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Analog Filtering of Large Solvent Signals for Improved Dynamic Range in High-Resolution NMR

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The large solvent signal from samples in H_2O solvent still challenges the dynamic range capability of any spectrometer. The solvent signal can be largely removed with a pair of simple resistor–capacitor (*RC*) high-pass filters when the solvent frequency is set at center band (zero frequency) using quadrature detection, with *RC* ∼ 0.5 ms. However, an ∼0.5-ms transient remains at initial time, which we reduce fourfold for a short time only, just before the A/D converter, by means of a variable-gain amplifier, and later restore with software. This modification can result in a nearly fourfold increase in dynamic range. When we converted to a frequency-shifted mode (A. G. Redfield and S. D. Kunz, 1994, *J. Magn. Reson. A* 108, 234–237) we replaced the *RC* high-pass filter with a quadrature feedback notch filter tuned to the solvent frequency (5.06 kHz). This filter is an example of a class of two-input/two-output filters which maintain the spectral integrity (image-free character) of quadrature signals. Digital filters of the same type are also considered briefly. We discuss the implications of these ideas for spectrometer input design, including schemes for elimination of radiation damping, and effects of probe bandwidth on extreme oversampling. © 1998 Academic Press

Key Words: **quadrature; feedback; analog; solvent; dynamic range.**

I. INTRODUCTION

In the context of NMR, dynamic range means the ability of an NMR instrument to cope with large signals while not adding extra noise above input thermal noise. Most often such signals arise from the single large solvent H_2O signal in aqueous samples. The spectrometer must be able to deal with such signals without requiring that the gain of the detector amplifier stages be set so low that the noise introduced by the analog-to-digital converter (ADC), at the input to the computer, contributes significantly to overall noise. Apparently, this means that input noise that is amplified, frequency-converted, and filtered must have an amplitude at the input to the ADC that is somewhat greater than the input voltage increment that makes the ADC digital output change by one unit (*1, 2*). Since the H_2O signal is typically more than 2^{16} times the thermal noise, a 16-bit ADC does not have the dynamic range required to handle it.

The need for high dynamic range is diminished considerably by the use of well-known methods for reducing the solvent signal (*3–5*), including selective pulses (*6*), solvent presaturation, and use of gradients and flip-back pulses with isotope-labeled samples (*7*). Nevertheless, it is always useful to improve the dynamic range of a spectrometer provided that it can be done without increasing difficulty of operation, if only for the purpose of increasing convenience and productivity.

Here we discuss a method of increasing dynamic range for most types of proton NMR, based on analog filtering, which has not been described previously to our knowledge except as a preliminary unevaluated proposal (*8*). We then describe this method in the context of oversampling combined with carrier shift, as described in a previous article (*1*) which we refer to as RK1. Oversampling refers to the use of an ADC sampling rate that is considerably greater than the minimum rate needed to faithfully extract the spectrum from the free induction decay (FID), as commonly expressed by the Nyquist criterion.

We are concerned only with improvements in dynamic range that might be achieved by modification of the receiver signal chain, ADC, and computer treatment. Therefore, we discuss only changes in dynamic range in the form of changes relative to typical current practice, namely use of a 500-MHz spectrometer with a 16-bit ADC set to observe a 10-kHz (20 ppm) spectral width. In this case 10,000 samples per second are required, usually in the form of 5000 complex quadrature pairs of samples per second. The dynamic range would improve by a factor of 2 for each extra bit of ADC precision if the ADC has no sources of error other than the digitization round-off error resulting from representing the input continuous voltage by an integer. We will evaluate various strategies below as improvements in dynamic range relative to this standard, in the form of a ratio, or its base 2 logarithm stated as bits of increased A/D resolution that would yield the same performance.

The ADC in any spectrometer is always preceded by an analog antialiasing filter whose width is approximately equal to half the sampling rate (or to the rate of quadrature pairs

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of samples per second). This filter takes the form of two closely matched low-pass filters which cut off at half the sampling rate, or 5 kHz for the example above. Since positive and negative frequencies are distinguished by quadrature detection, the effective width is twice the width of each filter, or 10 kHz.

For those unfamiliar with oversampling, it can be easily explained as follows: increasing the spectrometer output filter width to 40 kHz increases the noise power by 4, and its root mean square amplitude by $\sqrt{4}$, allowing the receiver gain to be decreased by 2 while maintaining the same noise level at the ADC input and achieving greater dynamic range by a factor of 2, or one bit equivalent of ADC resolution. In order to avoid aliasing out-of-band noise into the spectrum, the sampling rate also must be increased by a factor of 4, and, for the same frequency resolution, the number of data points recorded in the computer memory must likewise be quadrupled. Oversampling in this way can be performed on any NMR spectrometer, but is not always done because the increase in memory storage and computation time is a nuisance, and the resulting increase in dynamic range is modest. As the reasoning above indicates, the increase in dynamic range is proportional to the square root of the increase in spectral width and sampling rate (*2*). These problems can be alleviated by digital filtering and decimation-in-time as described in RK1. Such decimation could be usefully performed on-line or off-line by most standard spectrometers, but is much easier to perform using a digital signal processor and associated memory as a buffer between the ADC and the computer. These features are now increasingly available in commercial instruments. Oversampling and digital filtering are widely believed to yield improved baselines, a topic which we will not discuss. The filters described in the present article have no effect on baseline roll.

The following section describes a simple instrument modification for increasing dynamic range for samples in H_2O for instruments that use the mode of data collection with the H_2O signal at center band. In Section III we present a way to achieve the same result when the center frequency is shifted away from zero, as described in RK1, and Section IV extends the previous ideas to digital filters. Some of these sections are technical and might be skimmed by the general reader. Section V concludes with a brief discussion of various architectural variants of the recently dominant type of instrument.

II. HIGH-PASS ANALOG FILTERING

An obvious way to reduce a strong solvent signal is to remove it with an analog filter. In the usual mode of operation the water resonance is placed at zero frequency, and it is then trivial to put a high-pass filter of the type shown in Fig. 1 in series with each of the two antialiasing filters. We use a time constant *RC* equal to 0.5 ms resulting in reduction

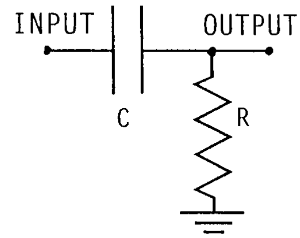

FIG. 1. High-pass filter. Two filters like this are used, fed from conventional antialiasing filters which have zero output impedance, and feeding the separate ADC track/hold circuits which have infinite impedance. The time constants *RC* of the two filters must be matched, but not as carefully as for the antialiasing filters because mismatch will give quadrature images only close to zero frequency. The filters are disabled by a manual switch which shorts the capacitors.

of signals of 30% or more within 300 Hz of the water resonance. The filter introduces phase and amplitude distortion of the form

$$G = 1/(1 - i(\omega RC)^{-1}), \qquad [1]$$

where ω is the angular frequency difference between the water frequency and the resonance frequency and G is the complex gain of the filter pair, which is zero at the water frequency. This distortion could easily be computer corrected to within a few hertz of the water frequency, as would be desirable for experiments with ^{13}C-labeled proteins. Lines within 300 Hz of water can still be usefully observed, but with possible increased ADC noise as well as the phase shift indicated by Eq. [1], and interference from shoulders of the solvent resonance.

Such a modification does not by itself improve the dynamic range. As shown in Fig. 2, the first few points of the FID digitization, within 0.5 ms of the start of the FID, are still as large as the incoming signal, and overload of the ADC still occurs at the same gain level.

In order to be able to increase the gain and dynamic range using the filter we add another feature acting in cooperation with the high-pass filter described in Fig. 1. We add a ‘‘gain changer’’ circuit (*8*) that reduces the gain just before the A/D for a time of the order of the time constant *RC* of the filter (Fig. 1). To do this, we put a gain-programmable instrumentation amplifier after all the filters, and just before the A/D converter, to decrease the gain by a factor of 4 for the first N_g paints of the FID. This amplifier's gain is controlled by the ‘‘borrow’’ line of a preset counter, into which the number N_g is loaded from a hardware register before the start of the FID. The register in turn is loaded with the number N_g by the computer at the start of the run. This counter then counts down once on each digitization strobe and is inhibited by its own borrow line which also increases the instrumentation amplifier's gain by 4. To compensate for this gain change, the first incoming N_g points are

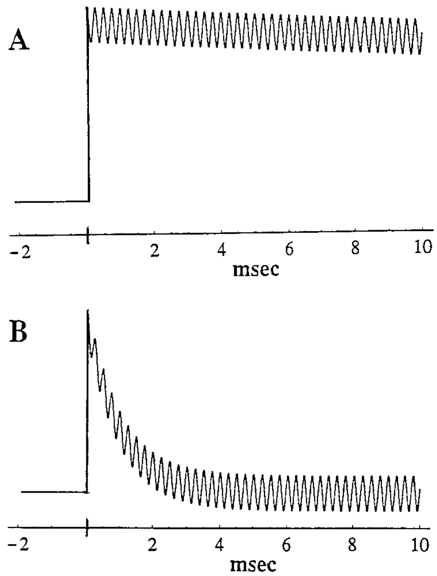

FIG. 2. (A) Typical input signal to one of the high-pass filters of Fig. 1, consisting of a large zero-frequency signal from water, added to a small high-frequency signal. The signal is zero for time less than zero, and only the first part is shown. (B) The signal after it has passed through the filter. The high-frequency signal is unchanged and the water signal is decreased over most of the FID, but it is still just as large at the beginning of the free induction decay.

multiplied by 4 in the computer before any processing of digital filtering takes place. If digital filtering is performed ‘‘on the fly’’ in order to time-decimate the data, rather than later, then this multiplication must be done on the fly also, before filtering and decimation. In our system the number N_g is generally set at a default value as indicated above, corresponding to the first 4 ms of digitization, or else it is set to zero if the high-pass filter is not needed, for example, in D_2O solvent. This implementation is hardly noticed by the user, since the spectrum appears similar with or without it, except that the receiver gain can generally be increased before overloading by about 4 (about 12 dB) compared to when the filter/gain changer is disabled. It is also noticeable, when unintentionally implemented, if the spectrum has only a small solvent signal and there are useful lines near the solvent, since these are dephased and attenuated in our system. Then the user has to realize that the filter/gain changer and corresponding software must be disabled. This implementation obviously does not take care of large proton signals such as spin echoes and radiation-damping signals that may arise more than 4 ms after the start of digitization. The programmed gain change described here could usefully be replaced by some sort of commercial or homemade automatic ranging A/D converter to take care of such signals. Baseline offset, and a baseline step when the gain is changed due to imperfection in the instrumentation amplifier, is eliminated by the 180° part of CYCLOPS phase cycling (*9*), or by most phase cyclings used in multidimensional NMR.

The first points of the FID are underdigitized in our implementation, increasing digital noise. The mean square digitizing noise for a 40-ms total digitizing time, of which the first 10% is digitized at 1/4 gain, is expected to be increased by a factor of $(0.1)(4^2) + 0.9 = 2.5$, compared to digitization noise with no gain change. The resulting increase in noise amplitude is $2.5^{1/2} = 1.6$, giving an increase in dynamic range of at least $4/1.6 = 2.5$. The values we use, of gain change amplitude (times 1/4) and time (4 ms), have not been optimized.

III. ANALOG FILTERING WITH A FREQUENCY-SHIFTED SIGNAL

In RK1 we described frequency shifting of the spectrometer frequency by 5.06 kHz, just before the start of digitization, mainly as a way to eliminate images and artifacts. In this way, the nuisance solvent signal was shifted from zero (center band) to 5.06 kHz. Obviously, the high-pass filter of Fig. 1 cannot then be used to filter the solvent. Instead we built an inherently quadrature filter circuit shown in Fig. 3. We know of no prior general discussion of this type of filter in the NMR or engineering literature. It is a ‘‘quadrature’’ filter in the sense that any monochromatic quadrature signal that is input to A_r and A_i results in a quadrature output at B_r and B_i. Stated formally, if $A_r = A_0\cos(\omega t)$ and $A_i = A_0\sin(\omega t)$, then the complex output $B_r + iB_i = B$ is given by $B = G(\omega)(A_r + iA_i)$, where $G(\omega)$ is the complex gain of the filter which is time independent. These equations define the term ‘‘monochromatic quadrature signal’’ used herein. The values of the input voltages A_r and A_i and the output voltages B_r and B_i are all real.

The usual pair of independent antialiasing filters found on all modern NMR machines form a quadrature filter if they are exactly matched in gain and phase shift for all frequencies. However, they always have the property that $G(\omega) = G(-\omega)^*$, where * denotes complex conjugate, so that G is real for zero frequency. On the other hand because of the feedback connections between channels, the filter of Fig. 3 does not have this property; G is nonreal for zero frequency, a fact which we need not discuss further but which the reader can verify.

The first stage of the filter (amplifiers 1 and 2 in Fig. 3) is a simple independent pair of low-pass antialiasing filters of the type mentioned just above, with half-cutoff frequency of 30 kHz, somewhat less than the complex digitization rate. This rate is now variable in our system, to produce a decimated spectral width compatible with data produced by our commercial instrument, but it is in the range of 40–60 kHz. A sharp-cutoff filter is not needed here because the NMR spectral range is small compared to 30 kHz for the samples we studied. The complex gain of amplifiers 1 and 2, defined as $G_a = (C_r + iC_i)/(A_r + iA_i)$, is

$$G_a = -1/(1 + i\omega RC_a). \quad [2]$$

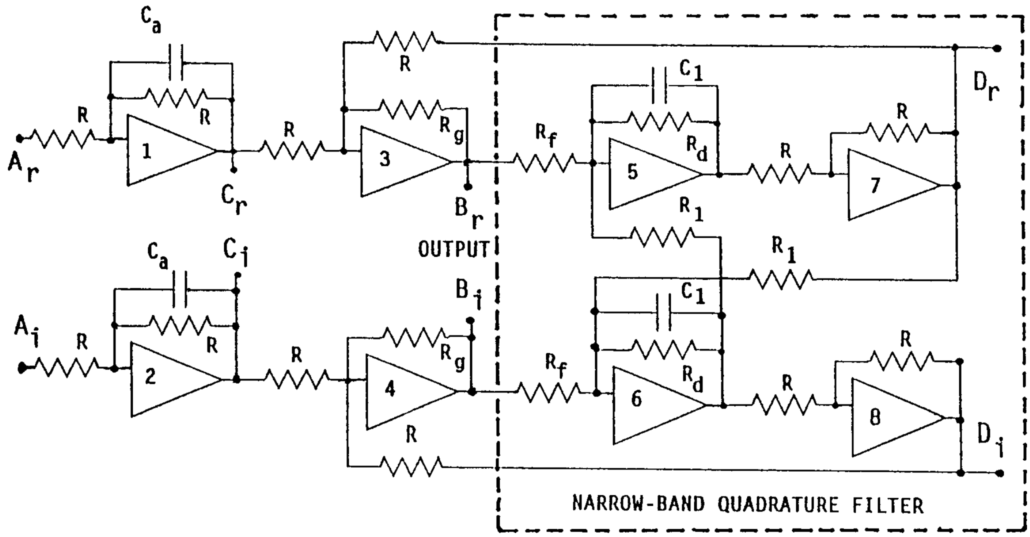

FIG. 3. Antialiasing and notch filter used for frequency-shifted operation. The dotted line delineates the section of the filter referred to in the text as the narrowband quadrature amplifier. Operational amplifiers are all Analog Devices OP27, and their grounded positive inputs are not shown. All resistors labeled R are 3.5 kΩ, and C_1, C_a, and R_f are .032 μf, 1360 pf, and 47 kΩ, respectively. The damping resistors R_d are omitted except for testing of the narrowband quadrature filter, when they are in the range of several hundred kΩ. The resistors R_g are adjustable from 15 to 16 kΩ to give equal gain for each channel far from the notch frequency, and resistors R_1 are adjustable between 1 and 2 kΩ, to determine the notch frequency. Not shown are 20-pf stabilizing capacitors across resistors R_g, and two low-pass *RC* input filters in series with each channel having time constants of 5 and 0.5 μs. Also not shown are relays which connect small (100 Ω) resistors across capacitors C_1, to disable the notch filtering when it is not needed.

The overall gain is G_aG_n, where G_n is the gain of the second state of the filter.

We will show that the second state of the filter in Fig. 3 is a notch filter which removes the positive frequency $\omega_1 = (R_1C_1)^{-1}$ and *not the negative frequency* ω_1. This filter would permit the spectrometer to observe lines undistorted at $-\omega_1$ while filtering out the solvent at $+\omega_1$; more important, it permits construction of the very simple filter of Fig. 3 to act as an arbitrarily narrow non-zero-frequency notch filter, for extension of the scheme described in Section II to non-zero solvent frequency. The output stage of the filter consists of the operational amplifiers 3 and 4, which are simple low-gain inverting amplifiers having gain $-R_g/R$, together with the complex feedback amplifier consisting of operational amplifiers 5, 6, 7, and 8 which is the block surrounded by the dotted line. Defining the gain of the latter block as $G_f = (D_r + iD_i)/(B_r + iB_i)$, or $G_f = D/B$, the overall notch filter gain is given by the usual feedback expressions for input gain $-R_g/R$ and feedback gain $-G_fR_g/R$:

$$B = -(R_g/R)(C + BG_f). \qquad [3]$$

Here we have implicitly assumed, from the notation used, that the filter inside the dotted line of Fig. 3 is a quadrature filter in the technical sense defined above; we will show this shortly. From Eq. [3], the gain of the entire second stage is

$$G_n = B/C = -[(R/R_g) + G_f]^{-1}. \qquad [4]$$

The feedback element, amplifiers 5 and 6 and the simple inverters 7 and 8, can be viewed as an analog computer which simulates a damped driven simple harmonic oscillator. It also simulates the transverse terms of the Bloch equations below saturation, or the Liouville equation for a density matrix coherence element in the limit of weak excitation. One of us constructed a filter of this type years ago, using vacuum-tube operational amplifiers, as a demonstration of the Bloch equations. We refer to it as a narrowband quadrature filter. Virtually the same filter, with only a single input, is described in detail by Lancaster (*10*), together with an interesting display of ''quadrature art'' obtained from it, and is called a biquad filter.

In quadrature notation we assume as usual an input to the block $B = (B_r + iB_i) = B_0e^{i\omega t}$ and that the output $D = (D_r + iD_i)$ is also monochromatic and quadrature, and of the form $D = (D_r + iD_i) = G_fB$, where G_f is the complex gain, and B_r, B_i, D_r and D_i are ordinary real signals. The behavior of the circuit is obtained by equating the current flowing into the inputs of amplifiers 5 and 6 to zero:

$$-C_1dD/dt - D(R_d^{-1} - iR_1^{-1}) + B/R_f = 0. \qquad [5]$$

The reader can verify that the real and imaginary parts of this equation give the correct input current-null equations for amplifiers 5 and 6 separately. The gain G_f is found immediately from the fact that $dD/dt = i\omega D$ which follows from the definition of the quadrature signal D. It is

$$G_f = D/B = (R_d/R_f)/\{1 + iR_dC_1(\omega - \omega_1)\}, \quad [6]$$

where the frequency ω_1 equals $(R_1C_1)^{-1}$. This is a narrowband filter with peak gain at the (real) frequency ω_1. Stimulated by a short pulse at its input, its response would be of the form $e^{i\omega_1 t}e^{-td}$, where $d = (R_dC_1)^{-1}$. It corresponds to a filter of $Q = R_d/R_f$ and it has no resonant response at negative frequency, unlike conventional pairs of separate narrowband filters.

In practice the damping resistor R_d is omitted in the final notch filter (Fig. 3). It is useful to include R_d for testing the behavior of the narrowband quadrature filter alone when its inputs are disconnected from the outputs of amplifiers 3 and 4. If $R_d \gg R_1$, then the outputs D show a nearly circular pattern on an oscilloscope x–y (real–imaginary) display even if the input is pure real ($B_r = B_0\cos(\omega t)$ and $B_i = 0$), when $\omega \cong \omega_1$. If R_d is removed, the narrowband filter has infinite gain at $\omega = \omega_0$ and tends to oscillate by itself. An oscillator of this type was published decades ago in the classic applications manual published by the G.A. Philbrick Co., originators of the operational amplifier. It is stabilized against oscillation when connected in the feedback loop with amplifier pair 3 and 4.

The overall gain of the notch filter (amplifiers 3–8, connected as in Fig. 3), for R_d infinite, is, from Eqs. [4] and [6],

$$G_n = -(R_g/R)/\{1 + iR_g[R_fRC_1(\omega - \omega_1)]^{-1}\}. \quad [7]$$

The gain is zero when $\omega = \omega_1$, and is decreased in magnitude by 0.707, relative to its gain far from the notch frequency ω_1, when $|\omega - \omega_1| = R_g\,(R_fRC_1)^{-1}$.

This filter has properties strongly analogous to those of the simple RC filter of Fig. 1, Eq. [1], except that ω is replaced by $\omega - \omega_1$ and RC is replaced by R_fRC_1/R_g. The latter quantity is equal to 0.5 ms for our filter. Just as for the earlier circuit, the filter removes the solvent signal only for time long compared to 0.5 ms. To achieve high dynamic range we use the gain-changer in conjunction with it, exactly as in Section II, with the gain-programmable amplifier after the filter of Fig. 3. The discussion of dynamic range in Section II applies equally in this case.

This circuit has never oscillated in 2 years of use, and it filters as expected. The circuit as originally built filtered at 16 kHz and we intended to try to use even higher frequencies, but the final choice of 5.06 kHz was forced on us for reasons described in RK1. At higher filtering frequencies, wideband operational amplifiers might be required to get the results predicted above. The circuit was originally built using such operational amplifiers, but it then showed parasitic oscillation. High-frequency construction technique (i.e., a good ground plane with compact feedback and good bypassing) is needed, and we do not know what the practical frequency limit of construction of this type of filter is.

The circuit of Fig. 3 can be simplified to form a versatile notch filter of a single nonquadrature signal for use with spectrometers which do not use quadrature detection. More than one circuit of this type could be used in series to filter out buffer signals from strong signals other than solvent. The circuit could be made to have programmable width and frequency, by incorporation of resistor arrays of the type used in digital-to-analog converters.

IV. EXTENSION TO DIGITAL FILTERS

Any analog filter can be approximated by a digital filter. Our treatment of digital filtering will look similar to a conventional treatment (*11*) with two exceptions: first, the coefficients connecting the input and output arrays are complex numbers; second, the inputs and outputs are complex numbers as usual, but these complex numbers are not to be interpreted as representing real numbers by their real part, as is common in electrical engineering notation, but instead they are arrays of pairs of numbers, one for the real part and the other for the imaginary part of the complex number. In the case of quadrature data, these numbers could be input directly from the two quadrature inputs. If quadrature detection is not used, the single-channel input data would become the real input to be the complex filter, and the imaginary input to be the digital filter would to be set to zero. In that case the input would be an equal sum of positive and negative frequencies but the complex digital filter output (especially for the narrowband filter emulated below) might be nearly pure positive frequency (or negative frequency) alone.

We consider first a narrowband feedback filter analog (known in the literature as an infinite impulse response filter, or IIR filter) of the simplest form. The kth complex output number of the filter D_k is related to the input number B_k, and the previous output number D_{k-1}, by

$$D_k = D_{k-1}e^{i\omega_1\tau} + B_k, \quad [8]$$

where ω_1 is a real number which will turn out to be the resonance frequency of the filter, τ is the time between input samples, and ω_1 is the desired peak gain frequency. We will discuss only the steady-state response of this filter to a sampled pure sinusoidal quadrature input $B_k = Be^{i\omega k\tau}$, where B is complex and ω is real. These B_k's could be inputs from a pair of ADCs sampling quadrature wave forms of the type defined in Section III.

The reader does not have to have prior knowledge of traditional digital filtering terminology to comprehend what follows. We define $Z = e^{i\omega\tau}$, and can then write $B_k = BZ^k$. A reasonable trial solution for the output of the filter, assuming that it is stable, is that it is also periodic with the same frequency: $D_k = BG_fe^{i\omega k\tau} = BG_fZ^k$, where the gain G_f, like B, is a complex number, dependent on ω but not k, and is the gain of the filter. These inputs and trial outputs inserted into Eq. [8] yield, after canceling a factor Z^k on each side,

$$BG_f = BG_f Z^{-1} e^{i\omega_1\tau} + B. \quad [9]$$

The gain is then

$$G_f = (1 - Z^{-1} e^{i\omega_1\tau})^{-1} \cong (i(\omega - \omega_1)\tau)^{-1}, \quad [10]$$

where in the second equality we expanded Z in a Taylor series $1 + i\omega\tau + \cdots$ and kept only the lowest order terms, as is appropriate if the input frequency ω is small compared to the sampling rate τ^{-1}, and similarly for the other exponential. The second form of Eq. [10] is similar in form to the response of the narrowband quadrature filter in Section III (Eq. [6], with R_d equal to infinity).

The reader can verify that the filter defined by Eq. [8] can be incorporated into a second filter with negative feedback to yield a notch filter, as in the analog filter of Fig. 3, by defining new inputs C_k and using the B_k as outputs, processed as

$$B_k = C_k - gD_k, \quad [11]$$

where D_k is given by Eq. [8]. Equation [11] is analogous to Eq. [3], and the overall gain for $\omega\tau \ll 1$ is similar to that of Eq. [4] above, if $g/\tau = R_g/R_f RC_1$. The parameter g must be real and positive, and would be small compared to one, for a narrow notch. A notch filter of this type might be used in conjunction with narrowband digital filters to get a sharp-cutoff filter.

In the language of digital filtering, this notch filter has a zero on the unit-Z circle at $Z = e^{i\omega_1\tau}$, and a nearby pole at $Z = e^{i\omega_1\tau}(1 - g)^{-1}$. It is similar to a standard notch filter (*11*) that also has a zero and pole at $e^{-i\omega_1\tau}$ and $e^{-i\omega_1\tau}(1 - g)^{-1}$.

By cascading several such narrow passband filters, or similar feedback filters with more terms connecting B_k with B_{k-1}, B_{k-2}, etc., with damping added, a narrowband filter of many poles could be constructed. Apparently six real multiplications per pole are needed, and a five-pole filter can probably be calculated on the fly on the input data for a fast digital signal processor operating at $\tau = 2$ μs (1-MHz digital quadrature bandwidth).

Use of such a narrowband filter with decimation provides a possible alternative to the current practice of a frequency shift of the data followed by filtering at zero frequency. For example, input data and noise within a 1-MHz bandwidth, with the spectrum occupying somewhat less than 100 kHz, centered at n times 100 kHz, where n is an integer, could be filtered using such a filter having a passband centered at $n*100$ kHz and width less than 100 kHz. Following time decimation by 10, the signal would be aliased to the nominal range −50 to +50 kHz, requiring storage of 0.4 MB per second of FID sampled, without requiring an explicit frequency-shift calculation. These numbers are appropriate for spectra occupying 200 ppm at 500 MHz. Other special ranges and decimations would be useful for other types of spectra, and filtering could also be done at the end of acquisition of several FIDs as described in RK1, and/or in two stages, or with several resolutions from the same data.

We have not used digital filters of these types in our spectrometer. Our treatment of them is included because it may be unfamiliar, and is analogous to the hardware filters described above.

V. DISCUSSION

We conclude with a brief discussion of the design parameters for the input stage of an NMR instrument, as they relate to the issues mentioned above.

An important variable in the operation of an NMR instrument is the center frequency of the NMR signal presented to the ADCs, which is zero for the usual recent practice, and was 5.06 kHz in the modification of RK1. A frequency in the range of 50 to 100 kHz is reasonable, since it would be high enough to move the entire NMR spectrum to one side of zero for almost any case, and low enough so that filtering circuits like that of Fig. 3 can probably be made. Frequency-shifted operation (*1*) is still not standard, and instead users of commercial instruments achieve acceptable results using CYCLOPS (*9*) for one-dimensional NMR, or hardware (*8*) or software adjustment of the quadrature detector for multidimensional NMR. In fact, frequency shifting can be made nearly invisible to the user, but it is most efficiently performed using a single digital signal processor to process both quadrature outputs, especially as described above.

Direct conversion of the intermediate frequency at several megahertz is now feasible (below) and can eliminate quadrature detection, but construction of a versatile narrowband analog filter in the megahertz range may be difficult. While it is attractive to simplify the spectrometer in this way, and the need for frequency shifting of the FID is eliminated, the quadrature detection which is eliminated is simple and well understood, and removing it decreases flexibility. It is trivial to build a quadrature detector with very wide bandwidth, to achieve good dynamic range. All of the above remarks apply equally to the use of anti-image narrowband filtering at intermediate frequency followed by nonquadrature conversion to low frequency (*12*). Therefore, a quadrature detector remains a desirable feature of a modern spectrometer.

Two groups have proposed use of feedback circuitry to eliminate radiation damping effects, and such capability seems very desirable for any spectrometer (*13, 14*). These methods were demonstrated for spectrometers operating with the water frequency at zero frequency, but it should be possible to use similar feedback when the solvent frequency is shifted. Broekaert and Jeener (*14*) discuss the feedback-stability requirements of their method in detail, and use a pair of single-pole (*RC*) filters as the single dominant element limiting the feedback bandwidth, as is often done with any high-gain feedback. At finite solvent frequency, whether in the range of a few kilohertz or higher, their simple pair of *RC* filters would be replaced with a narrowband quadrature filter similar to the block inside the dotted line of Fig. 3. This filter would have to be the only narrowband element in the radiation-damping feedback loop. It would have to be switched in during the free induction decay, and otherwise the *RC* filters described (*14*) would be used for the radiation-damping elimination. A notch filter (Section III) would still be usable to increase dynamic range, but placed after the radiation-damping feedback loop, just before the ADC.

Digital signal processors (DSPs) are primarily devices that save money by providing buffer storage and high-speed parallel processing, permitting use of inexpensive slow main computers, and they should be used on all NMR systems, no matter how humble. By use of two ADCs with a top-line DSP, an input sampling rate of 10^6 per second, or 1-MHz bandwidth, is probably easy, with 16-bit accuracy. Digital downconverters (DDCs) perform frequency downconversion, digital filtering, and time decimation, at input sample rates exceeding 10 MHz (*15*). They normally would be in front of a DSP and two would be needed for quadrature detection, while one would be needed for direct detection at the intermediate frequency as mentioned above. Unfortunately, ADCs that can sample at this rate are not as precise as the lower speed ADCs and their use would not improve dynamic range much, at this writing (*2*). Use of these high sampling rates may be more attractive in the future, or justified on the ground that their potential utility justifies the relatively low cost of implementing them. It seems prudent for the instrument designer to plan for future upgrade to this technology, using two DDCs and whatever ADCs may be available. At the same time, it is possible that a 1-MHz bandwidth with analog filtering as described here, giving a factor of over 30 in dynamic range compared to the typical conditions described in the Introduction, will satisfy the desires of the NMR spectroscopist for high dynamic range.

So far we have assumed that increasing the filter bandwidth with oversampling as in RK1 will increase the noise at the ADC and increase dynamic range. In fact the analog bandwidth of modern NMR systems is limited by the resonance width of the NMR probe to less than 1 MHz, especially for superconducting probes which are now available. The noise outside this bandwidth, and perhaps within it, can be supplemented by introduction of artificial noise carefully filtered so that it does not appear in the NMR spectrum (*16, 17*). This is known to engineers as ''out-of-band dither'' (see, for example, *18*). Since out-of-band dithering does not rely on the noise from the spectrometer input, it seems conceivable that the gain of the receiver system and the level of dithering can be adjusted separately to further optimize dynamic range. This is a topic worthy of future investigation.

We conclude by noting that Sections III and IV of the present article are largely concerned with a point of view, namely exploitation of the representation of real pairs of signals, carrying harmonic data, as complex numbers, which has been used in the NMR literature since the first quadrature detectors were developed (*19*). On the other hand, although quadrature detectors are now commonly described in electronic engineering texts as used in ''pulse code modulation'' (90° phase shifting of an RF carrier to represent a binary signal), one seldom finds mention in these texts of the outputs of a quadrature detector as being real and imaginary parts of a complex signal. A possible reason for this neglect of a simplifying representation, other than tradition and fear of possible confusion with the dominant prior use of complex numbers to represent single real signals, is that quadrature signals as used here are unstable against small imperfections in hardware which will introduce image frequencies. This is, of course, not a problem for a quadrature digital filter (Section IV above).

The circuit of Fig. 3 viewed as a single-channel amplifier can be correctly described merely as a ''biquad'' filter (*9*) used as the feedback element of a negative feedback amplifier. What is gained by quadrature notation? The circuit of Fig. 3 is simpler than any pair of notch filters, it is single-sideband, and it is probably superior in performance to any alternative. Quadrature notation, like imaginary numbers notation, is not strictly necessary, but provides insight and convenience.

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