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Aplicability of TNT "super-Q detection" to multipulse sequences

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The use of high-Q probes to increase the sensitivity in NMR and NQR is a well-known technique, however very high Q values are associated with several limitations. This paper explores the ^{14}N NQR multipulse detection of trinitrotoluene (TNT) signal-to-noise ratio as a function of the pickup coil Q factor, with a particular emphasis on the "super-Q" regime, where probe bandwidth becomes narrower than the NQR linewidths. We have used a mixed experimental–theoretical approach to find the TNT Q-dependent signal-to-noise value which avoided the inconvenient construction of a probe at every Q. The process has been repeated for a range of excitation/detection frequencies and a 2D sensitivity map was obtained. Our analysis suggests, that sensitivity is maximum and practically Q-independent when $400 < Q < 4000$. However, because the conflicting requirements of the SLSE excitation and the "super-Q" detection, only a gain of ~ 6 dB is obtained compared to a conventional $Q \sim 100$ coil.

1. Introduction

One of the basic techniques to increase the sensitivity in nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) is the use of a high-Q probe [1] consisting of a tuned pickup coil with a high quality factor Q, where the underlying assumption is sensitivity scaling with $\sqrt{Q}$. However, there is a practical limit of increasing Q beyond any measure, which is determined by the high-Q probe limitations. First, a high-Q probe has a very long dead-time, typically an order of magnitude longer than its characteristic time constant

$$\tau_c = \frac{Q}{\omega_0}, \tag{1}$$

where ω_0 is the excitation/detection frequency. The problem is very pronounced at low ω_0 and remedies in the form of active damping just after the RF pulse [2,3] are quite complicated. Second, the probe bandwidth is proportional to ω_0/Q and becomes very narrow at high Q, eventually, in the "super-Q" limit [4] even narrower than the resonance line under investigation. This results in a severe lineshape distortion. And finally, a high-Q probe is not easy to build. Conventional solenoid coils at RF frequencies have Q's around 100 [5]. This value can be optimized by an appropriate coil geometry, but the increase is modest. Another option, suitable only for low frequencies, is the use of a Litz wire, which increases Q by roughly a factor of two. Coils with a higher Q can be obtained with a superconductor [6,7], but with obvious difficulties.

There are however applications where the intrinsic sensitivity is so low, that dealing with the above nuisances can be acceptable. One of these is certainly the detection of explosives by ^{14}N NQR [8,9]. The set of the NQR frequencies, which is defined by the electric field gradients at the site of ^{14}N nuclei in the sample, serves here as a unique fingerprint to identify the material. Unfortunately, these frequencies tend to be very low, typically between 500 kHz and 5 MHz, resulting in a poor sensitivity. The already low sensitivity is then further reduced by the requirement of remote detection, e.g. the detection of buried landmines, or by a small filling factor, e.g. detection of explosives hidden in luggage. Nevertheless, the necessity for a reliable detection has in recent years seen the development of several techniques with enhanced sensitivity for NQR detection of explosives [10–20].

One of the recently investigated methods suitable for the detection of trinitrotoluene (TNT) is a combination of a multipulse sequence for excitation/detection and a matched filter (MF) [12]. The benefit of using a MF is its simplicity, which provides an easy way to optimize the detection sensitivity. For example, it was here predicted and experimentally confirmed that a spin-lock spin-echo (SLSE) pulse sequence [21]

$$90^\circ_{\pm y} - (\underbrace{\tau - 90^\circ_x - \tau}_{t_{\rm seg}})_N \tag{2}$$

with a short repetition time $t_{\rm seg}$ and consequently a low spectral resolution, produces a much higher sensitivity compared to a simi-

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lar detection with a longer t_{seg} and a high spectral resolution. Nevertheless, TNT NQR detection still requires further enhancements. A promising direction seems to be the "super-Q" detection [4], which we are exploring in this article.

We are confronted with two principal difficulties when "super-Q" detection is applied to TNT: the first is related to multiple closely spaced resonance lines in TNT, while the second to the short available acquisition time which is imposed by the multipulse sequence. Whereas closely spaced resonance lines can be considered only as a nuisance of finding the frequency yielding the best sensitivity, the short acquisition time severely undermines one of the key requirements for the effectiveness of the "super-Q" detection; acquisition time substantially longer than τ_c. Because the construction of a "super-Q" probe is difficult, we first decided to estimate whether the sensitivity of a TNT multipulse "super-Q" detection is improved compared to a conventional detection and if the improvement is large enough to warrant the development of such a probe.

The paper is organized as follows: in Section 2 we first overview the principles behind a "super-Q" detection on an exponentially decaying signal. In the next step we extend the analysis to include the off-resonance excitation/acquisition and multipulse excitation with segmented acquisition, as appropriate for TNT. In the last part of this section we develop an algorithm to predict the TNT NQR response for an arbitrary Q probe from an experimentally obtained TNT response with a chosen low-Q probe. In Section 3 we present a two dimensional predicted TNT sensitivity $\omega_0 - Q$ map, which suggest the optimal range of Q values and frequencies for maximum detection sensitivity. We also discuss the feasibility of optimal probe construction. In Section 4 we summarize our conclusions.

2. "Super-Q detection

"Super-Q" detection is in NMR/NQR defined by a much narrower probe bandwidth compared to the intrinsic linewidth of the resonance line under the investigation. Because of this, the acquired signal at the spectrometer becomes a band-limited version of the induced signal in the pickup coil. However, at the same time the observed signal amplitude becomes much higher due to a high Q, and a net sensitivity increase is experienced. This effect will now be quantified for several model signals by assuming a very common NQR detection circuit [22] as presented in Fig. 1.

2.1. Model detection circuit

The primary detection element is a pickup coil with inductance L and resistance R, whose associated quality factor is $Q = \omega_0 L/R$. The precession of magnetization induces a voltage across the pickup coil which is here represented by a source $V_{in}(t)$ in series with the coil. The resistor thermal noise is represented by a voltage source $V_{th}(t)$, with $\overline{V_{th}^2(t)} = 4kTR\Delta\nu$, where $\Delta\nu$ is the bandwidth of interest. The probe, consisting of the pickup coil and the two capacitors C_t and C_m, has an overall impedance $Z(\omega)$ at frequency ω. The capacitors are used for matching purposes and are assumed as noiseless. The preamplifier is connected directly to the probe and is modeled with four elements [23,24]: an ideal amplifier with voltage gain G, a parallel current noise source $I_n(t)$, a series voltage noise source $V_n(t)$, and a noiseless input impedance Z_0. The quantities $Z_0, I_n(t)$, and $V_n(t)$ define the probe optimal $Z(\omega_0)$, where sensitivity is maximal. Here, the preamplifier noise factor F, defined by the ratio of its input and output signal-to-noise value, is minimal. In our case, F for uncorrelated noise sources is

$$F = 1 + \frac{\overline{V_n^2(t)} + \overline{I_n^2(t)} \mid Z(\omega_0)|^2}{4kT\Delta\nu \operatorname{Re}(Z(\omega_0))} \tag{3}$$

with a minimum value F_{min} when

$$Z(\omega_0) = \sqrt{\frac{\overline{V_n^2(t)}}{\overline{I_n^2(t)}}}. \tag{4}$$

The preamplifier and the probe are said to be noise matched. The other condition for optimal $Z(\omega_0)$ is maximum power transfer achieved when the preamplifier and the probe are impedance matched

$$Z(\omega_0) = Z_0^*. \tag{5}$$

In practice, the parameters $\overline{V_n^2(t)}, \overline{I_n^2(t)}$, and Z_0 can not be chosen independently so some compromise has to be made. For this analysis however, we will assume perfect noise matching as well as perfect impedance matching exactly at the excitation/detection frequency ω_0 so that

$$Z(\omega_0) = Z_0 = \sqrt{\frac{\overline{V_n^2(t)}}{\overline{I_n^2(t)}}}. \tag{6}$$

If the preamplifier gain is sufficiently high, then we can neglect all noise sources in subsequent stages and the compound noise is specified with a single parameter F_{min}, the preamplifier minimal noise factor or more commonly with its noise figure $NF = 10\log(F_{min})$.

2.2. Signal

The signal of interest $V_{sig}(t)$ is the voltage just before the ideal amplifier (see Fig. 1) and is related to the pickup coil voltage $V_{in}(t)$. In NMR/NQR the linewidths are usually much smaller than ω_0, so that to a good approximation the fast oscilating term $\exp(i\omega_0 t)$ can be removed with the introduction of $\widetilde{V}_{sig}(t)$ and $\widetilde{V}_{in}(t)$ via

$$V_{sig}(t) = \widetilde{V}_{sig}(t)\exp(i\omega_0 t) \tag{7}$$

$$V_{in}(t) = \widetilde{V}_{in}(t)\exp(i\omega_0 t). \tag{8}$$

The expression connecting the voltages $\widetilde{V}_{sig}(t)$ and $\widetilde{V}_{in}(t)$ simplifies to

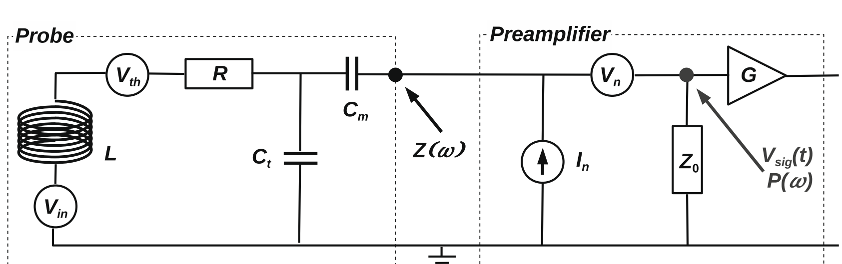

Fig. 1. Model detection circuit.