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Communication

# A 'Hi-Fi' Cartesian feedback spectrometer for precise quantitation and superior performance

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**Abstract**

The use of Cartesian electronic feedback for effecting a major improvement in the functioning of magnetic resonance instrumentation is reported. The dependences of both flip angle and signal strength upon probe loading, matching, and tuning are virtually eliminated. Thus, for a chosen probe, sample geometry and flip angle, the free induction decay signal strength is rendered solely dependent upon the number of nuclei. The instrument therefore becomes capable of absolute calibration. In addition, phase and amplitude distortion of selective pulses, introduced by crossed diodes, power amplifier heating, etc., is virtually eliminated, as are radiation damping and phase modulation caused by probe vibration. The use of multiple probes at the same frequency, for example quadrature probes and phased arrays, is also simplified as the effects of interactions between such probes are typically reduced by two orders of magnitude.


*Keywords:* NMR; MRI; MRS: quantitation; Electronic feedback; Cartesian feedback; Distortion; Selective pulse

## 1. Introduction

There are numerous defects in, and deficiencies of, magnetic resonance instrumentation, arguably the most serious being that a spectrometer or imager is uncalibrated in an absolute manner. When transmitting, a change in or of the sample (e.g., non-conducting to conducting, polar to non-polar, etc.) necessitates a change of pulse power or length, even if the probe has been re-tuned and re-matched—and the latter may not be possible if automatic sample-changing is employed. Concomitantly, upon reception, even if different samples contain the same number of nuclei, the amplitudes of their free induction decays (FIDs) following a 90° pulse (i.e., the integral of the spectrum) may differ. With an ideal instrument, such changes would not occur. Thus, to take but two examples among many, there would be no need to worry that the swelling of a perfused heart would change the pulse length and the signal strength of some metabolite of interest, or that the breathing of a patient in an imaging experiment would do likewise.

These shortcomings are caused by the tuned and matched probe, for its $Q$-factor and tuning are dependent on its environment; in particular, both variables are sample-dependent. A related defect is that tuning can be modulated by movement and vibration, the latter causing extra "$1/f$" noise about a resonance and "t1" noise in two-dimensional spectra via phase modulation. Such vibration can come from air flow, from spinning the sample, from gradient noise, etc. Spinning the sample in high resolution or magic angle experiments can also directly modulate the probe tuning if there is any heterogeneity or asymmetry in the electric susceptibility of the sample. This causes extra spinning sidebands. If more than one tuned probe coil at the same frequency is used, these sensitivities can increase greatly due to coupling. Examples are high resolution quadrature

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probes, coils in rotating frame imaging experiments, phased array coils, etc. While "paddles" [1] or capacitor–resistor leakage bridges [1,2] can cancel both reactive and resistive interactions, the sensitivity of the balance still renders such solutions susceptible to the factors mentioned above. Further, cancellation of resistive interactions diminishes sensitivity. Change of temperature also affects probe tuning and $Q$-factor, causing $B_1$ field and signal strength to drift in amplitude and phase.

Now during signal reception, the use of pre-amplifiers that are noise-matched but power-mismatched (typically low input impedance devices but high input impedance designs can also be employed) has been known for many years to reduce the *effective* probe $Q$-factor, without affecting signal-to-noise ratio [3–6], thereby ameliorating the problems. During transmission, the equivalent is to over-couple the transmitter [3], but gains in this regard come at great expense, as the transmitter power specification has to be seriously increased for a useful effect to be obtained; further, maintaining a consistent degree of over-coupling is difficult with systems designed for only 50 Ω use. Thus, problems during transmission remain unresolved.

Turning to other ills, when the signal is very strong, "radiation damping" can be a nuisance. It is usually partially dealt with by detuning the probe while the flip angle may also be reduced to maintain an approximately exponential decay; however, other solutions pertinent to this paper exist [7–9]. The use of a power-mismatched pre-amplifier can again help in this regard, its beneficial effect first being observed in about 1970, but in some cases this solution may be inadequate. Next, crossed diodes in probe protection circuits cause considerable non-linearity at low pulse powers and as a result, can greatly distort selective pulses. PIN diode circuits help considerably here, but even they are not distortion-free and their switching times are often excessive. Further, the design of direct current paths that do not compromise the performance of some imaging probes is sometimes problematic. Finally, high power transmitters are renowned for changes of power and phase during a pulse as components rapidly heat and with poor designs, power supply voltages droop. Pulses are then distorted in amplitude and phase and of course, ambient temperature changes have their destructive role to play here too. However, our purpose in this Communication is not merely to detail defects, but to describe a solution to all these ills using feedback.

## 2. Negative feedback stability

Negative feedback has been renowned since the pioneering work of Black [10] for its ability greatly to reduce amplifier distortion, stabilise gain, and change input and output impedance. Essentially, it functions by sampling the output of an amplifier, comparing it to that desired and correcting the output to cancel any error. Thus, in a magnetic resonance context, an obvious example of its use would be during transmission. With a small sense loop, or by monitoring a small fraction of the voltage across a tuning capacitor, we could directly or indirectly sample the $B_1$ field produced by a probe and compare the monitored signal with that desired. With sufficient open-loop gain round the feedback loop, any distortion introduced by the power amplifier or by crossed diodes would then be reduced to negligible levels. However, the Bode criteria for stability [11] must always apply: with change of frequency, the open-loop gain must have diminished to less than unity by the time the phase has changed by 180°. It is axiomatic that these criteria are normally difficult or impossible to fulfil at very high frequencies (VHF), and the conventional wisdom is that RF feedback circuits oscillate. NMR in this frequency range is no exception, particularly as there are normally long lengths of cable between the magnet and the transmitter and receiver that sit outside the magnet's fringe field.

Now a standard method of dealing with problems of oscillation in video-frequency operational amplifier design is to ensure that the frequency response $H(\omega)$ of the amplifier is dominated by a single-pole, low-pass RC filter. The equivalent at VHF would be to ensure domination by a *band-pass* filter of centre-frequency $\omega_0$ whose transfer function is of the form

$$H(\delta\omega) = \frac{H_0(\delta\omega)}{1 + \mathrm{j}\delta\omega\tau}, \tag{1}$$

where $H_0(\delta\omega)$ is the unmodified response of the amplifier, $\tau$ is the time constant of the filter and $\delta\omega = \omega - \omega_0$. If $H_0(\omega_0) \gg 1$, the gain is unity with a phase shift $\sim\pm 90°$ *from the filter* when $\delta\omega \sim \pm|H_0(\delta\omega)|/\tau$. Thus, provided the phase shift $|\angle H_0(\delta\omega)|$ from the *unfiltered* amplifier at these frequencies is less than 90° (in practice, for safety, 45°), the amplifier will not oscillate if negative feedback is applied. The problem here is the long value of filter time constant $\tau$ typically needed; it requires a highly stable filter with a $Q$-factor $\omega_0\tau/2$ of, say, 40,000. A solution to this problem was first proposed in the communications industry in 1983 [12] and has since been given there the appellation "Cartesian feedback," the name we have adopted here. It was mentioned independently for application to an NMR spectrometer in 1989 [13] and described in detail theoretically under the title "quadrature feedback" in 1991 [14]. A precursor in 1980 was the use of a rectified (single-quadrant) feedback method for creating distortion-free selective pulses [15].

The implementation of the equivalent of the required high-$Q$ filter, centred on 10 MHz, is shown as part of Fig. 1—it is the heavily outlined section. In-phase and

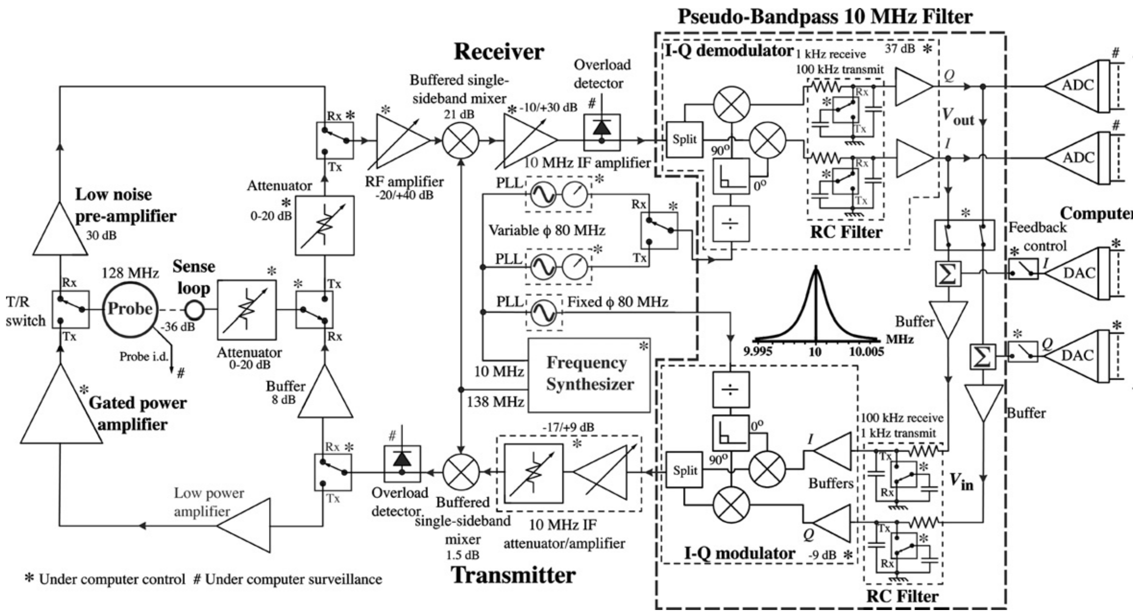


Fig. 1. Avoidance of oscillation via bandwidth reduction with the aid of Cartesian feedback. Both the transmitter and receiver are on continuously to form a feedback loop, albeit with different gains, phases and paths during transmission and reception. (The switch positions shown are for signal reception.) Note that the position of the constituent baseband RC filters changes with transmission or reception so they are always in the forward path.

quadrature baseband signals (phase-sensitive quadrature detection) are obtained from the intermediate frequency (10 MHz) section of the receiver. These signals are filtered with identical low-pass RC filters and then applied to a quadrature (*I–Q*) modulator to regenerate an intermediate frequency signal. The available bandwidth about the centre-frequency is clearly set by the low-pass filters. Note that the absolute phase of the signal from this pseudo-band-pass filter can be set to ensure that on resonance, the feedback is truly negative. It should not be thought that the bandwidth of a negative feedback system employing such a filter is limited to $\Delta\omega = 2/\tau$. The bandwidth is increased by the open-loop gain of the system $H_0(\omega_0)$ once the feedback loop is closed, allowing the usual NMR bandwidths (e.g., 200 kHz) to be employed. Rather, the full *advantages* of the feedback only pertain over the bandwidth $\Delta\omega$.

## 3. Negative feedback advantages

To appreciate those advantages, we assume for simplicity that we are on or close to resonance so that we may ignore the finite bandwidth of the filter. We begin with transmission and apply a voltage $V_{in}$ to the quadrature (*I–Q*) modulator at the beginning of the transmitter chain. (Voltage $V_{in}$ might, for example, be a complex selective pulse $V_p$ derived from twin digital-to-analogue converters.) Following amplification in the transmitter, and the tuning and matching of the probe, a current

$$i_p = \alpha V_{in} \exp(j\omega_0 t) \tag{2}$$

flows in the probe and generates the $B_1$ field. Here $\alpha$ is the effective transconductance of the transmitter chain and importantly, it includes the effects of tuning and matching and any losses or change of gain caused by the transmit/receive switch. If these alter for some reason, then $\alpha$ alters too. The $B_1$ field created by the current induces a monitoring voltage in a nearby sense coil, and this voltage is passed to the spectrometer's receiver and thence to the quadrature demodulator. Let the voltage at the demodulator be $\beta i_p$, where $\beta$ is proportional to the mutual inductance between the sense coil and the probe. Following demodulation, which is equivalent to multiplication by $\exp(-j\omega_0 t)$, the quadrature voltage out is given by $V_{out} = \beta i_p \exp(-j\omega_0 t)$. If feedback is now applied, we must let $V_{in} = V_p - V_{out}$. With appropriate demodulator phasing, this is one of the configurations possible in Fig. 1. We then have from Eq. (2) that

$$\begin{aligned} i_p &= \alpha V_{in} \exp(j\omega_0 t) \\ &= \alpha[V_p - \beta i_p \exp(-j\omega_0 t)] \exp(j\omega_0 t). \end{aligned} \tag{3}$$

Solving for the probe current,

$$i_p = \frac{\alpha V_p \exp(j\omega_0 t)}{1 + \alpha\beta}, \tag{4}$$

and it follows that if the open-loop gain $\alpha\beta \gg 1$ (we typically use 100), then $i_p \cong (V_p/\beta)\exp(j\omega_0 t)$. Most importantly, the current is independent of $\alpha$, the transmitter gain and the tuning and matching. Rather, the probe current in transmission is dependent on the effective sense coil/*receiver* gain $\beta$, one of the more confusing aspects of working with negative feedback. Another way of looking at the effects of feedback here is to regard it as having changed the dynamic output impedance of the transmitter, a facet that will be exploited to the hilt in the next Communication [16]. The transmitter essentially becomes a constant current source in series with the probe coil, and errors of tuning and matching are then largely irrelevant provided sufficient power is available to cope with the error.

Turning to signal reception, the roles of the sense coil and of tuning and matching are now reversed. The probe is connected as usual to the pre-amplifier and thence to the receiver and quadrature detector, while the sense coil is connected to the transmitter. (The high power amplifier is bypassed.) Let a voltage $V_c \exp(j\omega_0 t)$ be induced in the probe coil. It comprises an FID voltage $\xi \exp(j\omega_0 t)$ and whatever is mutually induced by any current in the sense coil. Reusing the conventional symbols $\alpha$ and $\beta$, the voltage is passed to the receiver with gain $\alpha$ and demodulated to give a quadrature output voltage $V_{out} = \alpha V_c$ that is passed to analogue-to-digital converters in the traditional manner. Note that once again gain $\alpha$ includes any contribution from the tuning and matching. We now also pass the output to the RC filters, re-modulate and pass, via the sense coil, a fraction $\beta$ to the probe coil. (The phase of the demodulation must, of course, be appropriate.) Thus

$$V_c = \xi - \beta V_{out} = V_{out}/\alpha. \tag{5}$$

Solving for $V_{out}$, we obtain

$$V_{out} = \frac{\alpha\xi}{1+\alpha\beta} \tag{6}$$

and once again, if the open-loop gain $\alpha\beta \gg 1$, the output voltage $V_{out} \cong \xi/\beta$ is essentially independent of gain $\alpha$ and of the vagaries of tuning and matching. Rather, it is the gain/attenuation of the low-power *transmitter* section of the spectrometer that determines the *receiver* gain. Just as with the transmitter the negative feedback was considered to have greatly increased the former's *output* impedance, so now the effective *input* impedance of the pre-amplifier can be considered to be greatly increased. From above, the voltage $V_c$ present in the probe coil is greatly reduced as:

$$V_c = \xi - \beta V_{out} = \xi - \frac{\alpha\beta\xi}{1+\alpha\beta} = \frac{\xi}{1+\alpha\beta}. \tag{7}$$

Concomitantly, current flowing in the probe in the presence of the FID $\xi$ is also reduced by one plus the open loop gain $\alpha\beta$, which has clear implications for "radiation damping" [7–9] and for coupling to another tuned circuit nearby—both are greatly lessened. One could say that the feedback is striving to keep at zero the voltage in the probe.

## 4. Results

The Cartesian feedback spectrometer of Fig. 1 was constructed. In the experiments to be described, an open-loop gain of 100 was used with 1 kHz filters. Thus, the gain-bandwidth product of the system was 200 kHz. A full description of the engineering details will be given in a later paper. To test in a severe manner the theory given above, a simple pulse-and-acquire experiment was designed in which the flip-angle and the signal strength were both highly dependent on coil loading. The instrument was used with 360 mL doped (7.5 mM $CuSO_4$) saline samples in bottles (o.d. = 53.5 mm, length = 187.4 mm) and a 3 T imaging magnet (Magnex, UK). The probe was a shielded, 79.6 mm diameter Alderman and Grant design [17] ($Q_{unloaded} = 310$, $\nu_0 = 127.6$ MHz) to which a small $B_1$ field sense coil was attached. The attenuation between the matched probe input with no sample and the sense coil output was 36 dB—the sense coil was very weakly coupled. The probe was fixed-tuned and fixed-matched for an "average" sample (20 mM NaCl, 7.5 mM $CuSO_4$, $Q_{loaded} = 86$), with the aid of a capacitive bridge and a $\lambda/2$ balun. In-line matching (outside the magnet), to accommodate other probe loadings, was provided by a $\Gamma$-section variable filter, which has a greater dynamic range than the more usual T- or $\pi$-section filters [18]. 1 kW of class AB transmission power (PA10-90, Intech, Santa Clara, CA) was available. The lines between the spectrometer and the probe were 12 m long with a velocity factor of 0.8. In both transmission and reception, the full open-loop gain of 40 dB was realised and we encountered no instability.

Four samples of the doped saline (0, 10, 20, and 40 mM NaCl) provided an extreme range of probe loading that would rarely be encountered in practice in a single experiment. The pH of the sample was held slightly below 7 by the addition of a very small amount of HCl to prevent precipitation of the copper. The samples were intended to act as "phantoms" for biological experiments. With the least conducting (highest $Q$) sample, the flip angle $\theta$ was set to approximately 10° (2 W, 40 µs) with a repetition period of 0.9 s. Now for a power-matched probe, the flip angle for a given pulse power and duration depends on $\sqrt{Q}$ while transverse magnetisation $M_{xy}$ varies as $\sin\theta$. Thus, $dM_{xy}/dQ = d\theta/dQ\ dM_{xy}/d\theta \propto \cos\theta$ and a small flip angle ($\cos\theta \cong 1$) therefore gives the strongest dependence of transverse magnetisation on $Q$. For a tuned and matched probe, the output signal following *a fixed flip-angle* pulse is also proportional to $\sqrt{Q}$, and so the combination of *non-fixed* small flip-angle and signal dependencies implies that the output should be proportional to $Q$. In turn, $Q$ is inversely proportional to effective probe resistance which comprises copper losses and sample loss. The latter is proportional to NaCl concentration $\sigma$ plus a constant amount from the doping and acid. To summarise, when not employing feedback,we expect the received signal from a tuned and matched probe, with a low flip-angle pulse of constant power and duration, to be inversely proportional to $\sigma_0 + \sigma$, where $\sigma_0$ is a constant. This is shown to be so in Fig. 2 where the amplitude of the resulting FID is plotted against salt concentration.

Also plotted in Fig. 2, however, are the results of applying feedback under various conditions. For all plots, the probe was initially in-line tuned and matched for the doped sample with no NaCl. All voltages were measured on an oscilloscope, with an estimated error ~±0.5%. The feedback results most immune to sample conductivity were those for which the open-loop gain of the system was reset with each sample change. This task can easily be automated and rendered transparent to the user. The increase in initial FID voltage (at 0 mM NaCl) when the loop is closed was a consequence of the limited gain resolution of 1 dB (12%). When the system is automated, this change can easily be assessed and corrected by the computer. Summarising, as expected there is a large change in amplitude in traditional open-loop mode that matches the theory above, but very little change in closed-loop mode. Thus, both the flip angle and the received signal have been stabilised.

A second experiment is shown in Fig. 3. Using a crossed diode transmit/receive switch and at low power, the transmitter output was modulated with a 1 kHz sine wave. The receiver output, which monitored the strength of the $B_1$ field, is shown in the figure with and without feedback. Without feedback, there is classic crossover distortion, caused by the crossed-diode transmit/receive switch, but note too the distortion in the waveform (arrows), probably caused by the 1 kW power amplifier. The distortion vanishes when the feedback loop is closed. This facet of the Cartesian feedback technique is important for maintaining the fidelity of lower power and selective pulses, and should also allow PIN diodes with their attendant problems to be dispensed with in many instances. A further bench experiment, involving two square surface coils, and of import for the future use of phased array coils in high-field imaging studies, is described in the next Communication [16].

## 5. Discussion

There are numerous details of engineering involved in the design of a feedback spectrometer if it is to be successful and these are more suited to a specialised paper.

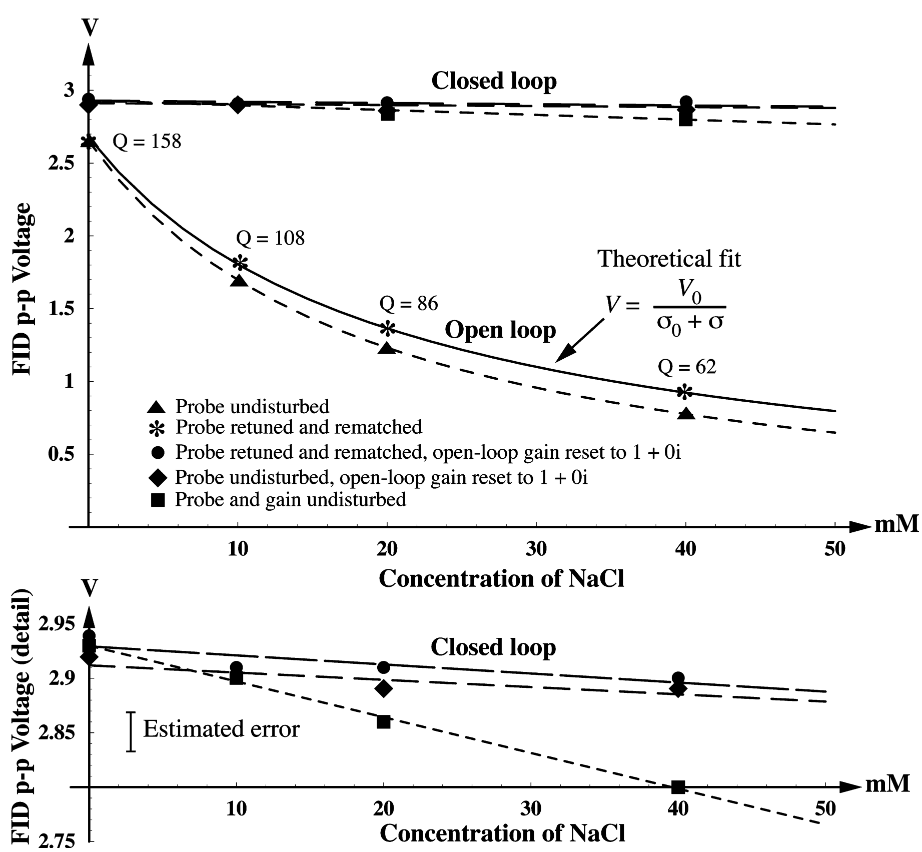


Fig. 2. The free induction decay voltage, as a function of sample NaCl concentration, with the spectrometer in open- and closed-loop modes and subject to various manipulations. The flip angle was nominally 10°. Probe loaded $Q$-factors are for isolated unconnected probes. The loop gain was increased by 100 when the loop was closed.

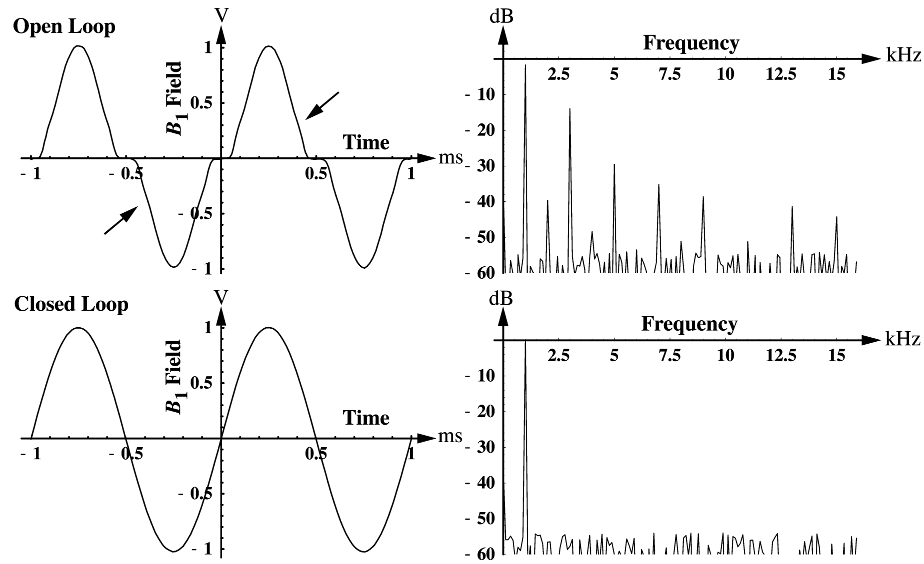


Fig. 3. The $B_1$ field, as monitored by the sense loop and the receiver, when a small sinusoidal voltage (e.g., a portion of a selective pulse) is applied to the transmitter modulator. The power spectra of the waveforms are shown on the right.

We therefore discuss briefly only the most important issues here.

*Implementation.* A primary design decision is whether to construct essentially two instruments that intersect at the probe (transmitter and feedback ⇒ probe ⇒ receiver and feedback) or to utilise the receiver for feedback when transmitting, and then use the transmitter for feedback when receiving, albeit with the omission of the power amplifier. Both methods have their advantages and drawbacks that can only be properly debated if both approaches have been attempted. Somewhat arbitrarily, we opted for the second method, as shown in Fig. 1. It is emphasised that with this method, the receiver and transmitter chains are on at all times.

*Modulation and demodulation.* As digitised feedback systems can oscillate with 1-bit amplitude, the instrument is perforce analogue at this time. Thus, of prime importance are the matching of the two ($I$ and $Q$) RC low-pass filters that should dominate the closed-loop performance, and the orthonormality of the quadrature detection and re-modulation processes. We currently achieve an accuracy of 0.1% in amplitude and phase. Note that once the loop is closed, any quadrature-phase errors propagate round the loop. Thus, digital sampling at an intermediate frequency does not remove them.

*D.C. offsets.* Direct voltage offset on the FID is usually considered unimportant as it can be removed during data analysis. However, with a feedback spectrometer, voltage offset during reception translates into a constant small signal at the Larmor frequency's being injected into the probe, which could cause nuclear saturation.

*Phase.* Feedback must be negative and so demodulator detection phase in both reception and transmission is important. Both open-loop gain and phase can be monitored at any convenient time by a computer and adjusted accordingly. However, widely different phases are typically needed during transmission and reception and thus rapid phase switching is needed. To this end, we employ three synchronised phase-locked loop (PLL) oscillators. One fixed-phase oscillator is the reference for the $I$–$Q$ modulator, while the other two variable-phase oscillators are references for the receiver quadrature demodulator.

*Noise.* It is an interesting point that if Cartesian feedback preserves the amplitude of the FID, the noise floor must rise if the $Q$-factor of the probe drops with change of sample. This is the exact opposite of the usual behaviour, where the probe is re-matched to 50 Ω with change of sample and the signal then drops while the noise remains constant. Note that the feedback neither decreases nor increases the signal-to-noise ratio ($S/N$) unless there is an engineering error.

*Group delay.* With multiple stages of amplification and/or attenuation in both transmitter and receiver at radio and audio frequencies, group delay round the feedback loop can increase frighteningly quickly. Particular attention must be paid to the various filters needed and the bandwidth of the audio amplifiers. By scrupulous attention to detail, we have been able to reduce the group delay through the electronics to about 250 ns, to which must be added the line lengths to the probe and the transfer function of the probe itself. It is worth noting that, at least in theory, compensation for the delay can be introduced in the intermediate frequency sections of the receiver and transmitter chains. We are actively exploring the introduction of what is sometimes known as "negative group delay" [19], but this is a particularly difficult area with many trade-offs involved, and our current instrument incorporates no such compensation.

*Calibration*. There is a known and fixed relationship between the strength of the $B_1$ field during transmission and the voltage induced in the sense coil. Equally, during reception there is a known and fixed relationship between the FID, the voltage induced in the probe by the sense coil and the current therein. It follows that as both voltage and current are accurately measurable during the NMR experiment, absolute calibration of a spectrometer is possible.

## 6. Conclusion

In conclusion, we believe that the application of Cartesian feedback is eminently feasible for both the transmitter and receiver of an NMR spectrometer, and holds such great advantages that any instrument manufacturer that could incorporate it in a routine fashion into its product could change the manner in which NMR is practised. In particular, absolute calibration of a probe/sense coil could be made in the factory. Shipping the probe with an embedded chip that the spectrometer's computer could access would allow the computer immediately to set the desired flip angle and to express areas under spectral lines in moles. The operational key would lie in letting the computer control the set-up and calibration of the instrument, while the instrument design key lies in minimising, then compensating for, group delay and having reproducible and accurately defined gain settings. We continue to research intensively both topics.

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