Signals and Communication Technology

Cristian Monea
Nicu Bizon

# Signal Processing and Analysis Techniques for Nuclear Quadrupole Resonance Spectroscopy

Springer

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# Signal Processing and Analysis Techniques for Nuclear Quadrupole Resonance Spectroscopy

Springer

Cristian Monea
Research and Development Department
Mira Technologies Group
Voluntari, Romania

Doctoral School of Electronics,
Telecommunications and Information
Technology
Politehnica University of Bucharest
Bucharest, Romania

Nicu Bizon
Faculty of Electronics, Communications
and Computer Science
University of Pitesti
Pitesti, Arges, Romania

Doctoral School of Electronics,
Telecommunications and Information
Technology
Politehnica University of Bucharest
Bucharest, Romania

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# Foreword

This book brings new literature reviews on nuclear quadrupole resonance (NQR) techniques, appropriate signal processing techniques proposed for NQR spectrometers and implemented NQR spectrometers developed to date.

The signals obtained from NQR spectroscopy are simulated to propose an NQR signal model to be used on the comparative analysis (based on a new set of performance indicators proposed here) of the main signal processing methods that have been developed in the literature.

So, this book proposes a new approach to detecting the NQR signal by using artificial intelligence methods (such as deep learning techniques and other proposed advanced techniques). As a result of this study, the best performing solutions are selected, adapted for NQR detection and implemented in a customized NQR spectrometer and, finally, the NQR-based equipment was evaluated in real conditions.

The data set was acquired under different operating conditions and was analysed to evaluate the performance of the custom-designed NQR spectrometer.

It is worth mentioning that the implementation of the detection system is detailed in this book from both a hardware and a software point of view, and the initial deep learning technique proposed is further improved in the penultimate chapter by using transfer learning and autoencoders to allow its use in other spectrometers and at different noise levels.

Thus, the content of this book is interdisciplinary, involving knowledge of physics, electrical and electronics engineering, signal processing, signal analysis and artificial intelligence (machine learning, deep learning, etc.) and optimization.

Therefore, the content of this book is addressed to researchers studying the resonance of nuclear quadrupoles and its applications, and NQR equipment manufacturers and readers in the multidisciplinary fields mentioned above, who want to understand the NQR spectrometer and the techniques used in its design.

So, both researchers (physicists, engineers and computer scientists) and engineers working for manufacturers of security or laboratory equipment based on the NQR technique, as well as master's and doctoral students studying and researching NQR detection techniques, will all be interested to read this book because it proposes (i) a new and performant NQR signal detection techniques based on improved deep learning methods and (ii) a detailed description regarding the hardware and

software implementation of an NQR detection equipment that implements the above-mentioned solutions.

In conclusion, it is noteworthy that the content of the chapters is presented gradually and theoretically in detail as necessary to understand the problems and effective techniques for implementing the NQR, being highly recommended for study in education and research.

Baku, Azerbaijan Arif M. Hashimov
April 2021

# Preface

In recent years, global terrorism and organized crime, especially in the field of drug trafficking, have increased enormously, with more than 10,000 incidents per year reported in the global terrorism database since 2017. For example, in 2017, over 140 tons of cocaine and 5 tons of heroin were confiscated in the European Union, and the number of confiscations has increased every year. In this context, a number of prohibited substance control systems have been developed and installed worldwide (at airports, customs, post offices and border checkpoints) to combat illegal activity and ensure the safety of citizens.

Therefore, this book addresses the issue of improving the detection of prohibited substances using the nuclear quadrupole resonance (NQR) technique and takes into account the advanced signal processing techniques recently proposed in the literature, including by the authors of this book.

NQR is a confirmed analysis technique and recognized as a solution that meets the performance standards imposed for security checkpoints. In short, the NQR technique is based on scanning the object (package and luggage) which may contain a substance of interest. An electromagnetic pulse train (called the excitation sequence) is used for scanning, and the response is received at the end of the excitation sequence. The NQR technique has the advantage of a high specificity relative to a substance of interest, but it is also worth mentioning that it is very difficult to detect the response (the weak signal emitted by the substance).

This book analyses and proposes new signal processing and analysis methods for the detection of dangerous or contraband substances (such as explosives, narcotics or toxic substances). Also, the hardware solutions implemented in a custom NQR spectrometer (detector) are described, and the performances obtained are compared with similar ones reported in the literature.

The identification of prohibited substances by nuclear quadrupole resonance depends on the physical principle used and deployment location of the NQR equipment, because the received signal has a low signal-to-noise ratio and is susceptible to radio interference in the same frequency band. In addition, the spectral lines are dependent on the substance's temperature.

Because the detection time is critical and the number of false-positive and false-negative alarms must be minimized, the main signal processing challenges are related

to the ability to detect the response signal using a limited number of acquisitions, to perform real-time analysis of the response signal's characteristics in order to cancel radio frequency noise and compensate the temperature dependence of spectral lines, with the ultimate goal of maximizing the detection accuracy.

In the last decade, numerous laboratory NQR detection systems have been proposed and implemented for identifying prohibited substances, with detection probabilities of up to 90%. However, the detection performance decreases greatly in the operational environment due to the causes mentioned above. So, new hardware and software solutions are needed to increase the performance of NQR detection. Therefore, the purpose of this book is to present some hardware and software solutions to improve the performance of the NQR technique for detecting prohibited substances.

This book is structured in ten chapters, and Chap. 1 introduces the topic of nuclear quadrupole resonance detection of prohibited substances.

Chapter 2 briefly presents the methods and equipment for the acquisition and analysis of signals for detection of prohibited substances.

Chapter 3 continues the analysis started in Chap. 2, focusing on nuclear quadrupole resonance spectroscopy and presenting its physical principle, specific signal acquisition methods, and laboratory and commercial NQR equipment.

Chapter 4 presents in detail the specific pre-processing, post-processing and signal analysis techniques proposed for nuclear quadrupole resonance detection.

Chapter 5 presents the test signals that will be used in the following chapter to study the performance of the algorithms proposed in the literature for NQR signal processing and analysis.

The study of the performance of the NQR algorithms is presented in Chap. 6 in order to define a reference regarding the obtained performance. It considers specific performance indicators and a multi-criteria classification algorithm based on an objective function to improve the probability of detection.

The experimental results of the acquisition of nuclear quadrupole resonance signals are presented and analysed in Chap. 7 in order to identify new and improved NQR detection techniques.

Thus, Chap. 8 presents new signal analysis algorithms based on machine learning and demonstrates their improved performance in detecting substances using the NQR technique compared to those presented in the previous chapter.

Chapter 9 describes techniques for enhancing the performance of the machine learning algorithm proposed in the previous chapter that are based on transfer learning and noise reduction using autoencoders.

The last chapter presents the implementation of an NQR equipment used for signal acquisition, processing and analysis. The hardware and software implementations are detailed, and the system's performance in different operating conditions is evaluated.

Summarizing, the salient features of the book would be the following:

- Presenting a detailed literature review of the methods and equipment for signal acquisition and analysis for the detection of prohibited substances,
- Presenting the principle of nuclear quadrupole resonance spectroscopy,

- Providing a detailed literature review of the signal processing and analysis techniques applied in nuclear quadrupole resonance detection, with a new classification,
- Performing a modeling of the signals used in nuclear quadrupole resonance spectroscopy, with the proposal of a new signal model,
- Performing a comparative study of the signal processing and analysis algorithms, in order to verify and create its own reference for the performance indicators, that will be of help for comparing the newly developed solutions,
- Performing an analysis of the signals acquired from nuclear quadrupole resonance experiments with the aim of aiding the development of new detection solutions,
- Proposing new signal analysis algorithms based on artificial intelligence/deep learning in order to improve the detection of substances by NQR technique,
- Proposing new features for the classification of NQR signals using artificial intelligence/deep learning algorithms,
- Proposing new artificial intelligence/deep learning techniques for enhancing the performance of signal analysis algorithms,
- Detailing the hardware and software implementations of an NQR signal processing and analysis system,
- Helpful for researchers and practitioners in the areas of electrical engineering, signal processing and analysis, applied spectroscopy, as well as for security or laboratory equipment manufacturers.

In conclusion, electrical engineering students and specialists are eligible and guided to use the book effectively in their current activities.

Pitesti, Romania
April 2021

Cristian Monea
Nicu Bizon

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# Abbreviations

| | |
|---|---|
| ACC | Accuracy |
| AE | Autoencoder |
| AI | Artificial Intelligence |
| ALE | Adaptive Line Enhancement/Adaptive Line Enhancer |
| ALS | Alternating Least Squares |
| AML | Approximate Maximum Likelihood |
| ANC | Adaptive Noise Cancellation/Adaptive Noise Canceller |
| APES | Amplitude and Phase Estimator |
| API | Application Program Interface |
| AR | Autoregressive |
| ARMA | Autoregressive Moving Average |
| AU | Arbitrary Unit |
| AUC | Area Under Curve |
| BICETAML | Beamforming-based Interference Cancellation Echo Train Approximate Maximum Likelihood |
| CAPA | Capon Amplitude and Phase Estimator Average |
| CAPES | Capon Amplitude and Phase Estimator |
| CMA-ES | Covariance Matrix Adaptation Evolution Strategy |
| CNN | Convolutional Neural Network |
| CNN-LSTM | Convolutional Neural Network Long Short-Term Memory |
| cNQR | Classical NQR |
| ConvAE | Convolutional Autoencoder |
| ConvLSTM | Convolutional Long Short-Term Memory |
| CPMG | Carr–Purcell–Meiboom–Gill |
| CS | Clonal Selection |
| c-SEAQUER | Conventional-Subspace-based EvaluAtion of Quadrupole resonance signals Exploiting Robust methods |
| CTLMS | Continuous Time Least Mean Squares |
| CUDA | Compute Unified Device Architecture |
| CW | Continuous Wave |
| DB | Database |
| DBN | Deep Belief Network |

| | |
|---|---|
| DC | Direct Current |
| DCRCB-GLRT | Doubly Constrained Robust Capon Beamformer-Generalized Likelihood Ratio Test |
| DEPIC | Dual-channel Estimation of Phase and amplitude for Interference Cancellation |
| DFT | Discrete Fourier Transform |
| DL | Deep Learning |
| DLL | Dynamic-Link Library |
| DMA | Demodulated Approach |
| DMNB | 2,3-Dimethyl-2,3-dinitrobutane |
| DNN | Deep Neural Network |
| DNN-AE | Deep Neural Network Autoencoder |
| EC | Ensemble of Classifiers |
| EFG | Electric Field Gradient |
| EGDN | Ethylene Glycol Dinitrate |
| EI | Expected Improvement |
| EPIC | Estimation of Phase and amplitude for Interference Cancellation |
| ESPIRE | Exploiting Spatial diversity and Polymorphism In Robust Estimation (of NQR signals) |
| ESPRIT | Estimation of Signal Parameters via Rotational Invariance Technique |
| ET | Echo Train/Extra Trees |
| ETAML | Echo Train Approximate Maximum Likelihood |
| ETCAPA | Echo Train Capon APES Average |
| ET-ESPRIT | Echo Train-Estimation of Signal Parameters via Rotational Invariance Technique |
| FDR | False Discovery Rate |
| FETAML | Frequency-selective Echo Train Approximate Maximum Likelihood |
| FFT | Fast Fourier Transform |
| FHETAML | Frequency-selective Robust Echo Train Approximate Maximum Likelihood |
| FICAML | Fourier analysis-based Interference Cancellation Approximate Maximum Likelihood |
| FID | Free Induction Decay |
| FLSETAML | Frequency-selective Least Squares Echo Train Approximate Maximum Likelihood |
| FN | False Negative |
| FNR | False-Negative Rate |
| FODETAML | Frequency-selective Offset-Dependent Echo Train Approximate Maximum Likelihood |
| FOR | False Omission Rate |
| FP | False Positive |
| FPGA | Field-Programmable Gate Array |

| | |
|---|---|
| FPR | False-Positive Rate |
| FRETAML | Frequency-selective Robust Echo Train Approximate Maximum Likelihood |
| FSAML | Frequency-Selective Approximate Maximum Likelihood |
| FSMC | Frequency-Selective Multichannel detector |
| FT-NQR | Fourier Transform NQR |
| GA | Genetic Algorithm |
| GBT | Gradient Boosted Trees |
| GDDR | Graphics Double Data Rate |
| GP | Gaussian Process |
| GPIO | General-Purpose Input/Output |
| HETAML | Hybrid Robust Echo Train Approximate Maximum Likelihood |
| HMTD | Hexamethylene Triperoxide Diamine |
| HMX | High Melting Explosive/Her Majesty's Explosive/High-velocity Military Explosive/High-Molecular-weight RDX |
| I2C | Inter-Integrated Circuit |
| ICAML | Interference Cancellation Approximate Maximum Likelihood |
| ICETAML | Interference Cancellation Echo Train Approximate Maximum Likelihood |
| ICFETAML | Interference Cancellation Frequency-selective Echo Train Approximate Maximum Likelihood |
| IDE | Integrated Development Environment |
| ILSVRC | ImageNet Large-Scale Visual Recognition Challenge |
| IMS | Ion Mobility Spectrometry |
| ISR | Interference-to-Signal Ratio |
| JSON | JavaScript Object Notation |
| k-NN | k-Nearest Neighbour |
| LMS | Least Mean Squares |
| LNA | Low-Noise Amplifier |
| LS | Least Squares |
| LSETAML | Least Squares Echo Train Approximate Maximum Likelihood |
| LS-FRETAML | Least Squares-Frequency-selective Robust Echo Train Approximate Maximum Likelihood |
| LSTM | Long Short-Term Memory |
| M3L | Model-Mismatched Maximum Likelihood |
| MDMA | 3,4-Methylenedioxymethamphetamine (Ecstasy) |
| MFD | Multi-criteria Fourier-based Decision algorithm |
| ML | Machine Learning |
| MLH | Maximum Likelihood |
| MSWF | Multi-Stage Wiener Filter |
| MUSIC | Multiple Signal Classification Spectral Estimation |
| NG | Nitroglycerin |
| NLS | Nonlinear Least Squares |
| NMOS | Negative-channel MOS |
| NMR | Nuclear Magnetic Resonance |

| | |
|---|---|
| NN | Neural Network |
| NORRDIQ | Noise and RFI Removal for Detection In QR applications |
| NPAPS | Non-Phase-Alternated Pulse Sequence |
| NPV | Negative Predictive Value |
| NQR | Nuclear Quadrupole Resonance |
| NS | Negative Scan |
| ODETAML | Offset-Dependent Echo Train Approximate Maximum Likelihood |
| PAPS | Phase-Alternated Pulse Sequence |
| PASLSE | Phase-Alternated Spin-Locked Spin Echo |
| PCC | Pearson Correlation Coefficient |
| PETN | Pentaerythritol Tetranitrate |
| PIN | PIN diode |
| PNP | PNP bipolar transistor |
| PostPA | Post-Processing and Analysis |
| PPV | Positive Predictive Value |
| PS | Positive Scan |
| PSL | Pulsed Spin Locking |
| QCPMG | Quadrupolar Carr–Purcell–Meiboom–Gill |
| RAM | Random Access Memory |
| RCB | Robust Capon Beamformer |
| RCDAML | Robust Correlation Domain Approximate Maximum Likelihood |
| RDX | Hexogen |
| ReLU | Rectified Linear Unit |
| REMIQS | Robust Estimation of MultIple polymorph QR Signals |
| ResNet-34 | Residual neural Network-34 |
| RESPEQ | Robust Evaluation using Subspace-based methods of Polymorphic nuclEar Quadrupole signals |
| RETAML | Robust Echo Train Approximate Maximum Likelihood |
| REWEAL | Robust Evaluation With conic subspace constraints of Estimation of Approximate maximum Likelihood |
| RF | Radiofrequency/Random Forest |
| RFI | Radio Frequency Interference |
| RLS | Recursive Least Squares |
| RMS | Root Mean Square |
| RNN | Recurrent Neural Network |
| ROC | Receiver Operating Characteristic |
| RTDAML | Robust Time Domain Approximate Maximum Likelihood |
| RX | Reception |
| SA | Simulated Annealing |
| SAMP | Spectral Average to Maximum Peak |
| SCB | Standard Capon Beamformer |
| SE | Spin Echo |

| | |
|---|---|
| SEAQUER | Subspace-based EvaluAtion of Quadrupole resonance signals Exploiting Robust methods |
| SF | Spectrometer Frequency |
| SLMP | Spin-Locked Multi-Pulse |
| SLSE | Spin-Locked Spin Echo |
| SMBO | Sequential Model-Based Optimization |
| SMF | Spectral Maximum Frequency |
| sNQR | Stochastic NQR |
| SNR | Signal-to-Noise Ratio |
| SOI | Signal Of Interest |
| SORC | Strong Off-Resonance Comb |
| SPA | Signal Processing and Analysis |
| SPI | Serial Peripheral Interface |
| SQUID | Superconducting Quantum Interference Device |
| SRAR | Spectral Regions Average Ratio |
| SRO | Super-Regenerative Oscillator |
| SSD | Solid-State Drive |
| SSFP | Steady-State Free Precession |
| SVM | Support Vector Machine |
| SW | Spectral Width |
| TATP | Triacetone Triperoxide |
| THC | Tetrahydrocannabinol |
| TN | True Negative |
| TNR | True-Negative Rate |
| TNT | Trinitrotoluene |
| TP | True Positive |
| TPE | Tree Parzen Estimator |
| TPR | True-Positive Rate |
| TX | Transmission |
| UART | Universal Asynchronous Receiver/Transmitter |
| USB | Universal Serial Bus |
| VGG-16 | Visual Geometry Group-16 |
| WICAML | Wavelets-based Interference Cancellation Approximate Maximum Likelihood |
| WPF | Windows Presentation Foundation |
| WURST-QCPMG | Wideband Uniform Rate Smooth Truncation-Quadrupolar Carr–Purcell–Meiboom–Gill |
| XAML | Extensible Application Markup Language |

# Chapter 1
# Introduction

The last decades have seen an unprecedented increase in global terrorism and organized crime, especially in the area of drug trafficking. The global terrorism database indicates over 10,000 incidents in 2017 alone [1], and recent events include the bombings from Sri Lanka, 21 April 2019, Kabul, 19 August 2019 or Beirut, August 4, 2020. In 2017, more than 140 tons of cocaine and 5 tons of heroin were reported to be seized in the European Union [2]. Figures 1.1 and 1.2 illustrate the evolution of heroin trafficking and terrorism at European and global level. In this context, a number of prohibited substance control systems have been developed and installed in airports, customs, post offices and border checkpoints to combat illegal activity and increase the safety of citizens.

The detection techniques applied range from trace detection, based on ion mobility spectrometry, chemiluminescence, colorimetric tests or mass spectrometry, to the detection of masses of substances, based on imaging techniques (X-rays, millimeter waves, computed tomography or terahertz waves) and nuclear techniques (thermal/fast neutrons, nuclear magnetic resonance or quadrupolar nuclear resonance). Also, there are various methods of signal processing and analysis, depending on the detection technique applied. They include statistical algorithms for signal detection and estimation, spectral processing, adaptive filtering, dedicated image processing algorithms or advanced signal analysis and recognition techniques based on machine learning (ML).

Nuclear Quadrupole Resonance (NQR) has been acknowledged as a technique for scanning prohibited substances that can meet the high requirements of security checkpoints. It has also been applied in landmine detection and its use is justified by the fact that there are currently over 100 million active landmines worldwide, killing or injuring, on average, 5,000 people annually [4].

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