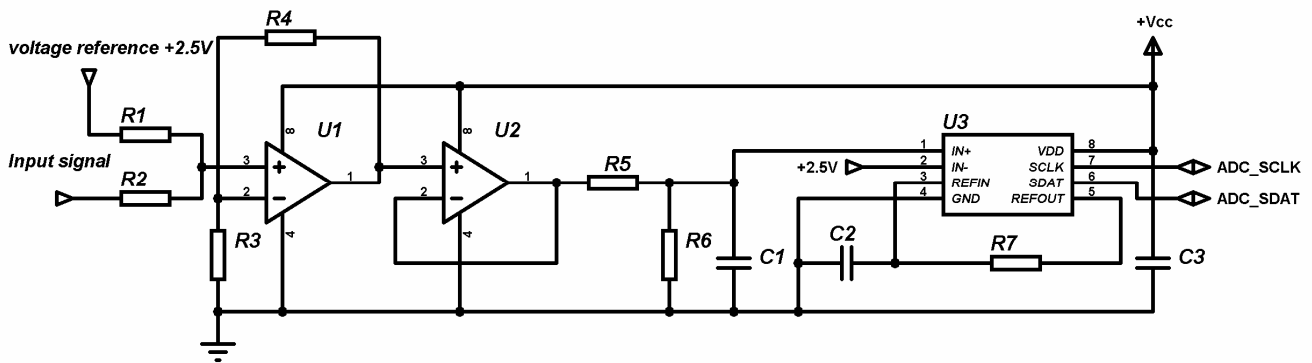


Figure 4. ADC input circuits

For providing of negative reference voltage we used circuit on a basis OpAmp AD8052. It carries out transformation of reference voltage value from +2,5 V to -2,5 V. Electrical circuit is represented in Fig. 5.

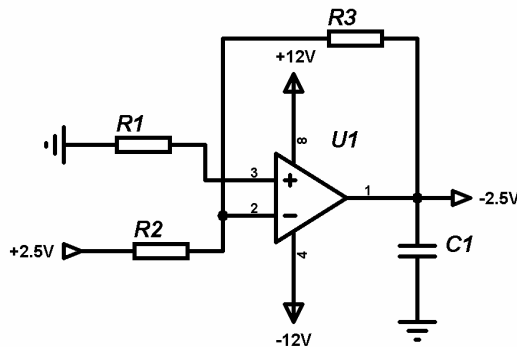


Figure 5. Schematic circuit diagram of reference voltage inverter

Personal computer software consists of 3 parts – user interface, mathematical part, and file manager.

The program allows to get an experimental data, to save them in a file, to carry out their treatment, to save results and to use for the next creation of data bases.

I. CONCLUSION

For the improvement of autodyne continuous wave quadruple resonance spectrometer a combined method of frequency setting in LC circuit is offered. Including to the autodyne oscillatory LC circuit of a combined capacitor (parallel connection of varicap and variable capacitor) decrease the drift of NQR signal datum line. Adjustment of the LC circuit operating frequency is realized automatically:

the rough setting is carried out by the change of variable capacitor capacity, and for exact setting varicap is used. Such method allows to decrease substantially dependence of the general Q factor of the circuit from operating frequency. The setting of the capacity of the variable capacitor is executed mechanically by the stepping motor. To control the NQR spectrometer with combined setting frequencies the specialized control unit on the microcontroller basis is developed. The unit executes such functions as measurement of LC circuit operating frequency and level of NQR response signal; stepping motor control, which kinematics is related to the rotor of variable capacitor; the varicap capacity control.

The rough frequency setting is realized with the step of 4000 Hz, and exact frequency setting has a step of 1 Hz. The cymometer resolution is of 1 Hz.

Setting of all operating parameters and the data capture is carried out by computer using protocol RS-232.

REFERENCES

- [1] Smith, J.A.S. "Nuclear Quadrupole Resonance Spectroscopy: General principles". Journal of Chemical Education, 48:39-49, 1971.
- [2] O.S.Stoican. NQR detection setup. Romanian Journal of Physics, Vol. 51, Nos. 1-2, P. 311-315, Bucharest, 2006
- [3] Hilferty, C. L. Design and Analysis of a Continuous Wave Quadrupole. Resonance Spectrometer. Thesis, Pennsylvania State University, 2003.
- [4] <http://www1.microchip.com/downloads/en/DeviceDoc/39564c.pdf>
- [5] <http://datasheets.maxim-ic.com/en/ds/MAX220-MAX249.pdf>
- [6] http://www.analog.com/UploadedFiles/Data_Sheets/REF19XSERIES.pdf