NMR Part II, Quadrature Detection

Quadrature detection uses two detector channels separated by 90 degrees. This distinguishes the direction of rotation (clockwise or counterclockwise) in the rotating frame of the spectrometer. This document shows how the quadrature signal is transformed to produce the real and imaginary spectra.

Signals Generated: This section defines the signals that are observed. You can change the amplitude, frequency, phase, and relaxation constants for each nucleus. The system will accept two different nuclei so that you can compare the effect of different settings.

	Wave a	Wave b
Amplitude of Wave	$A_a := 1$	$A_b := 1$
Frequency of Wave	$\nu_a := 1 \cdot Hz$	$\nu_b := -2 \cdot Hz$
Phase of Wave	$\theta_a := 0 \cdot rad$	$\theta_b := 0 \cdot rad$
Relaxation Constant	$T_a := 5 \cdot sec$	$T_b := 5 \cdot sec$

Sampling Parameters: This section defines the sampling parameters of the spectrometer. You can change the number of data points and the dwell time. These settings effect the resolution, spectral window, and acquisition time.

Number of Data Points Sampled $N := 2^{10}$ (must be a binary number)

Dwell Time $DW := 0.08 \cdot sec$

Non-Ideal Problems: These parameters reflect non-ideal conditions that occur in a real spectrometer. You can set these to non zero values to see how they effect the spectrum.

Error in Quad Phase Shift $\phi := \frac{0}{12} \cdot \pi$

Imbalance of Imaginary Amplifier Gain $Gain_{rel\_error} := 0 \cdot \%$

DC in Real Channel (% of Total Amplitude) $DC_{Real} := 0 \cdot \%$

DC in Imaginary Channel (% of Total Amplitude) $DC_{Imag} := 0 \cdot \%$

Calculated Parameters: The following are calculated from the above parameters.

Acquisition Time	$AT := DW \cdot N$	$AT = 81.92 \cdot sec$
Spectral Window	$SW := \frac{1}{2 \cdot DW}$	$SW = 6.25 \cdot Hz$
Resolution	$Resolution := \frac{1}{AT}$	$Resolution = 0.012 \cdot Hz$
Phase shift error		$\phi = 0 \cdot deg$
DC offset, Real channel	$DC_R := DC_{Real} \cdot (A_a + A_b)$	$DC_R = 0$
DC offset, Imaginary channel	$DC_I := DC_{Imag} \cdot (A_a + A_b)$	$DC_I = 0$
Amplifier Gain mismatch	$G_I := (1 + Gain_{rel\_error})$	$G_I = 1$
Angular Frequency Wave a	$\omega_a := 2 \cdot \pi \cdot \nu_a$	$\omega_a = 6.283 \cdot rad \cdot sec^{-1}$
Wave b	$\omega_b := 2 \cdot \pi \cdot \nu_b$	$\omega_b = -12.566 \cdot rad \cdot sec^{-1}$
Number of data points		$N = 1.024 \cdot 10^3$

Index: These indexes are used for various calculations

Index Counters

$$i := 0, 1 .. (N - 1)$$

$$j := 0, 1 .. \left(\frac{N}{2} - 1\right)$$

Time Index

$$t_i := i \cdot DW$$

Frequency Index

$$frequency_j := \frac{j}{N \cdot DW}$$

Frequency Index for Quadrature spectra

$$frequency_{quad_i} := \left(\frac{i}{N \cdot DW}\right) - \frac{N - 1}{2 \cdot N \cdot DW}$$

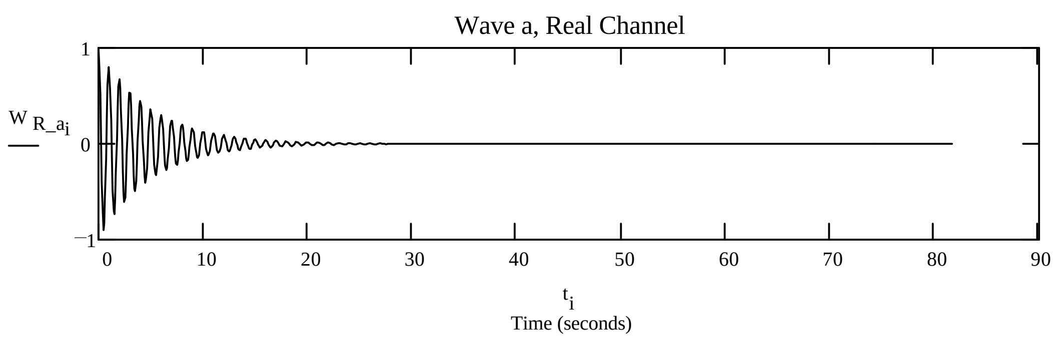
Real Channel: For quadrature detection, two signal channels are used. One is the called the real channel. The real channel produces a cosine wave. Below are the calculations used to generate the signal for this channel.

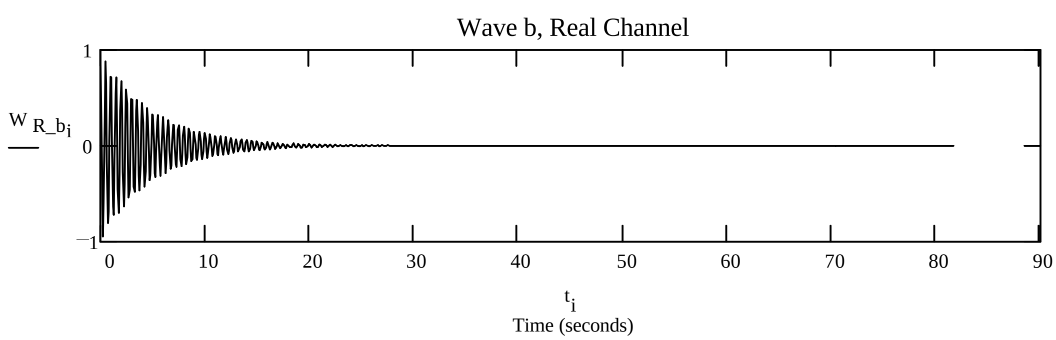
Calculate FID: FID for the real channel based upon the above information.

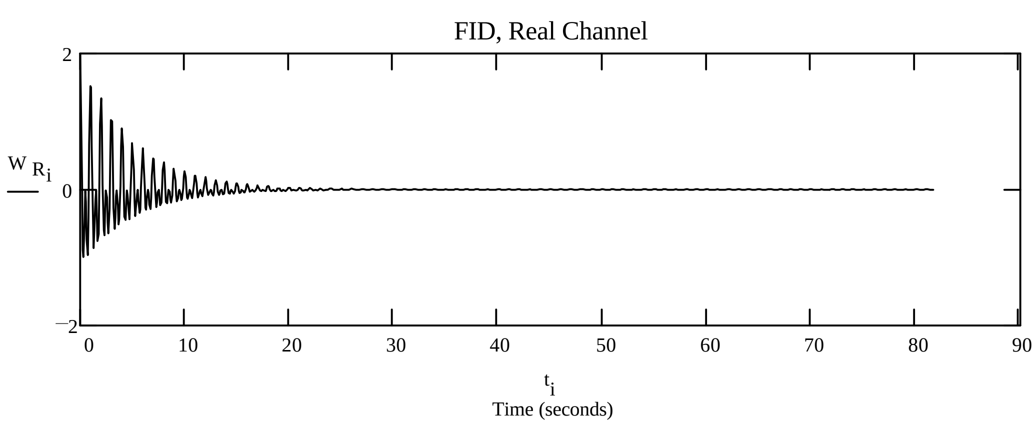
Wave a $$W_{R\_a_i} := A_a \cdot \cos\left(t_i \cdot \omega_a + \theta_a\right) \cdot e^{-\frac{t_i}{T_a}} + DC_R$$

Wave b $$W_{R\_b_i} := A_b \cdot \cos\left(t_i \cdot \omega_b + \theta_b\right) \cdot e^{-\frac{t_i}{T_b}} + DC_R$$

Sum of Waves a and b $$W_R := W_{R\_a} + W_{R\_b}$$





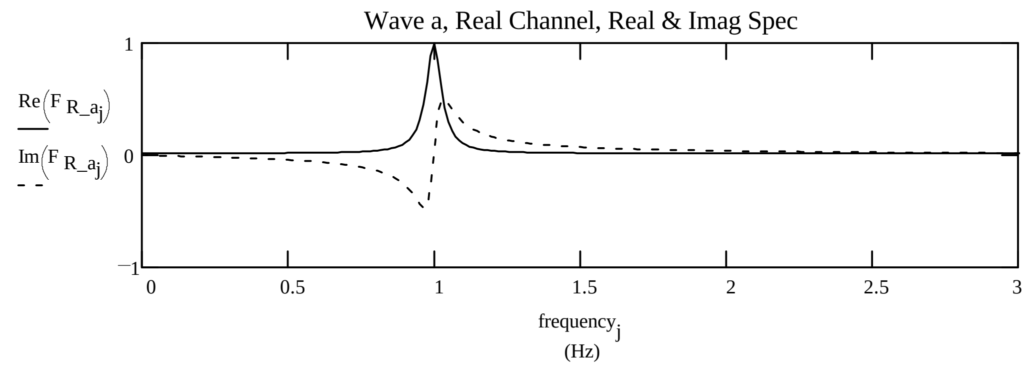


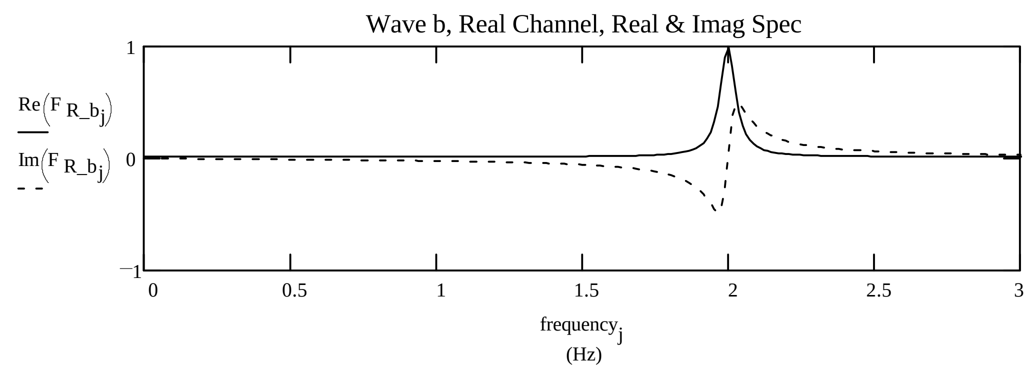
Fourier Transform Signal From Real Channel: The Fourier transform of the signal from the real channel produces a real and an imaginary spectrum. The real spectrum corresponds to the absorption mode spectrum or the cosine component. The imaginary spectrum corresponds to the dispersion mode spectrum or the sine component. These are labeled the real spectrum of the real channel (real of the real) and the imaginary spectrum of the real channel (imaginary of the real).

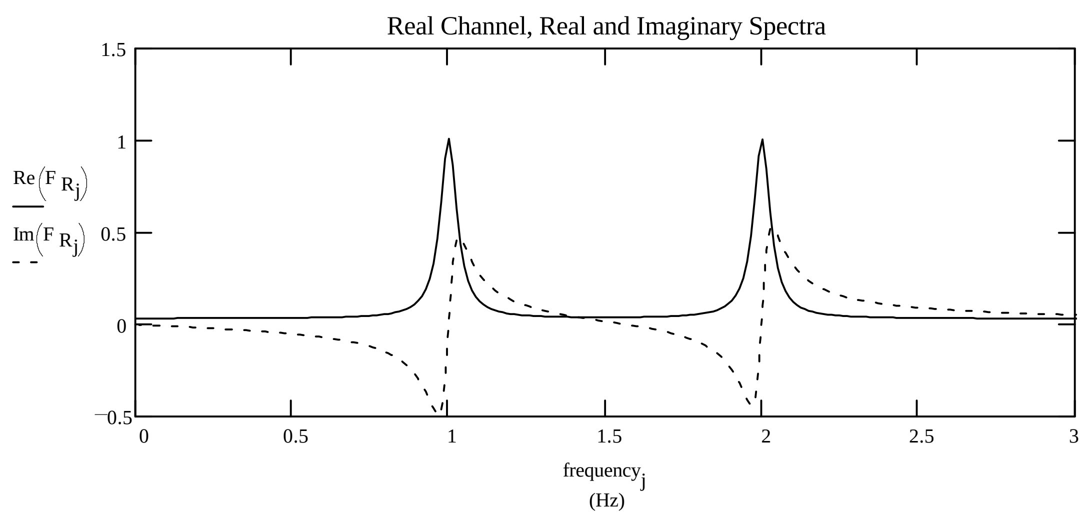
FFT of Real FID a $F_{R\_a} := \mathrm{fft}\left(W_{R\_a}\right)$

FFT of Real FID b $F_{R\_b} := \mathrm{fft}\left(W_{R\_b}\right)$

FFT of Real FID (Sum) $F_{R} := \mathrm{fft}\left(W_{R}\right)$







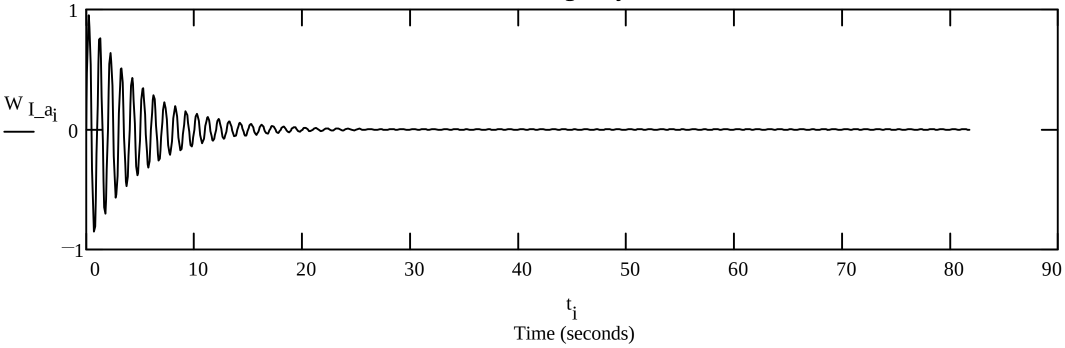
Generating Imaginary Channel. The second quadrature channel is called the imaginary channel. It is oriented 90 degrees from the real channel. This produces a signal that corresponds to a sine wave.

Generating FID:

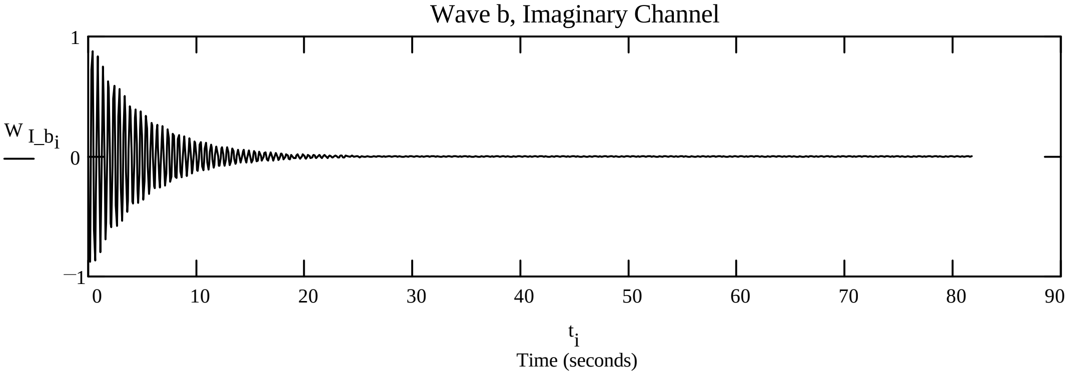
$$W_{I\_a_i} := G_I \cdot A_a \cdot \sin\left(t_i \cdot \omega_a + \theta_a + \phi\right) \cdot e^{-\frac{t_i}{T_a}} + DC_I$$

$$W_{I\_b_i} := G_I \cdot A_b \cdot \sin\left(t_i \cdot \omega_b + \theta_b + \phi\right) \cdot e^{-\frac{t_i}{T_b}} + DC_I \qquad W_I := W_{I\_a} + W_{I\_b}$$

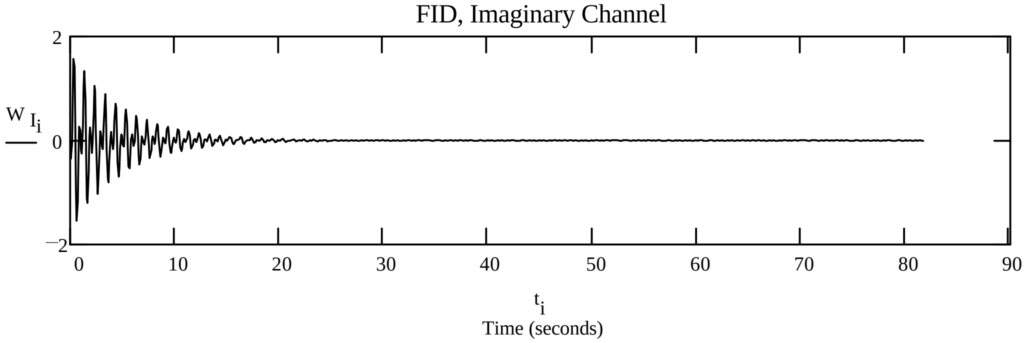
Wave A, Imaginary Channel



Wave b, Imaginary Channel

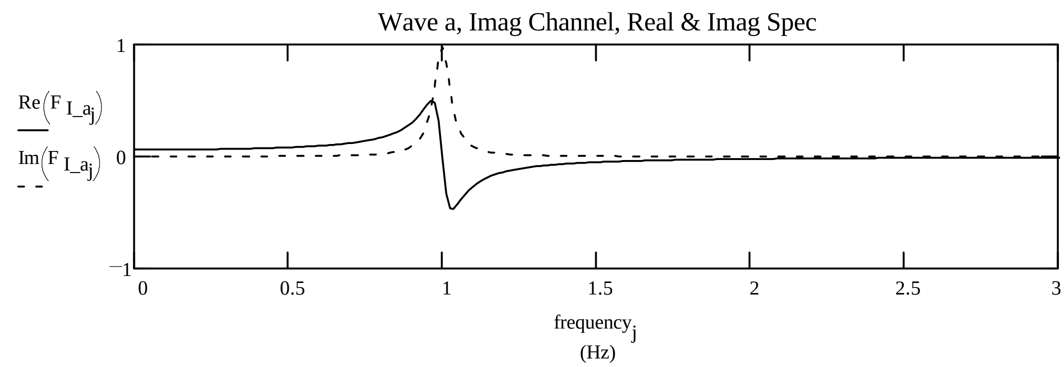


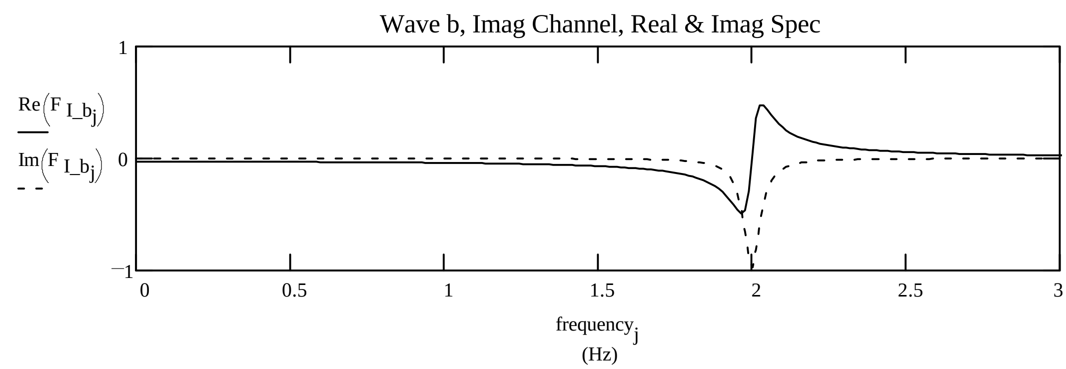
FID, Imaginary Channel

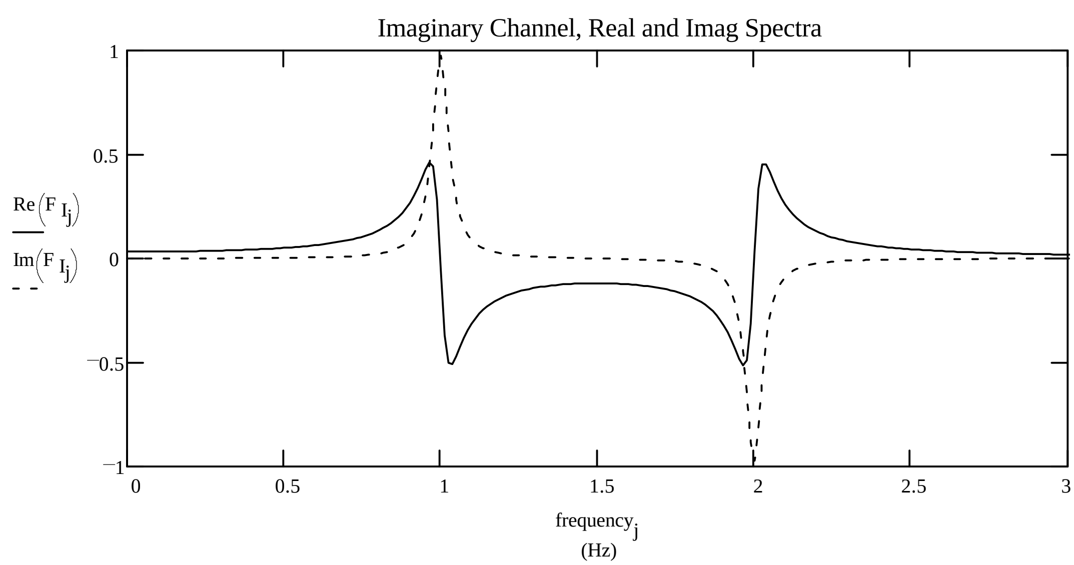


Fourier Transforms of Imaginary Channel FID: The FT of the imaginary channel also produces a real and imaginary spectrum. These are labeled the real spectrum of the imaginary channel, and the imaginary spectrum of the imaginary channel.

FFT of Imaginary FID a	$F_{I\_a} := \mathrm{fft}\left(W_{I\_a}\right)$
FFT of Imaginary FID b	$F_{I\_b} := \mathrm{fft}\left(W_{I\_b}\right)$
FFT of Imaginary Channel FID (Sum)	$F_{I} := \mathrm{fft}\left(W_{I}\right)$







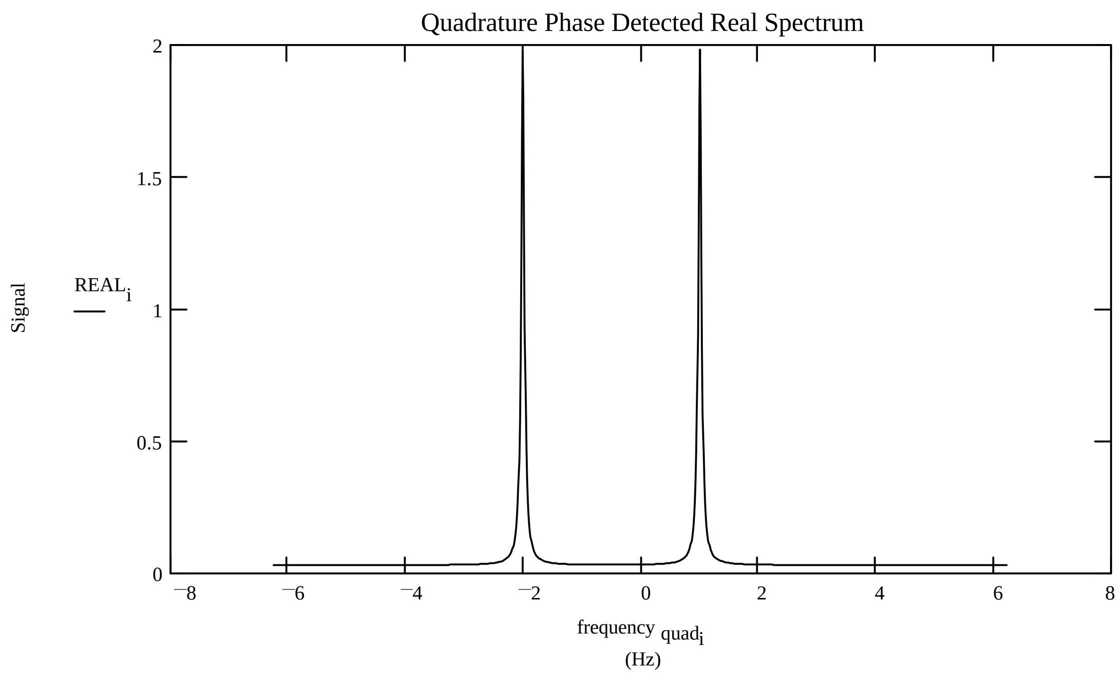
Quadrature Manipulation. The spectra from the Real and Imaginary channel are combined to produce a single set of quadrature detected real and imaginary spectra.

Generating the Real Spectrum: The real spectrum is generated from the real spectrum of the real channel and the imaginary spectrum of the imaginary channel. The left side of the real spectrum (frequencies less than the spectrometer frequency) is generated by subtracting the real of the real and the imaginary of the imaginary. The resulting matrix is inverted to follow convention for the display of spectra. The right side of the spectrum (frequencies greater than the spectrometer frequency) is generated by adding the imaginary of the imaginary and the real of the real. The final spectrum is displayed by placing the two spectra side by side. 0 Hz is in the center. To the right is increasing frequency, to the left is reduced frequency (relative to the spectrometer frequency). This conforms with standard NMR data presentation.

To understand how this spectrum is produced, examine the real spectrum from the real channel and the imaginary spectrum of the imaginary channel. Pay close attention to the phase differences between signals with positive and negative frequencies.

$$REAL_{left} := Re(F_R) - Im(F_I) \qquad REAL_{right} := Re(F_R) + Im(F_I)$$

$$REAL_j := REAL_{left}{}_{\left(\frac{N}{2}-1\right)-j} \qquad REAL_{\left(\frac{N}{2}+j\right)} := REAL_{right}{}_j$$

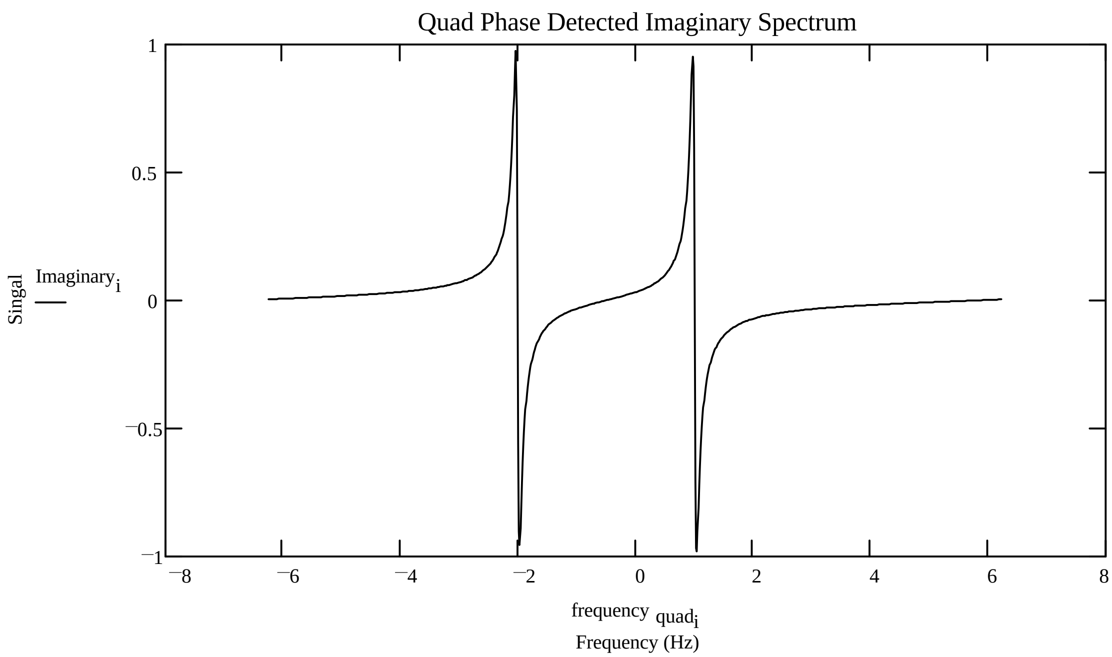


Generating the Imaginary Spectrum: The quadrature detected imaginary spectrum is produced in a similar manner using the imaginary spectrum from the real channel and the real channel of the imaginary spectrum.

To understand what happens here, examine the imaginary spectrum from the real channel and the real spectrum from the imaginary channel.

$Imaginary_{left} := Re(F_I) + Im(F_R)$ $Imaginary_{right} := Re(F_I) - Im(F_R)$

$Imaginary_j := Imaginary_{left_{\left(\frac{N}{2}-1\right)-j}}$ $Imaginary_{\left(\frac{N}{2}+j\right)} := Imaginary_{right_j}$



Questions

1. Change the signal frequency and observe how this changes the FID and the spectra. Pay close attention to the phase of the intermediate spectra, and think about how they are manipulated to produce the quadrature spectra.
   a. Change the frequency so that it is greater than the spectral window.
   b. Enter a negative frequency and see what happens.

2. Make changes to the non-ideal settings and observe how they effects the intermediate spectra and the final spectrum.

3. What advantages does quadrature phase detection have?

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