Improvement of simulated nuclear quadrupole resonance signals from explosive detection via a Red-Pitaya board

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Abstract. In Nuclear quadrupole resonance (NQR), the interaction of the nuclear magnetic moments of quadrupolar nuclei (spin greater than 1/2) with the electric field gradient of the surrounding molecular orbitals produces an energy splitting. Because the resonant frequency is very specific to the molecular structure, the NQR can be used to detect explosive materials very accurately and it is extremely useful for detecting modern bombs whose containers made from plastics and wood instead of metals. However, NQR signals are generally very weak so they are difficult to be detected. Recently, Red-Pitaya boards, a Field Programmable Gate Array (FPGA) on Single Board Computers, have been being utilized in many electronic applications due to their small size and low cost. Since the boards can generate and acquire radio frequency signals, they can be taken as the console of portable bomb detectors. In this work, we study an improvement of the NQR signals of an explosive, ammonium nitrate with a resonant frequency of 423.6 kHz, acquired by using a Red-Pitaya board (STEMlab 125-14). To construct the NQR signals, we simulate free induction decay (FID) signals (exponential decay of sinusoidal functions) and add real measured noises from an input port of the Red-Pitaya board. To mimic real situations, the FID amplitude is varied, frequency fluctuations and phase shifts are added. The results show that averaging of signals from repeat measurements can improve the signals in all cases. To distinguish the signals from the noises, a minimal number of measurements is required. This necessary number of repeat measurements increases with frequency fluctuations and phase shifts but decreases when the FID amplitude grows.

1. Introduction

In Nuclear Quadrupole Resonance (NQR), energy gaps are generated by the interaction of the nuclear magnetic moments of quadrupolar nuclei (spin greater than 1/2) with the electric field gradient of the surrounding molecular orbitals. NQR works by sending radiofrequency (RF) waves with resonant frequency to excite the sample and detecting the respond signal with the same frequency [1-3]. This resonant frequency is very specific to the molecular structure of the sample. Therefore, the NQR is very useful for detecting explosives, especially modern bomb s whose containers made from plastics and wood instead of metals [4]. However, NQR signals are very weak and difficult to be detected. The signal-to-noise ratio (SNR) of NQR is affected by several factors, including molecular dynamics of relaxation, interference signals, electronic noise, explosive amount, distance, temperature, and the design of the detecting system [5,6].

Recently, Red-Pitaya STEMlab 125-14, single board computers containing a field programmable gate array (FPGA), have been used as control units in many electronic applications [7-9] due to their small size and low cost. Since the boards can generate and acquire signals within a frequency range of NQR, they are a suitable console of portable bomb detectors.

In this work, we study an improvement of NQR signals when acquired by a Red-Pitaya board (STEMlab 125-14). Thereby, the amplitude, frequency fluctuation and phase shift of the signals together with the electronic noises from the acquisition board are considered. We search for a necessary number of repeat measurements until the average signals has a sufficiently high SNR of 5 - 10.

2. Methods

To mimic the NQR signal obtained after an RF pulse is applied to the sample, we calculate an FID signal, an exponential decay of sinusoidal function of time t, as

$$FID(t) = A\sin[2\pi(f_0 + \Delta f \times rand)t + \phi \times rand]\exp\left(-t/T_2^*\right) \tag{1}$$

where A: amplitude of the FID signal, f_0: the resonant frequency of the sample at a given temperature and T_2^*: the spin-spin relaxation time. For ammonium nitrate, f_0 and T_2^* are 423.6 kHz (at 27°C) and 6 ms, respectively [5, 6]. A frequency fluctuation and a phase shift are added to mimic real situations where a temperature fluctuation may present. Δf and ϕ are the amplitude of the frequency fluctuation and the phase shift, respectively and *rand* is a uniformly distributed random number between -1 and 1.

Electrical noises from a fast analog input of a Red-Pitaya board (STEMlab 125-14) are acquired when the port is connected to a 50-ohm plug. The sampling rate is set to 1.953 MHz, about 4.6 times of the resonant frequency 423.6 kHz. Each set of acquired noises has 16384 samples (limited by the 16K-buffer size of the board) which results in an acquisition interval of 8.389 ms. 1000 sets of noises are collected as a noise bank for the simulations.

To simulate an NQR signal $S(t)$ acquired from the Red-Pitaya board, we add a set of noise randomly taken from the noise bank to the signal, $S(t) = FID(t) + noise$. The added noise together with the frequency fluctuation and the phase shift lower the signal-to-noise ratio (SNR) of a single acquired signal. The SNR is improved by averaging the signals from multiple measurements. The SNR is defined in the frequency domain as in [2]. We calculate the fast Fourier transform FFT of the average signal $S_{av}(t)$ obtain from n simulated measurements and the signal level is taken as the magnitude of FFT at the resonant frequency f_0, namely the NQR peak. Similarly, the noise level is estimated from the same n measurements (without FID signals) but it is defined as the maximal peak (the noise peak) in f_0 ± 2kHz of the resonant frequency.

3. Results

Examples of signals in time domain and the corresponding FFT are shown in figure 1. An electronic noise, acquired by a fast analog input of the Red-Pitaya board, fluctuate roughly between -0.4 and 1.0 mV during the interval of 8.389 ms and it is composed of many frequencies around the NQR frequency, figures 1(a) and 1(a′). A pure FID signal $S(t)$ with amplitude of 10 μV has a clear FFT, figures 1(b) and 1(b′). When the noise is added to the signal, its SNR is quite low (~1.7) so the NQR peak (at 423.6 kHz) and the noise peak are difficult to be distinguished, figures 1(c) and 1(c′). After the measurement is repeated 10 times, the average signal $S_{av}(t)$ has a better SNR (~5.7) so the NQR peak is much higher than the noise peak, figures 1(d) and 1(d′).

To illustrate the influence of the amplitude of FID signal, on the SNR, we perform simulations with different values of A in equation (1) while the frequency fluctuation and the phase shift are not added, i.e., both Δf and ϕ are set to zeros. As ones can expected, in the presence of given noises from the Red-Pitaya board the SNR increases with the FID amplitude A. We search for a sufficient repetition number N of measurements to improve the signal quality until the SNR reach to 5 - 10.

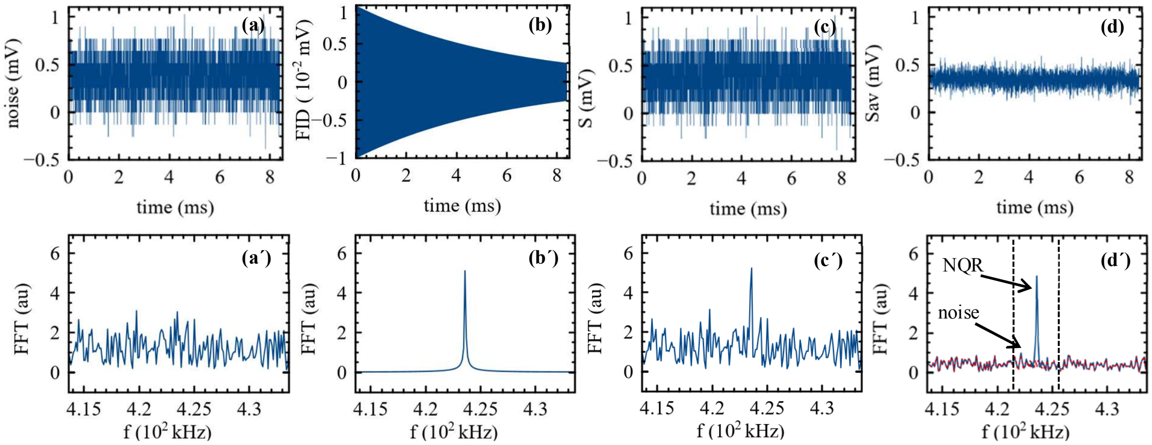

Figure 1. Examples of signals and their FFT. (a - a′) An electronic noise from a fast analog input of the Red-Pitaya board, (b - b′) an FID signal with amplitude of 10 μV, (c - c′) the signal with added noise $S(t)$, and (d - d′) the average signal $S_{av}(t)$ from 10 measurements. In (d′), the dashed line corresponds to the average of 10 sets of noise (without FID signals) and the vertical dot lines, depict the ±2kHz zone around the resonant frequency.

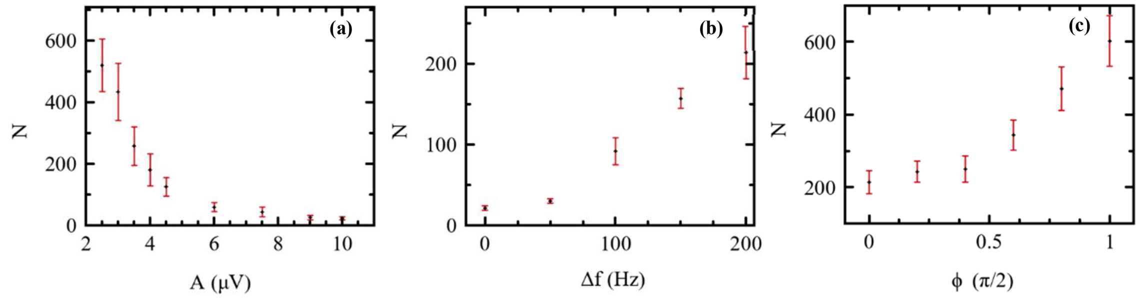

Figure 2. Repetition number N of measurements to reach the required SNR of 5 - 10 as functions of (a) amplitude A of FID, (b) amplitude Δf of frequency fluctuation, and (c) amplitude ϕ of phase shift. Each value of N is the average value obtained from 10 sets of experiments and the corresponding error bar shows the standard deviation.

To ensure that we get an appropriate approximation of N for each case of A, 10 sets of experiments are performed. For each experiment, a set of the repetition number n, that results in SNR 5 - 10, is collected. The average of 10 sets of n is taken as N and its standard deviation is also calculated. As shown in figure 2(a), N monotonously decreases when A increases. For very low A between 2.5 and 5.0 μV, N drops very fast. However, A gradually changes for 6 - 10 μV. In cases of high amplitude, $A > 50$ μV (data not shown), the SNR from a single measurement is sufficiently high (SNR > 10) so the repetition of measurements is not required.

Figure 2(b) shows the influence of the frequency fluctuation on the repetition number N of measurements. Note that the temperature coefficient for frequency of ammonium nitrate molecule is 91 Hz/K[6], thus the frequency fluctuation Δf is varied from 0 - 200 Hz to mimic a temperature fluctuation of about ±2°C during measurements. The amplitude A of FID is kept constant at 10 μV, the largest A in figure 2(a) and the phase shift is not added. These results shows that even for such high amplitude A, the repetition number N increases very fast as the amplitude Δf grows.

Figure 2(c) shows that one needs even larger N if phase shifts occur between the repeated measurements. This graph results from simulation with strong FID amplitude A = 10 μV and high frequency fluctuations Δf = 200 Hz. This graph shows that N grows with a very high rate for $\phi > \pi/4$. The maximal amplitude $\phi = \pi/2$ (the random phase shifts ranging between $-\pi/2$ and $\pi/2$) causes the number N increasing about 3 times in comparison to the case of no phase shifts $\phi = 0$.

4. Conclusion and discussion

We have demonstrated that averaging signals from repeat measurements could improve the SNR of the simulated NQR signals in a presence of electronic noise at Red-Pitaya board input. The method has been tested for different situations of signal amplitude, frequency fluctuation, and phase shift. In cases of low signal amplitudes or high frequency fluctuations as well as large phase shifts, one needs more repeat measurements to obtain a desired SNR.

We consider possible values of amplitude, frequency fluctuation and phase shift in real situations as follows. Typical NQR detection setups mainly consist of an NQR console, a transceiver unit, signal amplifiers, noise filters, a battery, and a probe. The amplitude of NQR signal depends on various parameters including the sample size, the sample-probe distance, and the gain of the electronic amplifiers. Based on an analysis in [10], the amplitude of amplified NQR signal reaching the console (e.g., a Red-Pitaya board) is in the order of μV. Concerning the frequency fluctuation, it has been shown that the NQR detection interval ranges from several seconds to minutes depending on the used pulse sequence type [6]. During such a detection interval, the temperature fluctuation of the sample under investigated is expected to be less than ±2°C so that the frequency fluctuation is possibly less than ±200 Hz in the case of ammonium nitrate. The phase shift depends on the timing of RF pulse excitations and NQR acquisitions which controlled by NQR console. Using the Red-Pitaya board as NQR console with the sampling frequency of 1.953 MHz, the resonant frequency of 423.6 kHz (at 27°C) and a given acquisition mismatch of ±0.5μs (i.e., the delay time between adjacent sampling points), the possible phase shift is about 0.43π radians. These considerations show that the ranges of amplitude, frequency fluctuation and phase shift of our study in figure 2 roughly correspond to those in real situations. Therefore, we expect that our simulation results can be utilized as a guideline for explosive detections.

Acknowledgments

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