AVANCES
EN CIENCIAS E INGENIERÍAS
ARTÍCULO/ARTICLE **SECCIÓN/SECTION A**

Implementing a Quadrature NMR Spectrometer based on a passive RC splitter-combiner network

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Editado por/Edited by: Cesar Zambrano, Ph.D.
Recibido/Received:10/25/2011. Aceptado/Accepted:11/05/2011.
Publicado en línea/Published on Web:12/20/2011. Impreso/Printed:12/20/2011.

Abstract

The present article will explain in some details the requirements of modulators and demodulators using quadrature splitters and combiners, and discuss the target specifications for these devices. The architecture of a passive *RC* network, useable as a quadrature splitter/combiner is then introduced, the design choices are described, the results of simulations and tests are given. Then, we present a full characterization of some of our modulators and demodulators along with a tuning strategy which achieves an outstandingly accurate quadrature signal processing, and characterizes the error terms of the device at the same time.

Keywords. NMR Spectrometer, Quadrature Signal Processing.

Resumen

El presente artículo describe la arquitectura de un espectrómetro NMR en cuadratura, se identifican los componentes claves que marcan el límite entre los mundos analógico y digital. Se explican en detalle los requerimientos de un modulador y demodulador que usan splitters y combiners en cuadratura y se discuten las especificaciones necesarias para estos elementos. Se introduce la arquitectura de una red RC pasiva utilizada como splitter-combiner, se describen las decisiones tomadas en el diseño y se presentan los resultados de simulaciones y test. Para terminar se presenta una caracterización total de algunos moduladores y demoduladores junto con las estrategias de calibración las cuales alcanzan una altísima presición en el proceso de señales en Cuadratura y caracterizan al mismo tiempo los errores del sistema.

Palabras Clave. Espectrómetro RMN, Proceso de Señales en Cuadratura.

Introduction

Nuclear Magnetic Resonance spectroscopy is an analytical technique used by chemists to investigate the properties of organic molecules, though it is applicable to any kind of sample that contains nuclei possessing spin. In order to increase the performance of NMR spectrometers new signal processing techniques has been introduced over the years. Quadrature signal processing will be described below together with its application on NMR spectrometers

Conventional signal processing implements operations upon real-valued functions while quadrature signal processing is best described by complex functions. Frequency conversion, filtering, modulation and demodulation are basic operations which may be performed with quadrature devices. Radio-frequency spectroscopies (in particular NMR) contributed significantly to development of quadrature techniques and devices which now find their main applications in telecommunication systems, such as mobiles phones and satellite communications. Quadrature signal processing is performed in digital and/or analog ways.

Digital processing can be made nearly ideal, but it is limited in the bandwidths (or frequencies) that it can cover [1]. The bandwidth/frequency limit in the analog

ISSN 1390-5384

domain is in the 1010 Hz range (2 or 3 orders of magnitude above the typical digital limit), but usually, accuracy of analog quadrature devices is relatively poor, and their bandwidths are small fractions of central frequencies. As we will see later these limitations mostly arises from either the quadrature splitter or the combiner and, in the worst case, from both of them. The analog quadrature splitter generates the Hilbert pair of signals from a single signal in input; the combiner performs the reverse operation. Both of them are inherently narrow-band devices, to the difference of radio frequency components such as amplifiers, attenuators, 0^o power splitters, adders, multipliers which are inherently broadband.

The broadband heterodyne NMR spectrometer

Figure 1 shows the conceptual scheme of the historic heterodyne NMR spectrometer. In the transmitter side (TX) the LO and IF signals are mixed and filtered to obtain the RF irradiation. In the receiver (RX), the response signal RF'$\sim$ RF is first translated into the IF band and then converted to baseband [2]. The baseband low pass filter has often a small width; we may record its response while sweeping the excitation (RF) or the response RF' by changing B^o (continuous wave methods). If the excitation is a pulse of duration smaller than the inverse bandwidth of RF', we have two possibilities: recording the integral response, when RF' is in the middle of the RF' band, or recording the entire spectrum, when we make sure that it lies entirely above (RF'>RF) or below (RF'<RF) the excitation; in the last case, the cutoff frequency of the baseband filter should be at least equal to the full width of spectrum.

The scheme is simple and essentially broadband. For example, with an IF = 170 MHz, and a LO variable in the 20-200 MHz interval, we may easily cover the transmitter range 1-150 MHz with a 150 MHz low pass filter having a stop band at 50 dB beginning around 190 MHz, and the 190-370 MHz range with a high pass filter having a 150-190 MHz transition region [3]. The requirement of a pure transmitted signal may appear not necessary since the resonant circuit of the probe acts as a filter.

However, if a broadband amplifier is used, substantial amounts of power may be reflected back, which may damage the amplifier or reduce its performance. Furthermore, some types of excitations, as homodecoupling, may require a spurious-free dynamic range as high as 100 dB in the RF' interval.

In the receiver side, the 170 MHz bandpass filter in the IF section may be few MHz wide while the final receiver bandwidth should be set by the adjustable baseband filter. The IF frequency is a forbidden one for the system; in spectrometers working with a fixed magnetic field, the IF is usually set between the frequencies of ^{31}P and ^{19}F where only the resonances of ^{203}Tl and ^{205}Tl occur [2].

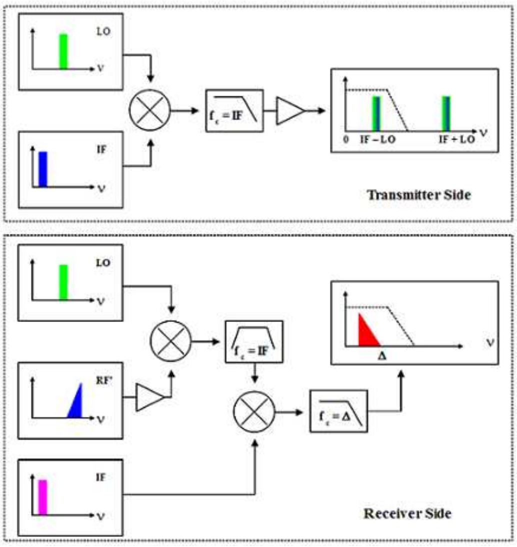

Figure 1: Block diagram of an Heterodyne NMR Spectrometer.

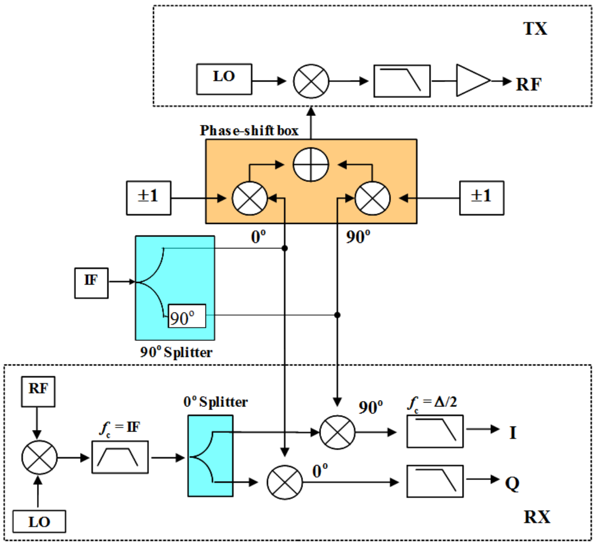

Figure 2: Block diagram of a quadrature NMR spectrometer.

The quadrature NMR spectrometer

Development of the NMR spectrometers over the past 30 years has spearheaded the introduction of quadrature techniques in the radiofrequency field. The classic scheme of a broadband spectrometer using these techniques in both the transmitter and receiver sides is a variation of the previous heterodyne spectrometer, (c.f. Figure 1).

The basic difference is a quadrature IF splitter which provides both the *cosine* and *sine* waves of the IF signal: IF (0^o) and IF (90^o). In the transmitter section, it is also shown a very simple phase-shift box, the so called quadraphase modulator, which permits changing the pha- se of the excitation in steps of 90^o. In the receiver section, after mixing with the LO and IF-filtering, the IF signal is equally split into two twins baseband converters, where it is mixed with IF 0^o and IF 90^o[4].

Relative to the previous design, the quadrature spectrometer has the following advantages:

- The phase of the excitation may be controlled in steps of 90^o, a feature required by most NMR experiments.
- The excitation may be placed in the center of the spectrum.
- The baseband filters may be set to half the spectral bandwidth, to Δ/2, rather than Δ, leading to a 3 dB gain in the signal-to-noise ratio (SNR). In fact, in the scheme of the heterodyne spectrometer, the noise comes from the – Δ, +Δ band while the entire signal is within only half of that band. In this case, instead, band of the noise and band of the signal are matched.

The disadvantages of this scheme are:

- Due to non-idealities, if the splitter is not well trimmed, and the two baseband converters are not exactly the same, ghosts are generated, i.e. a replica with reduced intensity, of the spectrum mirrored in the opposite side relative to the zero frequency.
- Every DC offset in the DC-coupled receiver yields a zero frequency spike.

Both these defects may be reduced by trimming, or suppressed by phase cycling. The tunable lowpass filters was cumbersome to build and added significantly to noise distortion. Today they may be replaced by their digital counterparts [5].

Blending new digital and analog signal processing technologies

After the quadrature spectrometer was conceived, the evolution in cost and performance of the analog components, driven by the telecommunication market, has been spectacular. Four quadrants multipliers, based upon Gilbert cells, are replacing the hybrid balanced mixers; inexpensive active components simplify impedance matching. Rather than filtering out the unwanted sidebands, it is becoming more convenient to use a single sideband mixer as the HPMX2001 from Hewlett Packard [6] schematically shown in Figure 3.

The two LO inputs accept frequencies up to 1.2 GHz; the modulation IF inputs go up to 700 MHz and are DC coupled. The narrowband part is usually the quadrature LO splitter, which is typically optimized over less than an octave. On the other hand, it seems natural to attain phase and amplitude modulation of the output by controlling the IF signals with digital techniques. An implication is that the IF signals should be, at most, in the 10^7 Hz range to allow high dynamic range (12 bits or more) digital signal processing.

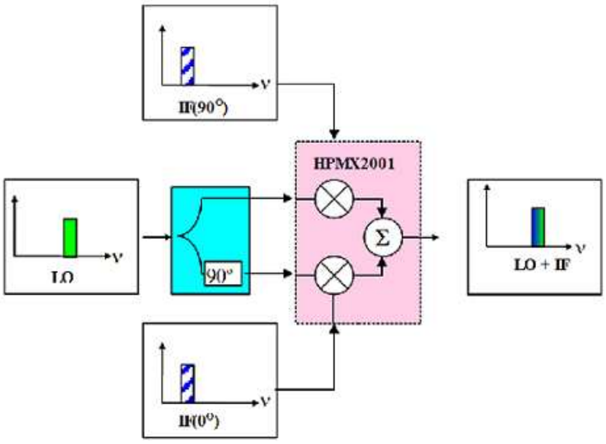

Figure 3: A transmitter scheme showing the Single Side Band Modulator (dashed box).

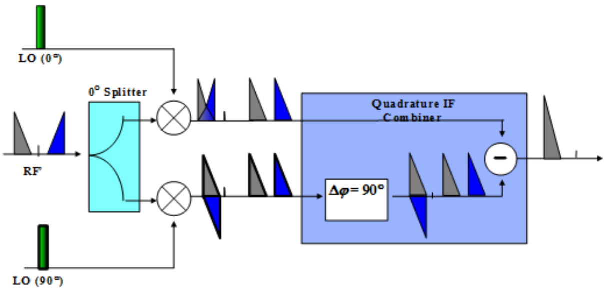

Figure 4: A band reject mixer, bold figures represent a 90^o out of phase.

In the analog portion of the receiver, quadrature techniques should be used to suppress the unwanted sideband arising from the LO-RF conversion. In fact, if the received signal is near LO-IF, also the noise at LO+IF would be converted into the IF band by a conventional mixer. The scheme of the band reject mixer (c.f. Figure 4) which suppresses the unwanted band and its noise is shown [7]. Here, the critical component is the quadrature IF combiner, and its figure of merit is the attenuation of the forbidden band relative to the allowed one. Obviously, such an attenuation will depend also upon the accuracy of the quadrature LO splitter.

After a proper bandpass filter, the IF signal should be digitized. The design of the Nyquist filter before the AD converter is not critical. For example, assume a sampling frequency of 10 MHz and require a flat response within 0.5 dB up to 3.5 MHz with an attenuation > 70 dB above 6.5 MHz; a 9 stages Butterworth filter will be enough. The high pass interference filter is even less critical, and selection of this cut-off frequency is mostly a matter of taste.

The baseband quadrature conversion of the IF signal, *S(t)*, can be performed digitally by mixing the digitized signal s_n, with two sequences of number representing the *cosine* and *sine* of the IF frequency [5]. Subsequent digital filters and decimators (DFD) achieve the desired receiver bandwidth and enhance the dynamic

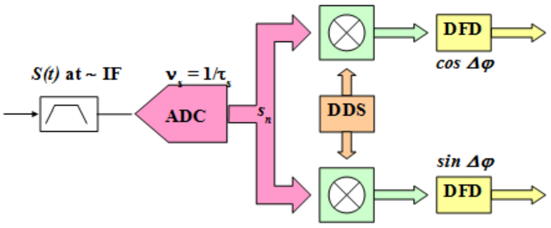

Figure 5: Block diagram of a Baseband quadrature converter.

range. The scheme of the digital quadrature detector is shown in Figure 5 [4].

A simple way to obtain the conversion is to set, $\Delta\psi = \pi/2$, which makes the multiplying numbers equal to ± 1 and 0. However, the full quadrature converter, including the quadrature Direct Digital Synthesizer (DDS), is now available as inexpensive single chips, which give an extra feature: user can choose the center frequency of conversion [8].

The Nyquist frequency of both data streams generated by sampling at 10 MHz is orders-of-magnitude larger than a typical high resolution spectrum. While the associated oversampling eases the design of the filter before the ADC and lowers the quantization noise floor (by spreading the quantization noise over a broader spectrum), it increases the requirements on the digital filter [9]. With an oversampling factor of 1000 and a 10^7 words/sec rate, we need about 10^{10} multiply & accumulate (MAC) operations per second to make a low-quality real-time Finite Impulse Response (FIR) filter. Since nowadays there is no way of accommodating the requirements of high quality narrowband filtering with a single-stage digital filter, more steps should be used. One of the possible configurations is the following:

- Averaging and decimating by *m*. The integrator should add at a υ_o = 10 MHz rate, which is easily achievable even with discrete TTL circuits.
- FIR filtering the output of the integrator followed by decimation to the desired bandwidth. This decimation should be of the order of ten, or larger, in order to achieve an acceptable integrator response, in terms of flatness and aliasing noise, it's verified only when the cutt-off frequency is about ten times smaller than the Nyquist frequency of the input streams.

The digital quadrature receiver has the following advantages over its analog counterpart:

- Since *S(t)* is AC coupled, analog DC offsets do not matter, and digital offsets are easily handled.
- No ghosts are generated because the two digital channels are identical by design and IF signals are perfectly in quadrature.

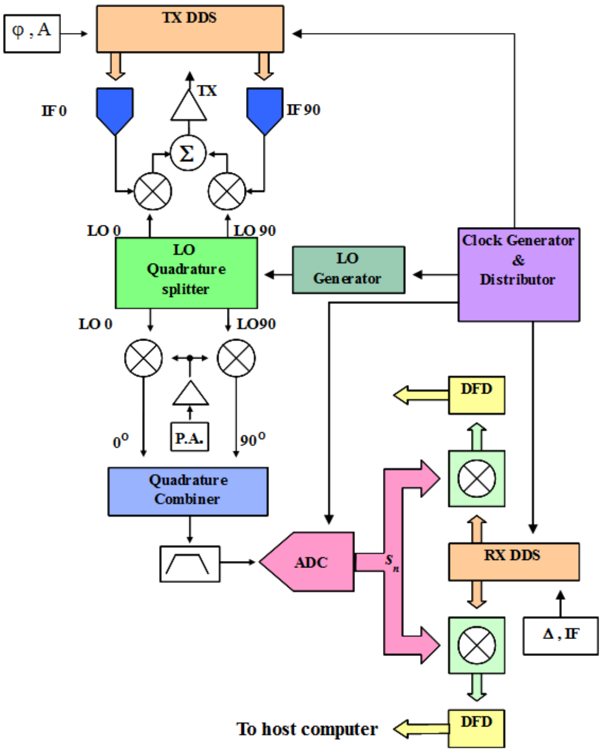

Figure 6: Block Diagram of a universal NMR transceiver.

- Quantization noise may, in principle, be reduced at will through oversampling, and the broadband nature of the fast ADC provides plenty of beneficial off band dithering noise; the digital system from the ADC on, may made nearly ideal [10].

Requirements and basic architecture of a universal NMR transceiver

Figure 6 shows a block diagram of an universal transceiver. TX is the signal to the power amplifier, PA is the signal from the preamplifier at the beginning of the receiver chain. No filter has been made before TX: the requirement is that the single sideband modulator should be able to suppress carrier and forbidden sideband by at least 50 dB and that the spurious-free region around RF is at least IF wide. The LO generator should be a source with very low phase noise (e.g.,-110 dB at 1 kHz), and the contribution of the clock to the ADC jitter should be negligible. The LO phase noise and clock jitter are the major sources of receiver noise.

In the receiver side, the combination of the LO splitter and quadrature combiner should suppress the unwanted sideband by more than 20 dB over the full LO range, and yield IF signals over more than a decade, from, say, 1 MHz to 30 MHz. The ADC should always work in the oversampling mode, with an input analog noise always larger than the least significant bit.

The DDS for digital baseband conversion has been represented separated from the one of the transmitter, while a superheterodyne spectrometer requires a unique IF source. One reason is that it is quite simple to synchronize

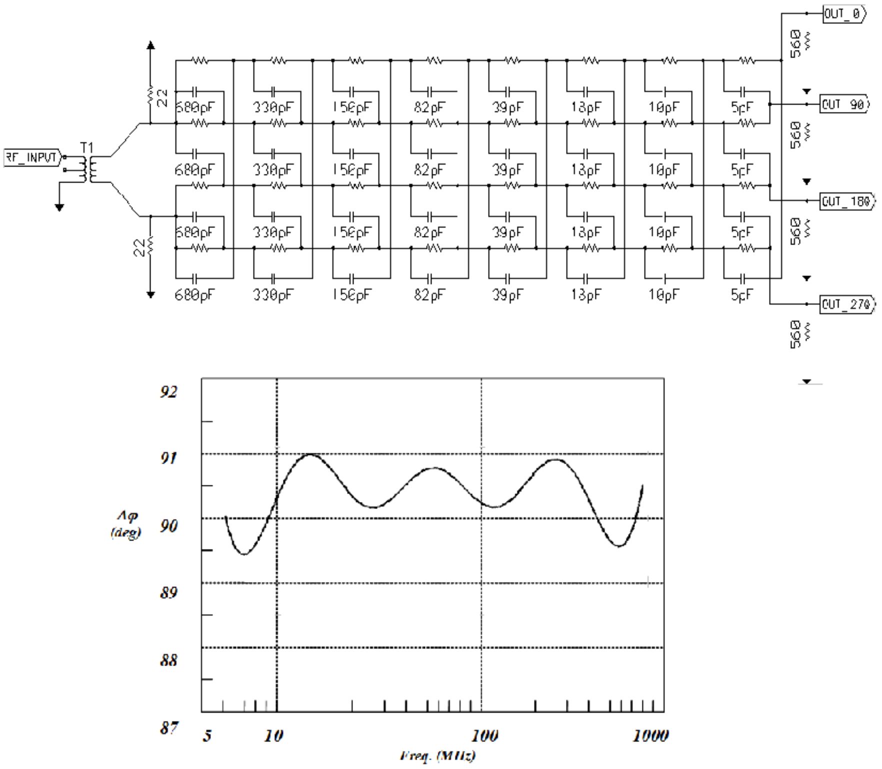

Figure 7: (a) Schematic of an 8-stages RC network, all R = 50 Ω and (b) Simulated response of the RC network (using Sigma Plot).

two digital oscillators, but quite difficult to bring many digital high speed signals from board to board.

Another reason is that the DDS often comes with the digital quadrature detector, and it may be desirable to irradiate at a different frequency relative to detection. Yet another reason is that a system with transmitter and receiver working simultaneously, rather than in time sharing, may be desirable, since it allows both continuous wave and pulse experiments to be performed.

The transceiver works with relatively low IF frequencies and has a “hole” near IF in the sense that the prescribed suppression of carriers and modulators may not be enough, for some applications, when LO-IF (i.e., the RF) is near IF.

Two possible schemes may be proposed:

- Fixed IF frequency of the receiver. By sampling at $\upsilon_0 = 4$IF we have the possibility of integer down conversion (as hinted above), but we need a high resolution LO generator to fine tune the position of the center of the receiver. On the other hand, the transmitter DDS may be set independently, and the frequency of excitation may be changed within the Nyquist limit of this DDS. The “hole” near IF is unavoidable.
- Adjustable DDS frequencies in the receiver and the transmitter. In this case, a coarse LO generator with large steps (say, 1 MHz or 10 MHz) may be used since the fine tuning of frequencies may be performed with the two DDS. The hole may be avoided (or shifted), and a broadband lock system may be implemented in this way.

Methodology

Besides the underlying control system, the only parts which are not commercially available in Figure 6 are the broadband LO quadrature splitter, working from IF + 1MHz to 1000 MHz, and the quadrature IF combiner, working from IF$_{min}$ – 1.5 MHz to IF$_{max}$+1.5 MHz. To obtain these broadband designs a specialized passive device has been studied, the so called *RC* network, which has been previously investigated by Halamek et al. [4]. The *RC* network consists of sections each consisting of a ring of four equal resistors and four equal capacitors. With *n*- sections having *RC* time constants organized according to a divide by two rule, roughly *n* octaves may be covered. Figure 7 (a) shows the schematics and Figure 7(b) the simulation of an eight sections *RC* network, which shows that the phase difference between the two outputs (0-180^o) and (90-270^o) is 90 $\pm$ 1^o from 5 to 700 MHz.

Implementation of this design requires a careful consideration of line transmission and impedance matching effects. After many attempts with home-made impedance transformers, a commercial balun-transformer in the input (Minicircuits T 1-1) [11] has been adopted, which brings the 50 Ω impedance of the single ended LO input

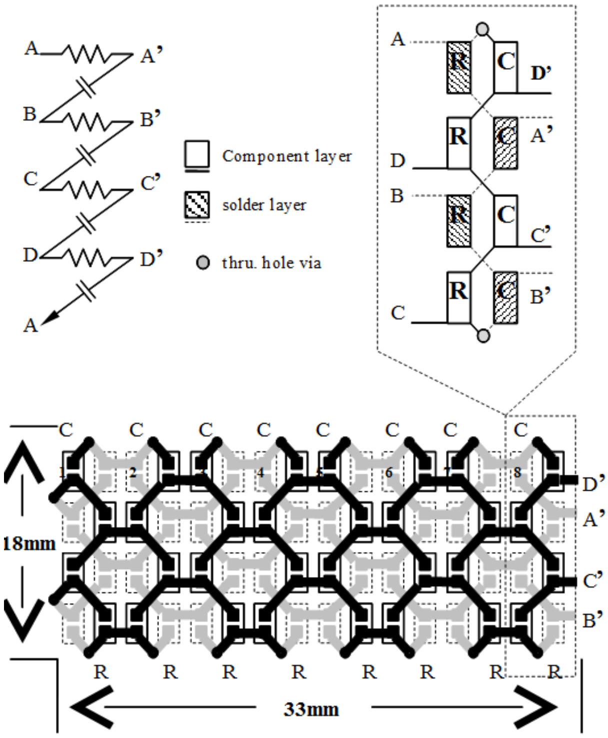

Figure 8: Physical Layout of the *RC* network

down to 12.5 Ω for each of the bipolar inputs, in order to achieve a rough impedance matching at the highest frequencies of the band. The four outputs should ideally be connected with a high impedance source, which has been set equal to 500 Ω in the simulation.

The physical layout is shown in Figure 8. A two layers PCB with connecting vias to tread the cycle of a section in a fully symmetrical way has been used. Furthermore, small surface-mounted *R*'s and *C*'s (0805 and 1206 size) has been used to achieve the smallest physical dimensions compatible with manual assembly. The requirements of the combiner are similar, but it should be used in the reverse way. Unfortunately, the simulation indicates that a typical 18 dB attenuation should be expected even with a 4 section /4 octaves device. To limit such an attenuation, the *RC* combiner consists of only 4 sections with a nominal range 0.5-8 MHz (or 2-32 MHz).

Results and Discussion

Test performed on prototypes indicate that the *RC* splitter-combiner is a viable solution for building a truly broadband and universal NMR transceiver. However, it is mandatory to introduce trimming possibilities to improve the selectivity of the receiver in the bands where it is marginally acceptable. Furthermore, the *RC* network needs a long assembly time; it is also very difficult to identify a bad connection or a wrongly placed component.

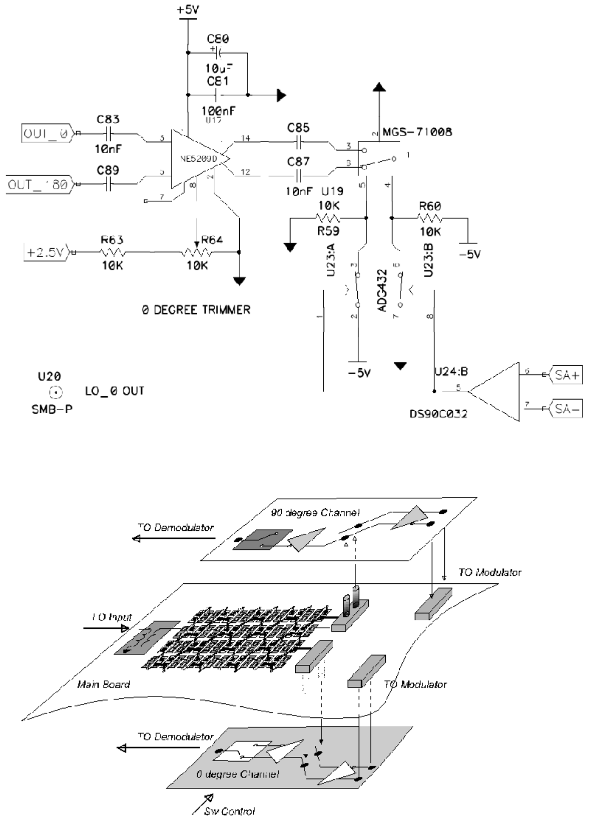

Figure 9: (a) Schematic of a variable amplifier based on NE529 (b) Physical and assembly layout.

A solution of the above mentioned issues is illustrated in Figure 9 (a). Each couple of outputs, 0 - 180^o and 90 - 270^o, of the *RC* network has been sent simultaneously to two variable differential amplifiers, the NE 5209, which has input impedances in the k Ω range.

A very special layout had to be chosen, with three PCB's piled one on top of the other to maintain the distances short and the traces symmetric to avoid transmission delay problems (c.f. Figure 9 (b)).

Figures 10 (a) and (b) give the amplitude and the phase errors of the splitter & modulator measured through the IF trimming parameters. This time the amplitude errors remain below 3% and the overall phase error is larger than 3^o only above 500 MHz, as it may have been expected.

The lines which go to the receiver may be trimmed in amplitude and two absorptive switches allow to select various combinations of positive and negative LO signals. The main purpose of these switches is to allow selection of the upper or lower sideband by selecting which of the two channels (A of B) follows by 90^o the other. Another purpose was to provide an alternative testing of the accuracy of the splitter by measuring the signal resulting by adding free induction signals acquired with the receiver LO phase-cycled with a 180^o step.

The results of testing are shown in Figure 10(a), (b) and (c). Figure 11 shows the DC offset values needed to achieve the same amplitude of LO signals at the input

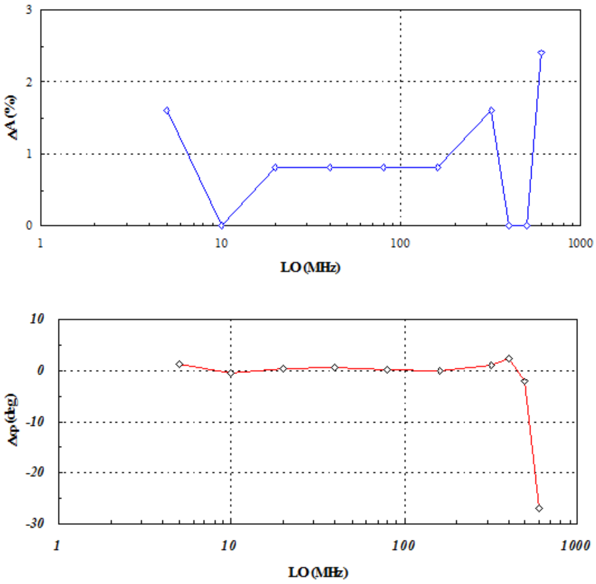

Figure 10: Amplitude (a) and Phase (b) as a function of frequency in *RC* network.

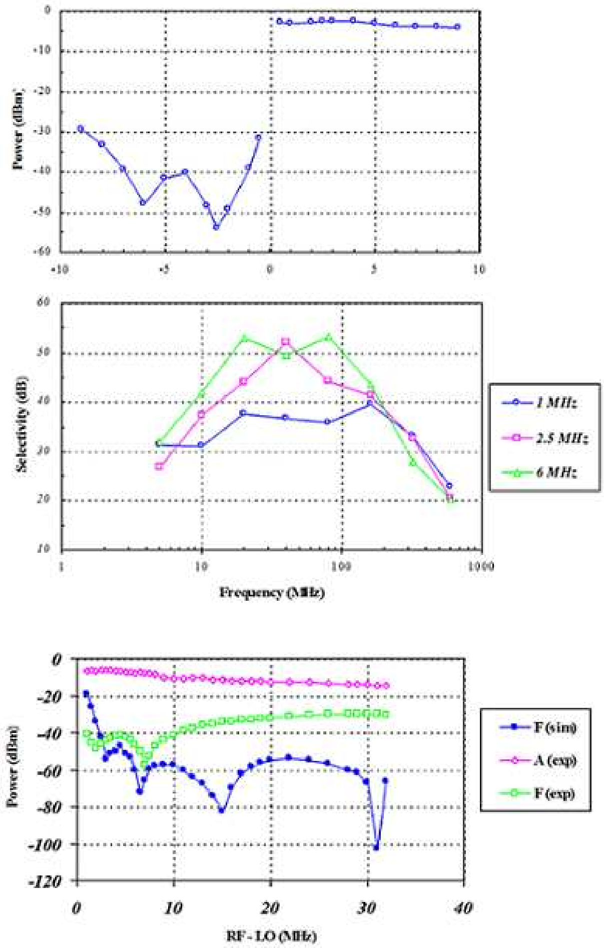

Figure 11: (a) Forbidden Band suppression and (b) selectivity of the receiver (c) Simulated versus experimental response.

of Single Side band Modulator; Figure 10 (b) shows selectivity using the same receiver circuit as below. Over most of the range, selectivity is above 30 dB and the response curve is essentially flat over the 0.5-9 MHz interval. As expected from the results obtained from the modulator section, amplitude trimming was minimal. The sideband switching behaved as expected.

Conclusions

This work demonstrates that a *Universal NMR transceiver* is possible thanks to a broadband *RC* splitter/combiner circuit. With some care, we have shown that this circuit may operate near 1 GHz, which we believe to be roughly the limit of a manually assembled, lumped elements version. Simple trimming procedures have been described which essentially cancel out the effects of imperfect quadrature processing, and lead to an accurate evaluation of these errors. Furthermore, the setting of these digitally controlled trimmers does not interfere with I&Q modulation, which may be programmed in the same way for all working frequencies.

We have shown that a quadrature modulator may achieve exceptional spectral purities over decades of working frequencies if appropriate trimming schemes are implemented. A consequence is that the quality of signal processing becomes essentially a function of the LO signal and the digital clock. In the case of NMR, LO signals with good coherence and exceptional phase noise specifications are needed. In fact, in the transmitter side, we may need to achieve a spurious free range larger than 100 dB over the entire spectrum of interest, which has typical width much smaller than our IF's (and does not include LO or forbidden sideband); in the receiver side, the LO phase noise contributes to the noise figure, and extremely "pure signals are needed.

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