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Phase-Sensitive Detection
Part II: Quadrature Phase Detection

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The problems associated with the use of a single phase-sensitive detector (PSD) in an NMR receiver are reviewed. These problems can be eliminated by the use of two PSDs, arranged in parallel. The references to the PSDs are derived from a single source, but one is phase-shifted by 90° with respect to the other. This arrangement is called quadrature phase detection (QPD). The free-induction decays (FIDs) obtained as outputs from the two PSDs are phase-shifted by 90° with respect to one another, and are referred to as a "real" and an "imaginary" FID. The PSDs and the electronic components associated with them, including amplifiers and filters, are called the "real" and the "imaginary" channels. The FIDs from these channels can be processed so that the problems associated with the use of a single PSD are eliminated. In practice, however, a different set of problems emerges with the use of a QPD system because it is not possible to balance the two channels exactly. A procedure called CYCLOPS, which phase-cycles both the transmitter and the receiver portion of the computer, can be used to overcome these difficulties.

INTRODUCTION

In Part I of this article (*1*), phase and the principles of phase-sensitive detection were covered in some detail, and readers are encouraged to review these principles before continuing with this part, particulary the portion of the Introduction that pertains to the use of the right-hand rule. In Part I, it was shown that the use of a single phase-sensitive detector (PSD) leads to two major problems in the detection of NMR signals. First, the pulsed radiofrequency (rf) must not be positioned between two Larmor frequencies, because a PSD cannot determine whether the Larmor frequencies are above or below the frequency of the reference. The result is that even if the spectral width is wide enough to prevent Nyquist "folding" (aliasing), one of the NMR signals will fold into the final spectrum, which then will exhibit an incorrect separation between the spectral lines. Second, even if the pulsed rf is positioned to one side of all the Larmor frequencies, the PSD cannot distinguish between the noise on the side containing the NMR signals and the noise on the opposite side. Both noise bands will appear in the final spectrum, and the signal-to-noise ratio (S/N) will be degraded by $\sqrt{2}$. A third disadvantage, which was not mentioned in Part I, is that the rf power is totally wasted on one side of where the rf is positioned — on the side opposite the side containing the Larmor frequencies. Quadrature phase detection (QPD), which uses two PSDs whose reference phases are 90° apart, eliminates these problems. It is now in general use, along with a phase-cycling procedure called CYCLOPS (*2*). The general principles discussed here are used extensively in two-dimensional NMR.

"FOLDING" WITH A SINGLE PSD

Suppose a 7.05-Tesla system is being used to obtain a proton spectrum of a sample that contains two resonance frequencies, 300,000,000 and 300,000,003 Hz, and that the pulsed rf is set at 300,000,001 Hz. This situation is depicted in Fig. 1, to which the following conditions apply:

(1) The arrow represents the position of the pulsed rf.
(2) The thin, vertical lines extending below the horizontal axis each represent a 1-Hz separation.
(3) The bold, vertical lines extending above the axis represent the two Larmor frequencies.

As described in Part I of this article, the two rf NMR signals are eventually fed to a PSD, which in this case has a reference input of 300,000,001 Hz. The PSD output, which is the free-induction decay (FID), is the absolute value of the differences between the two Larmor frequencies and the reference; 1 and 2 Hz, in this case. The final spectrum consists of two lines separated by only 1 Hz — not 3 Hz. It appears that the 300,000,000 Hz signal has been "folded" around the 0-Hz edge of the spectrum.

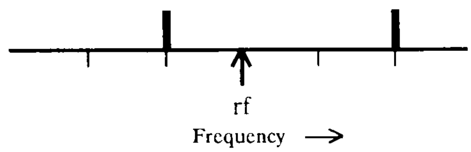


Figure 1. Frequency Scale Representation of Two Lamor Frequencies and a Pulsed rf.

Figure 2 illustrates some, but not all, of the components in a typical QPD receiver. The NMR signals are simultaneously fed to two PSDs. The output from the same oscillator (OSC) that is used

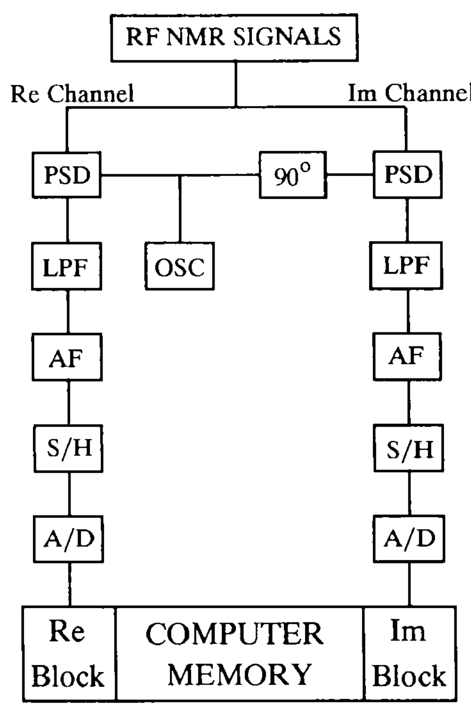


Figure 2. Block Diagram of a QPD Receiver.

for the pulsed rf is fed directly to the reference input of one of the PSDs and to a 90° phase shifter before being used as the reference input for the other PSD. Both outputs (FIDs) are passed through lowpass filters (LPF), whose band-widths are set to one-half of the total spectral width, to remove the upper sidebands and noise frequencies outside of the spectral window, and are then amplified by audiofrequency (AF) amplifiers. The FIDs are still analog signals at this point, and they must be digitized. A sample-and-hold (S/H) device samples the voltages at successive intervals called the "dwell time," which, to avoid Nyquist aliasing, is equal to the reciprocal of twice the band-width of the LPF. An analog-to-digital converter (A/D) reads the voltages held by the S/H, and deposits them into successive words in computer memory. Because the two PSD references are 90° out of phase with respect to each other, the two channels are called "real" and "imaginary." These terms are consistent with the general use of "cosine" for "real," and "sine" for "imaginary." The cosine and sine functions are ±90° apart — as are the real and imaginary FIDs.

REAL AND IMAGINARY (COMPLEX) FIDs WITH 0° PHASE ANGLES

The real and imaginary FID waveforms can be constructed by making use of the rotating frame, which when viewed from the top is considered to be rotating counterclockwise, and at the same frequency as the pulsed rf. Figure 3 shows the view into this frame, from the top and looking down onto the xy transverse plane. In this figure, the two net magnetization vectors are shown lying in the plane, and they are aligned along the $-y$ axis. These would be their positions after a 90° pulse is directed along the x axis. The low-frequency vector (L) rotates clockwise at a 1-Hz rate in this frame, and the high-frequency vector (H) rotates counterclockwise at a 2-Hz rate. For simplicity, the signals will be assumed to be nondecaying. Hence, as the vectors rotate, their magnitudes will be assumed to be constant. Furthermore, they will be assumed to have a length of unity. Also shown are vectors labeled Ref, the references to the PSDs. They do not rotate because they have the same frequency as the frame.

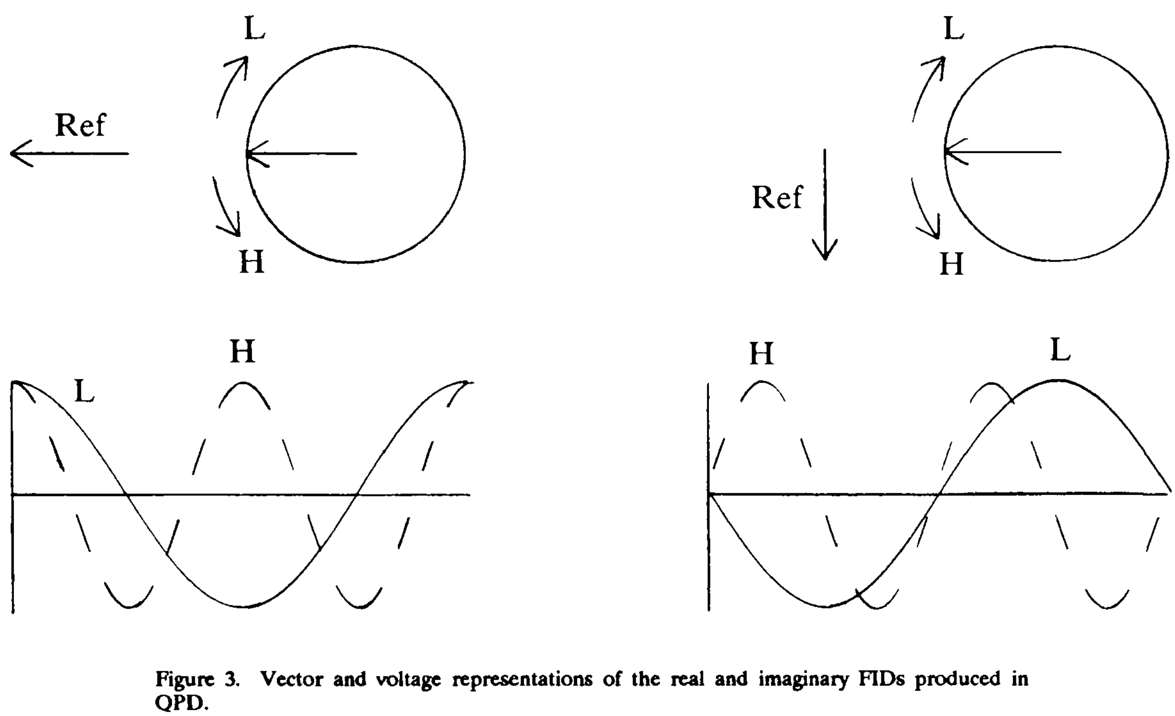


Figure 3. Vector and voltage representations of the real and imaginary FIDs produced in QPD.

For the real channel, it is assumed that all three rf frequencies are exactly in phase at the start of the collection of the signals by the A/D; at t = 0. At this instant, both magnetization vectors will produce an instantaneous, positive, 1-V dc. As the vectors rotate, they will go out of phase with respect to the reference. As the low-frequency vector rotates clockwise in the frame at a 1-Hz rate, it will produce the following instantaneous voltages at 0.25-second intervals, starting at $t = 0$: 1, 0, -1, 0, and 1. At intermediate time points, the voltages will produce the positive cosine waveform shown by the solid line. The high-frequency vector rotates counterclockwise at a 2-Hz rate, and it will produce the following instantaneous voltages at the same time points: 1, -1, 1 ,-1, and 1. It will form the positive 2-Hz cosine function shown by the dashed line. The actual real FID will be the point-by-point sum of these two individual signals.

For the imaginary channel, the reference vector is shown at a 90° angle with respect to the reference vector for the real channel, because the rf for this reference has been shifted by 90°. As time progresses, the angle between these two reference vectors will not change; they are of the same frequency. At $t = 0$, both net magnetization vectors produce 0 V because both are 90° out of phase with respect to the reference. As the low-frequency vector rotates, it first goes further out of phase and then begins to come into phase, producing the voltages 0, -1, 0, 1, and 0 at the same 0.25-second intervals. The resulting waveform is the 1-Hz negative sine waveform shown by the solid line in the figure. Similar reasoning leads to the dashed, positive sine waveform for the 2-Hz signal.

These two FIDs can be sampled and digitized (by the S/H and the A/D) either simultaneously or alternately. In either case, the two FIDs are collectively referred to as a complex FID. The Fourier transform (FT) of each FID produces a real and an imaginary spectrum, so that four subspectra are formed from the complex FID. It will be shown that these spectra can be combined to produce two final spectra, also referred to as real and imaginary. The FT performed in this way is called a complex FT.

PHASE AND SPECTRAL LINE-SHAPES

In Fig. 3, the FIDs are shown with constant amplitudes, but in practice, they decay exponentially. This decay produces a line-width that is a function of the time constant (T_2^*) for the decay. However, the spectral line-shapes obtained after the FT of a signal will depend on the phase of the signal. Figure 4 shows the real and imaginary line-shapes obtained from a Bruker AM-300 as a function of the phase of a decaying FID.

QPD SUBSPECTRA

The real and imaginary FIDs in Fig. 3 both contain 1- and 2-Hz signals, and the spectra obtained from these FIDs will show spectral lines located at 1 and 2 Hz from the 0-Hz origin. Although all of these spectra will show an incorrect separation between the lines, the final QPD spectra, which will be discussed in the next section, will have the correct 3-Hz separation. The FTs of each of the FIDs give a real and an imaginary spectrum. Hence, four subspectra are obtained, and these are the real (Re) and imaginary (Im) parts of the real and imaginary FIDs. They are designated RR, IR, RI, and II, respectively (Fig. 5). The line-shapes shown were obtained by making reference to the phases of the signals in the FIDs in Fig. 3 and the spectral shapes in Fig. 4.

FINAL QPD SPECTRA

The final, real QPD spectrum shown in Fig. 5 is generated by adding the RR and II subspectra and plotting the result to the left of the center, which now is 0 Hz. The II subspectrum is subtracted from the RR subspectrum, and the result is plotted to the right of center. The overall separation is now the correct value of 3 Hz. Note that the high-frequency line is plotted to the left, and the low-frequency line is to the right. This is in accordance with the accepted practice of plotting the most shielded line to the right. The final, imaginary QPD spectrum is similarly generated from the sum and difference of the RI and IR subspectra, and it is also shown in the figure. In the imaginary spectrum, the shape of the 2-Hz line appears to be the reverse of the result obtained from RI − IR. The shape appears reversed because the RI − IR line is plotted by starting from the center and proceeding toward the left edge of the QPD spectrum. The final spectrum is correct; both imaginary lines have a positive 90° phase shift with respect to their corresponding absorption mode lines.

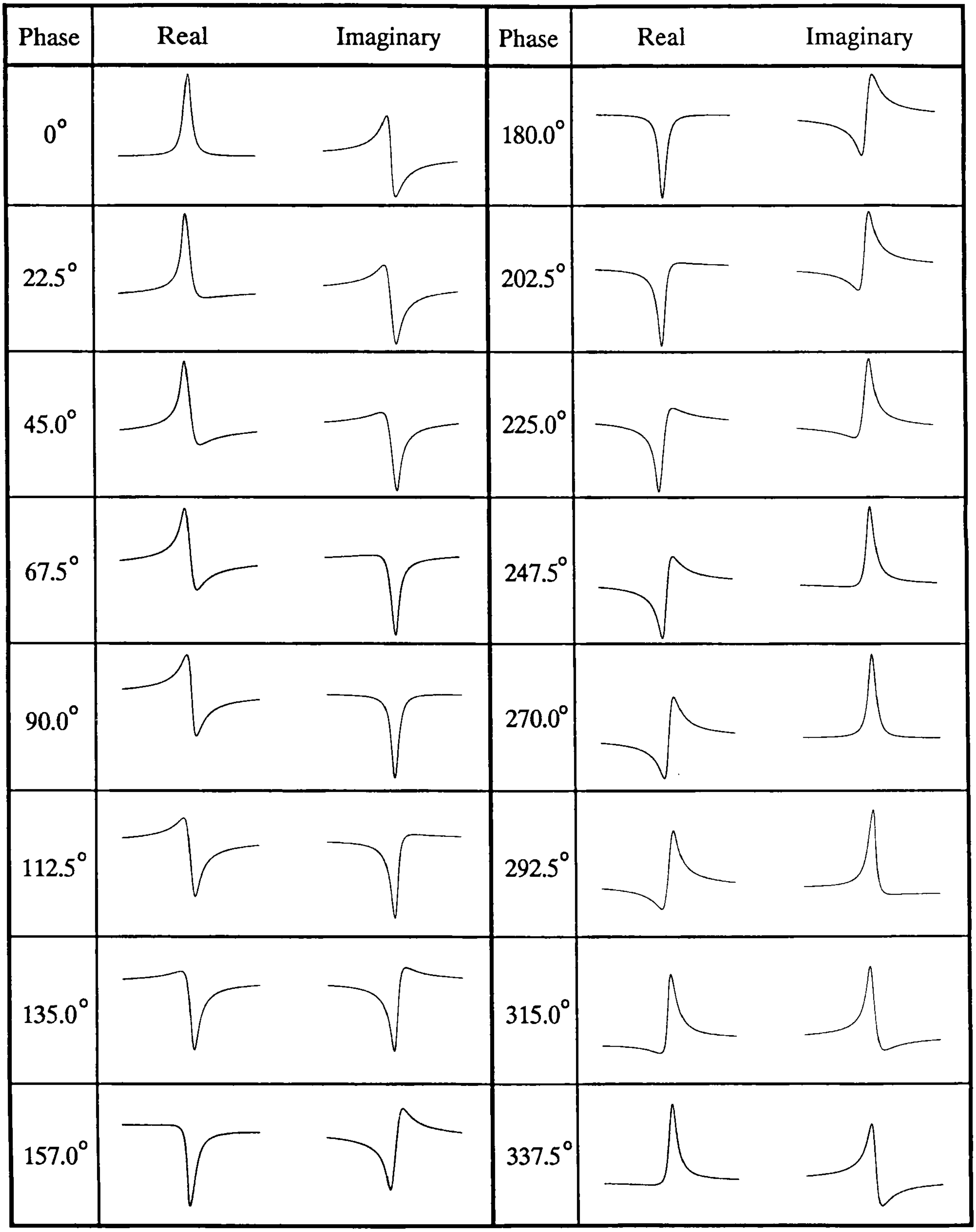


Figure 4. FID Signal Phase and Spectral Line-Shapes.

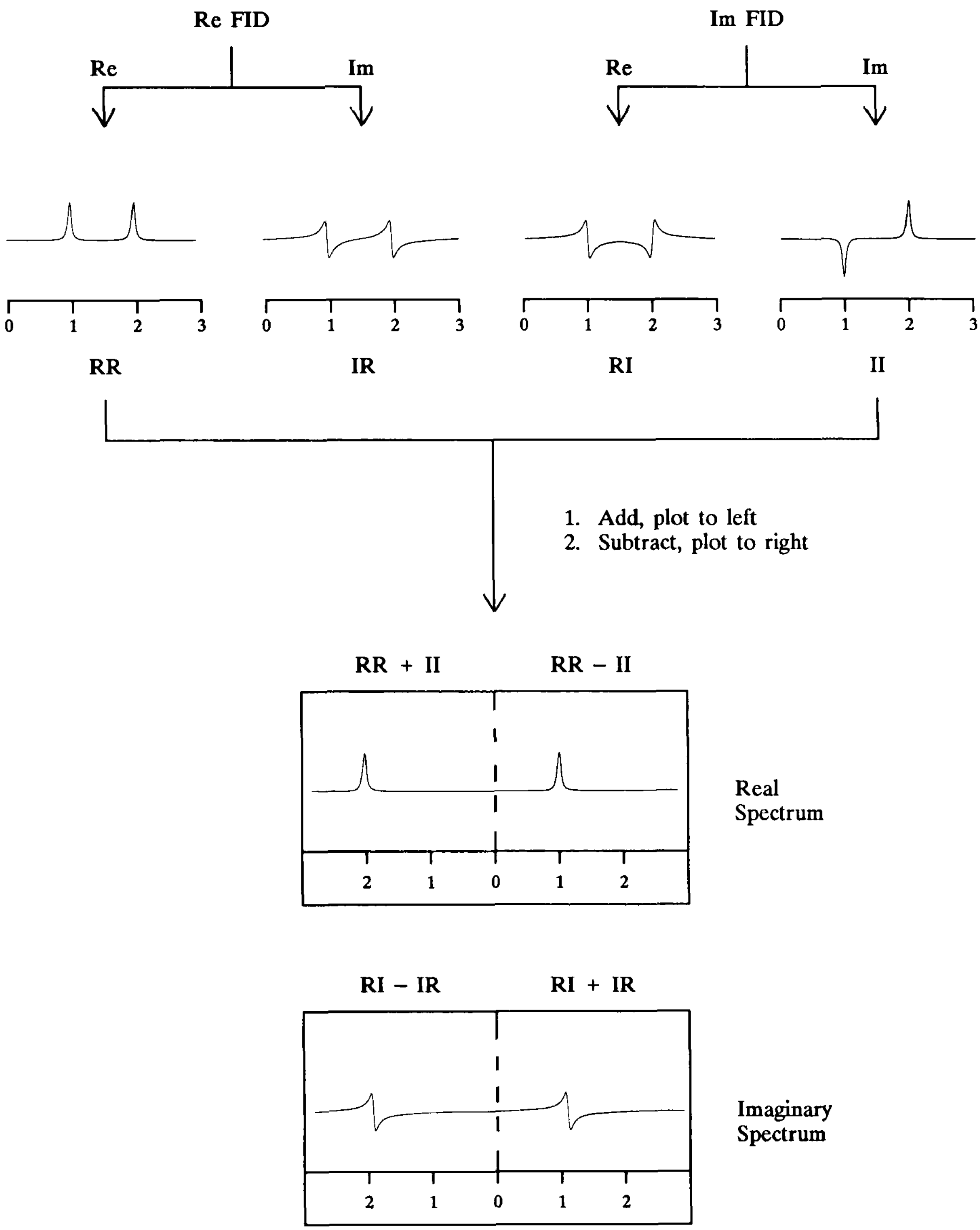


Figure 5. The four subspectra obtained from a real and an imaginary FID, and the final QPD spectra.

QPD SPECTRA FROM FIDs WITH ARBITRARY PHASE ANGLES

The procedure described above will produce the correct spectrum even if the phases of the signals in the FIDs are not exactly the same as those shown here. That is, the FIDs do not have to be pure cosine functions from one channel and pure sine functions from the other. The only requirement is that they are shifted from each other by ±90°. For example, suppose that the phase of the rf pulse is such that the magnetization vectors form a 45° angle with respect to the *-y* axis. Figure 6 shows the Re and Im FIDs, the four subspectra that would be obtained from them, and the appearances of the final Re and Im QPD spectra. Here again, the 2-Hz line appears to be reversed in both the real and the imaginary QPD spectra, for the same reason described above. The overall result is correct; both imaginary lines have a positive 90° phase shift with respect to their corresponding absorption mode lines.

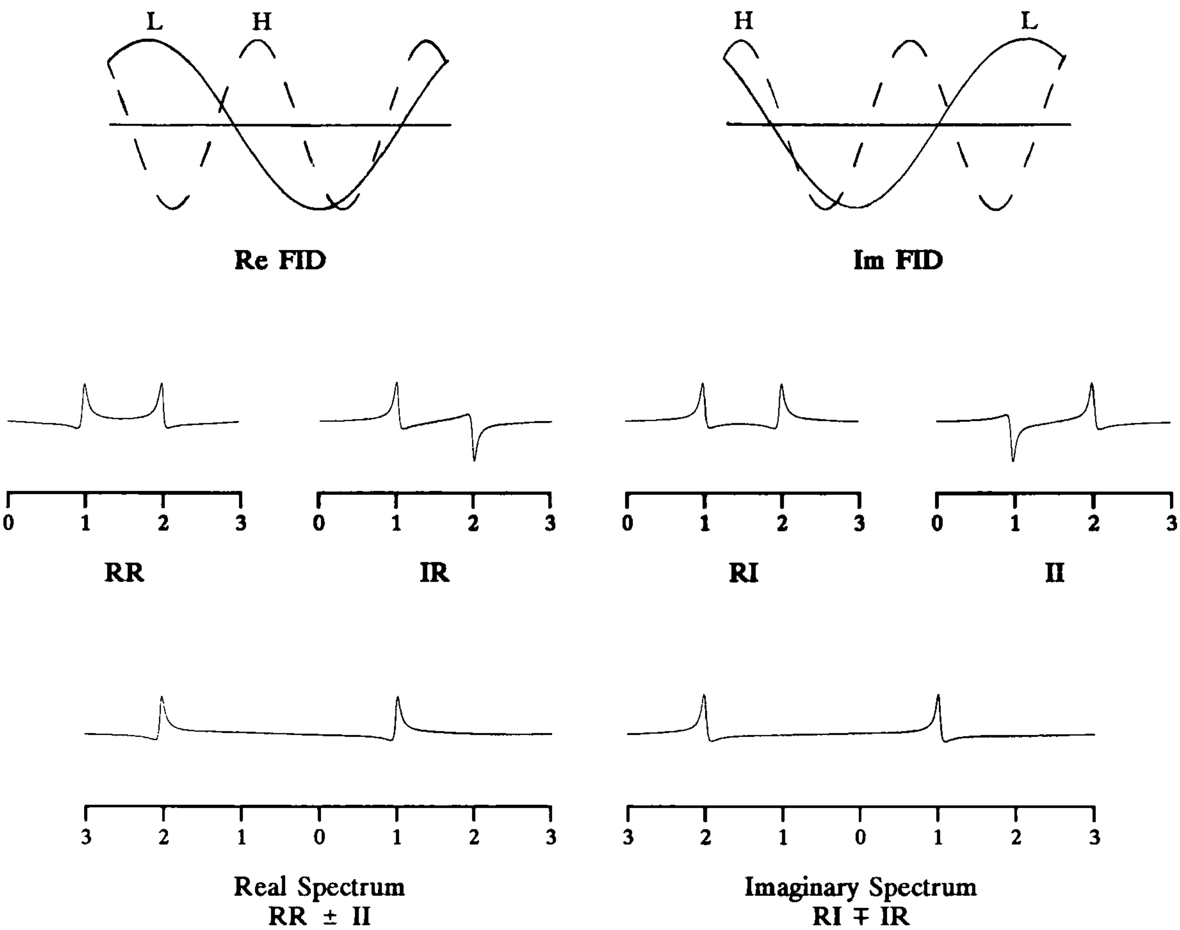


Figure 6. Subspectra and QPD spectra obtained from a 45° phase-shifted transmitter pulse.

CHANNEL IMBALANCES AND ARTIFACTS

The above procedure will not yield the correct final QPD spectra if certain instrumental conditions are not fulfilled. For example, the 1-Hz line in the II subspectrum in Fig. 5 must have the same magnitude as the corresponding line in the RR subspectrum, and these two lines must be 180° out of phase with respect to each other. If not, then complete cancellation will not occur upon addition of the spectra, and a small peak will appear 1 Hz to the left of center. Because the residual peak appears the same distance to the left of center as the actual line appears to the right, it is called a "quad" image. In addition to this image, another one will appear 2 Hz to the right of center after the subspectra are subtracted. The quad images, as well as other artifacts, appear because the two channels are not electronically balanced. These imbalances can be categorized into three general classes:

(1) Differences between the gains of the AF amplifiers in the two channels.
(2) Direct current offsets (outputs) from the amplifiers in the channels.
(3) Deviations from an exact 90° phase shift between the references to the two PSDs.

These three imbalances will be discussed separately.

Gain

The gain of an amplifier is the extent to which it will amplify, or multiply, an incoming signal. Gain is generally expressed in units of decibels (dB), defined as follows:

$$\text{dB} = 10\log(P_2/P_1)$$

P_2 and P_1 are the output and input power, respectively. Because power is directly proportional to the square of voltage or of current, dB also can be defined as follows:

$$\text{dB} = 20\log(E_2/E_1) = 20\log(I_2/I_1)$$

E and I are voltage and current, respectively.

Although the gains are adjustable for the two amplifiers used in QPD, and they are periodically adjusted during routine maintenance of a spectrometer, the gains will gradually drift. If they drift unequally, which is usually the case, then quad images can form, as described before. This will be discussed in more detail later.

DC Offset

When an amplifier is operating correctly, its output contains only noise if there is no input. If a signal is applied to the input, then the output should be simply a multiplied (amplified) reproduction of the input, plus noise. However, the output of an amplifier frequently contains a direct-current (dc) component, which often means a constant voltage that can be either positive or negative. When this occurs, the amplified FID will be shifted, either up or down, with respect to 0 V. This dc voltage is referred to as a dc offset, and it changes gradually with time. Figure 7 shows an amplified FID, without added noise, and the same FID shifted upward because of a positive dc offset. The offsets are adjustable on the amplifiers used in the two channels and are usually brought to zero during routine maintenance of the spectrometer. If this adjustment is not done, then a "spike" could appear at the center of the final QPD spectrum, as described later.

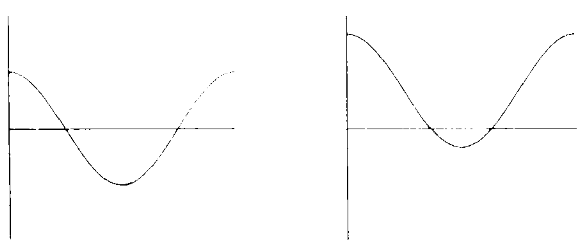


Figure 7. An FID Without and With a DC Offset.

Deviations in Reference Shift

As explained in the previous section, if the gains of the two amplifiers are not equal, then the magnitudes of the spectral lines will not be equal, resulting in incomplete cancellation of some of the lines during the addition of the RR and II subspectra. Although the spectral lines must be of equal magnitude, this condition is not itself sufficient. Even if the magnitudes are the same, the phases must be exactly 180° apart. In a properly operating system, this 180° shift is obtained from two 90° shifts. The first is from the shift applied to the references, and the second is from the combination of a real subspectrum (from one channel) with an imaginary subspectrum (from the other). Under normal conditions, the computer will provide an exact 90° shift between the real (cosine) and imaginary (sine) spectra. However, the phase-shifter that provides the shifts to the references is an electronic device, and hence is susceptible to drifting.

PHASE CYCLING: CYCLOPS

The effects from the three imbalances described above can be effectively eliminated by a phase-cycling routine. Hoult (*2*) was the first to report a procedure that accomplishes phase cycling in QPD, and it is still in general use today. The procedure is called CYCLOPS, an acronym for CYCLically Ordered Phase Sequence. CYCLOPS removes the effects of the three imbalances as described below.

Gain

Suppose that the voltage gains of the real and imaginary channels are 0.984 and 1.58 dB, respectively. After the first pulse, the relative amplitudes of the 2-Hz signals contained in their respective computer data blocks will be 1.12 and 1.20. If the inputs to these data blocks are then switched before receiving the next FIDs from the two channels, then the simple, algebraic sum of the amplitudes will be the same after time-averaging two FIDs: (1.12 + 1.20) and (1.20 + 1.12), or 2.32 for each. However, the two FIDs entering any given data block would not be phase-coherent. For example, for the real channel the first FID would be a cosine waveform; whereas the second would be a sine waveform. To make them phase-coherent, the phase of the transmitter for the second pulse is shifted 90°. If the first pulse produces a cosine and a sine for the real and imaginary FIDs, respectively, then the second pulse will produce a negative sine and a cosine for the real and imaginary FIDs, respectively; but because the two data blocks are reversed, the signals to be time-averaged will now be phase-coherent, but only for the cosine waveforms. For the sine waveforms, it is necessary only to subtract the second from the first. Note that the subtraction in the imaginary block does not reduce the amplitude — it adds them because the second waveform is inverted with respect to the first. The result is that the real data block would contain a cosine waveform with an amplitude of 2.32, which would match the amplitude of the sine waveform in the imaginary data block, also 2.32.

DC Offset

Suppose the offset from the real channel is 0.1 V. The output will be ($0.1 + \cos\omega t$), and an FT will produce a spectrum with two lines, one at 0 Hz and one at ω Hz: Recall from Reference 1 the important distinction between 0 Hz, which is a constant voltage that does not change with time, and 0 V, which is nothing at all. In the RR subspectrum, the NMR line would have a line-shape because the signal amplitude is decaying, but the 0-Hz line would be very sharp because the dc-offset amplitude is a constant and is not decaying. For the example illustrated in Fig. 5, both the RR and IR subspectra will show a spike at 0 Hz. After the addition and subtraction of the RR and II subspectra to form the final real QPD spectrum, a spike will appear at 0 Hz, exactly in the center of the spectral window. Similarly, a spike will appear exactly in the center of the final imaginary QPD spectral window. This spike is sometimes incorrectly called "pulse breakthrough."

"Pulse breakthrough" is actually the remnants of the ringdown from the rf pulse applied to the tuned receiver coil in the probe. When the pulse is applied to the tuned tank, the amplitude of the "flywheel" current (*3*) will decay exponentially with time. Immediately after the end of the pulse, this ringdown and the NMR signal are both present. Fortunately, the time constant for the ringdown is much shorter than that for most NMR signals, and it will decay to zero much more quickly. To avoid collecting the ringdown along with the NMR signal, a delay period is used that begins immediately after the pulse and ends at the beginning of acquisition of the FID. Various names are given to this delay, two of which are receiver delay and blanking time. If this delay is too short, then the tail of the ringdown "breaks through" into the acquisition time and corrupts the data in the FID.

To eliminate the 0-Hz spike, the rf phase of a third transmitter pulse is shifted 180° from the first. Then the output from the same amplifier will be ($0.1 - \cos\omega t$). Recall that the dc offset is a constant-voltage output from an amplifier, and as such, it is independent of the phase of the transmitter pulse. Subtracting the second FID from the first, in computer memory, gives $2\cos\omega t$, and eliminates the dc offset.

Deviations in Reference Shift

The elimination of artifacts from this imbalance is perhaps the most difficult to explain. Hoult (*2*) used Argand diagrams to show how CYCLOPS overcomes this phase problem. A very brief explanation will be given here, solely to introduce the concept. A more detailed one will be given later.

Suppose the phase shift between the references is 80°, instead of 90°. We begin by letting the phase for the real reference be 0°, and we use 80° for the imaginary reference. The choice of 0° does not represent a special case. We could have, albeit with some inconvenience, chosen 15°. It is important to note that an absolute phase has no physical meaning. It is significant only when it is measured with respect to another phase — two intersecting lines are needed to specify an angle.

After the first pulse, the real FID from the 2-Hz signal will be a pure cosine function (0°), but the imaginary FID will not be a pure sine. It will have a cosine component whose magnitude will be equal to cos(80°), or 0.174; the sine component will be equal to sin(80°), or 0.985. These results are shown in Fig. 8, which uses diagrams similar to those of Fig. 3. In this figure, **M** is the

Figure 8. Vector diagrams for real and imaginary references phase-shifted by only 80°, instead of 90°. These diagrams correspond to those in Fig. 3.

magnetization vector in the transverse plane after a 90° pulse, and Ref is the reference to the PSD. For the second pulse, if the phase of the transmitter is shifted 90°, then the real FID will be a pure negative sine function, but the imaginary FID will not be a pure cosine function; it will have a sine component whose amplitude is -0.174, as shown in Fig. 9.

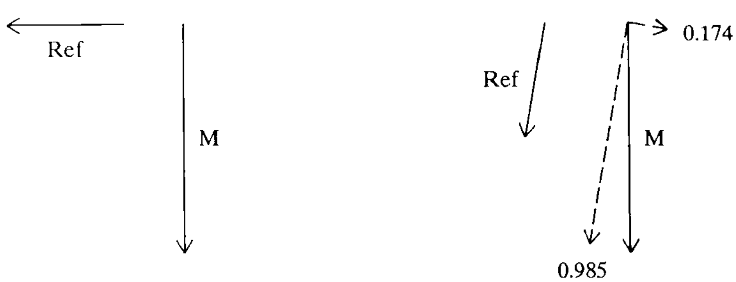


Figure 9. Vector diagrams for a 90° phase-shifted transmitter pulse. The references are also shifted as shown in Fig. 8.

As explained above, the final real FID is obtained by adding the first FID from the real channel to the second FID from the imaginary channel. The final imaginary FID is obtained by subtracting the real channel's second FID from the imaginary channel's first FID:

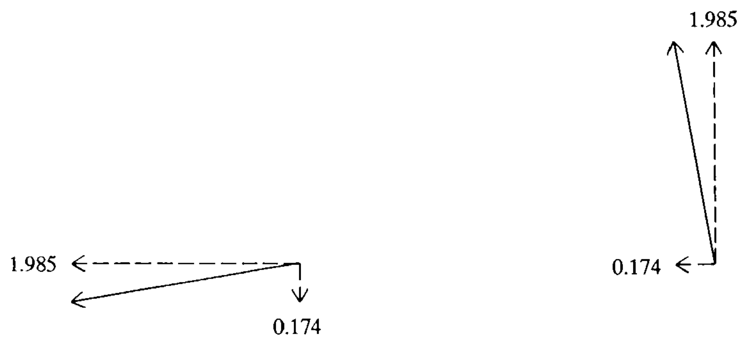
$$\text{Re FID} = \cos\omega t + 0.985\cos\omega t - 0.174\sin\omega t$$

$$= 1.985\cos\omega t - 0.174\sin\omega t$$

$$\text{Im FID} = 0.985\sin\omega t + 0.174\cos\omega t - (-\sin\omega t)$$

$$= 1.985\sin\omega t + 0.174\cos\omega t$$

The vector diagrams for the final FIDs are shown below. Note that the *resultant* vectors are now 90° apart, and not 80°.



Real Imaginary

COMPLETE CYCLOPS PROCEDURE

The complete CYCLOPS procedure accomplishes the elimination of artifacts, while simultaneously performing quadrature phase detection. The procedure is given in the table below; R and I are the FIDs obtained from the real and imaginary channels, respectively. Note that they are alternately placed in the computer data blocks labeled Re and Im. A negative sign indicates that the FID is to be subtracted.

TABLE 1
CYCLOPS Procedure

Transmitter Phase		0	90	180	270
Computer Data Blocks	Re	R	I	–R	–I
	Im	I	–R	–I	R

Figure 10 shows the vector diagram representation for the above sequence. Here, the most general case is assumed; the phase difference between the PSD references is not 90°, and the phase of the FID from the real channel is not 0°. The references to the PSDs are represented by vectors labeled Ref. For the real channel, *G* and *O* are gain and offset, and *A* is the 2-Hz signal vector, which rotates counterclockwise in this frame. The signal vector has magnitude *A* and is decomposed into two components; one parallel to, and the other perpendicular to the reference vector. The components are labeled *b* and *c*, and *b* is always the larger of the two. For the imaginary channel, the corresponding labels are *g*, *o*, *A*, *d*, and *e*. Finally, the symbols Re and Im are FIDs from the real and imaginary channels, and the numerals 1 through 4 are the FIDs obtained from the first through the fourth pulses.

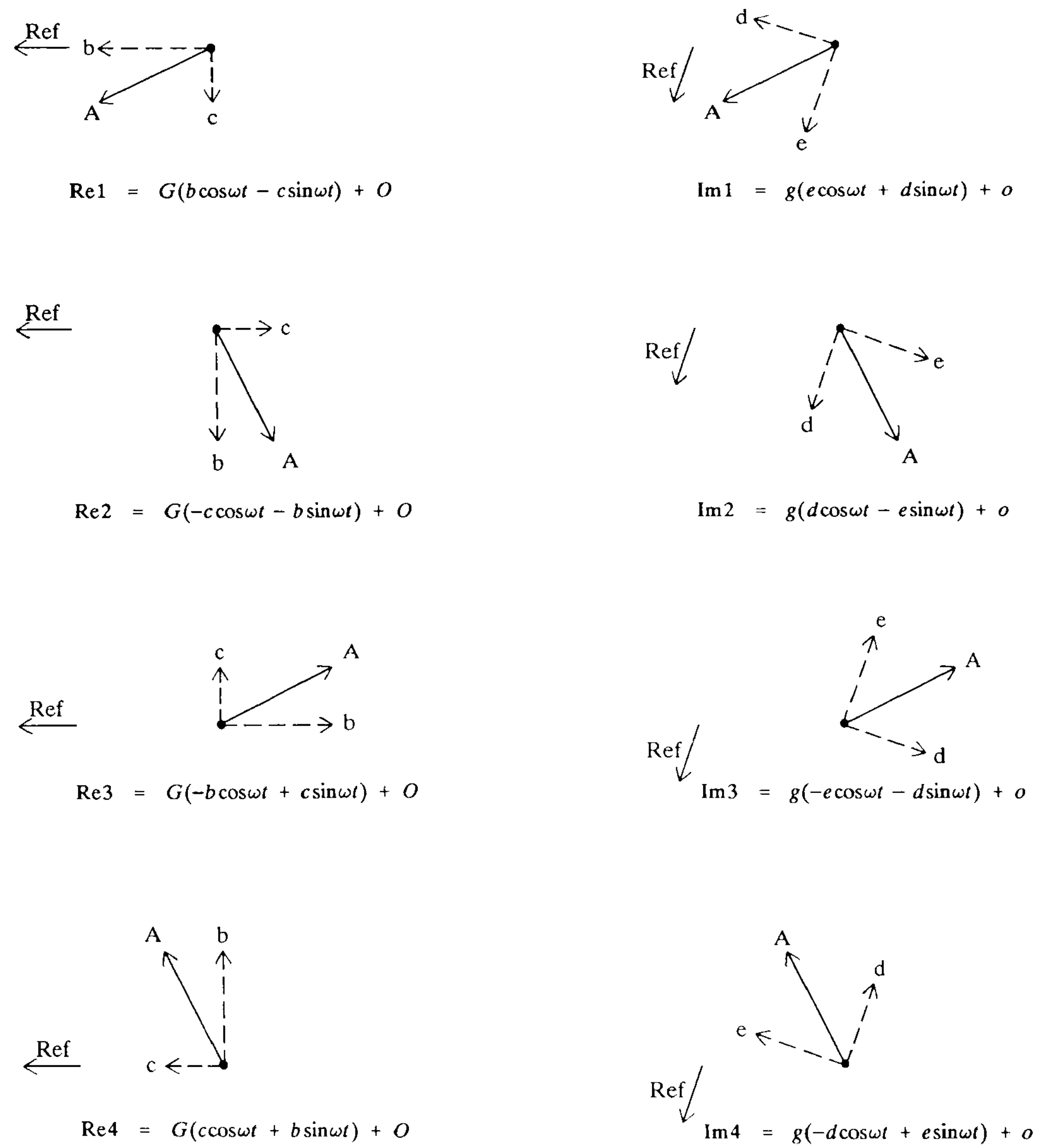


Figure 10. Signal vectors obtained from 90° phase-shifted transmitter pulses, and the vector components that are parallel and perpendicular to the real and imaginary references. The references are not shifted 90° from each other.

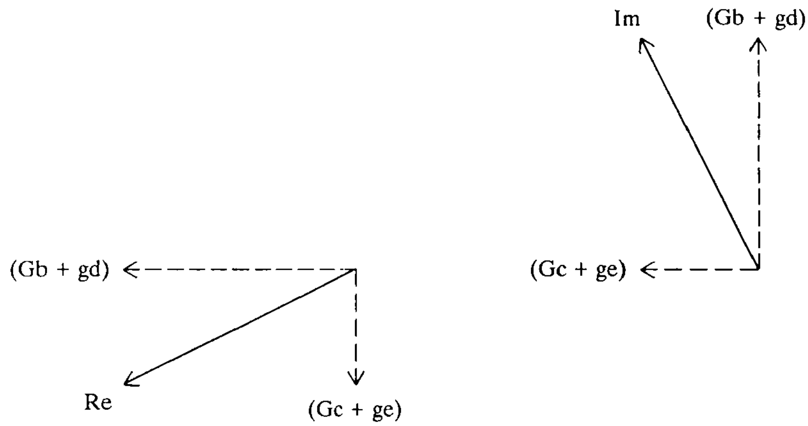
If the entries in Table 1 are replaced with those from Fig. 10, then Table 2 is produced. The final real and imaginary FIDs, and their respective vector diagrams, are shown below the table.

TABLE 2
CYCLOPS Procedure Using Figure 10

Pulse Number		1	2	3	4
Computer Data Blocks	Re	Re1	Im2	−Re3	−Im4
	Im	Im1	−Re2	−Im3	Re4

$$\begin{aligned}
\text{Final Re FID} &= \text{Re1} + \text{Im2} - \text{Re3} - \text{Im4} \\
&= [G(b\cos\omega t - c\sin\omega t) + O] + [g(d\cos\omega t - e\sin\omega t) + o] \\
&\quad - [G(-b\cos\omega t + c\sin\omega t) + O] - [g(-d\cos\omega t + e\sin\omega t) + o] \\
&= 2(Gb + gd)\cos\omega t - 2(Gc + ge)\sin\omega t
\end{aligned}$$

$$\begin{aligned}
\text{Final Im FID} &= \text{Im1} - \text{Re2} - \text{Im3} + \text{Re4} \\
&= [g(e\cos\omega t + d\sin\omega t) + o] - [G(-c\cos\omega t - b\sin\omega t) + O] \\
&\quad - [g(-e\cos\omega t - d\sin\omega t) + o] + [G(c\cos\omega t + b\sin\omega t) + O] \\
&= 2(Gc + ge)\cos\omega t + 2(Gb + gd)\sin\omega t
\end{aligned}$$



Real Imaginary

The phase cycling is now complete. Note the following points:

(1) The offsets from both channels have been eliminated.
(2) The vector sums in both of the above vector diagrams are equal; hence, the amplitudes of both FIDs are equal.
(3) The phase-angle difference between the resultant real and imaginary vectors is 90°.

ADVANTAGES OF QPD

A QPD system that uses CYCLOPS to eliminate artifacts has three major advantages over a single-PSD system. Each of these is described below.

Simplification of Spectra

As described previously for a single-PSD system, if the pulsed rf is positioned between resonance frequencies, then lines on one side will "fold" into the final spectrum, because this system cannot distinquish between frequencies that are above or below the pulsed rf. This folding produces a complicated spectrum that is difficult to interpret. A QPD system eliminates folding to produce a spectrum that is easier to interpret.

Conservation of Transmitter Power

In FTNMR, when a single frequency is pulsed, rf power is distributed on both sides of the pulsed frequency. When a single PSD system is used, the pulsed rf must be positioned to one side of all the resonance frequencies of a sample. Therefore, the rf power distributed on the opposite side is totally wasted. Furthermore, the power distribution on either side is not flat, and with increasing distance, it decreases gradually in frequency space from the pulsed rf. In a QPD system, the pulsed rf can be positioned in the middle of the resonance frequencies. Hence, rf power is not only conserved, but is flatter over the spectral range.

Increase in Sensitivity

When the pulsed rf is positioned completely to one side of all the resonance frequencies, the output from a single PSD contains all the audio frequencies from 0 Hz up to the spectral width (SW) set by the operator. As described here and in Reference 1, a lowpass filter is employed to attenuate all frequencies higher than this band-width. These higher frequencies are all noise, and if they are not attenuated, they will "alias" into the spectrum to reduce S/N. This aliasing is frequently called Nyquist folding. However, noise on the opposite side, which is called out-of-band noise, cannot be distinguished from noise on the side containing the resonance frequencies. This noise is called in-band noise. This out-of-band noise, which encompasses one band-width, will fold into the spectrum to reduce S/N by $\sqrt{2}$. This is depicted in Fig. 11A. On the other hand, with a QPD system, the highest frequency of interest in either FID is SW/2. The band-widths of the lowpass filters placed at the outputs of the two PSDs, as shown in Fig. 2, can now be reduced to one-half of that used for a single-PSD system; to SW/2, instead of to SW. Now, no out-of-band noise will fold into the spectrum, and the S/N is increased by $\sqrt{2}$ over that obtained from a single-PSD system (Fig. 11B).

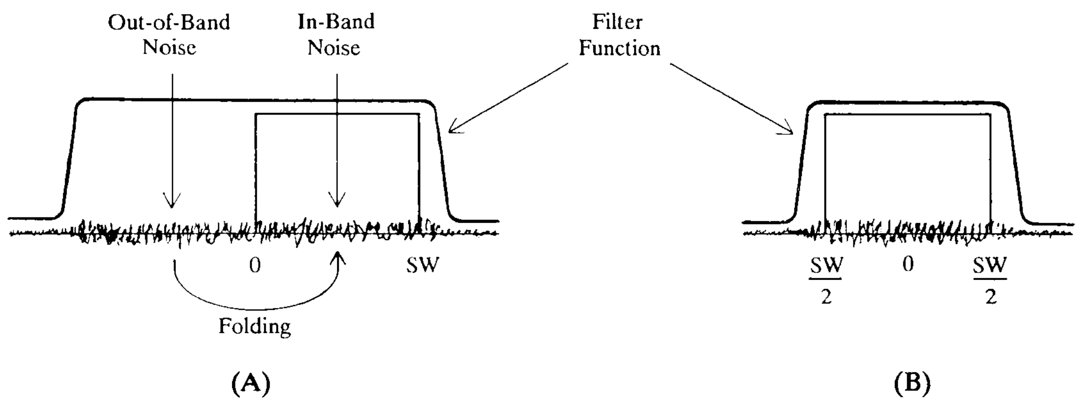


Figure 11. Effects of low-pass filters in (A) single and in (B) quadrature PSD systems.

SUMMARY

When only one PSD is used in the receiver section of an NMR spectrometer, NMR resonance frequencies on one side of the pulsed rf will "fold" into the spectrum, because a single PSD cannot distinguish between frequencies that are lower than the reference frequency and those that are higher. This folding can easily complicate the interpretation of the spectrum. Hence, the pulsed rf must be set to one side of all the resonance frequencies. This requirement allows out-of-band noise to fold into the spectrum and to reduce S/N by $\sqrt{2}$. It also wastes one-half of the transmitter power and produces a relatively large power drop-off as a function of frequency.

A QPD system uses two PSDs to eliminate the problems mentioned above. The references to the PSDs are derived from the same source, but one is phase-shifted by 90° with respect to the other. Two FIDs are obtained from the PSDs; one is called the real FID and the other is called the imaginary FID; the combination is a complex FID. When an FT is performed on each FID, a real and an imaginary spectrum are produced. The four subspectra can be combined to produce one real and one imaginary spectrum — neither one containing folded lines — even when the pulsed rf is positioned between resonance frequencies.

The electronic components used in the two channels have properties that gradually change with time, causing imbalances between the channels that can produce images in the final spectra as well as a spike in the center. A phase-cycling procedure, called CYCLOPS, can effectively eliminate these artifacts. The procedure requires that four pulses be applied, with the phases of the rf being successively shifted by 90°. In addition, the FIDs from the two PSDs are alternately placed into two separate computer data blocks, with the appropriate addition or subtraction of the FIDs to maintain phase coherence.

Because a QPD system used in conjunction with CYCLOPS allows the pulsed rf to be positioned between resonance frequencies, the power drop-off as a function of frequency is less, and power is conserved. In addition, the band-widths of the LPFs can be reduced to one-half of the spectral width. Hence, out-of-band noise is prevented from aliasing into the spectrum, resulting in overall S/N that is $\sqrt{2}$ greater than that obtained from a single-PSD system.

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