NMR Part III, Quadrature Phase Cycling

Quadrature phase cycling removes spectral artifacts created by non-ideal conditions in the NMR electronics. These artifacts are caused by DC offset, gain mismatch, and phase error in the receiver amplifiers. Phase cycling eliminates these artifacts by changing the transmitter phase in the sequence 0, 90, 180, 270. The computer combines the real and imaginary spectra from each channel for each step of the sequence to generate the final phase cycled spectrum. In this process the signals add, but the artifacts cancel. If you look closely at the intermediate spectra you can see how this works.

Signals Generated:

	Wave a	*Wave b*
Amplitude of Wave	$A_a := 1$	$A_b := 1$
Frequency of Wave	$\nu_a := 2 \cdot Hz$	$\nu_b := -5 \cdot Hz$
Phase of Wave	$\theta_a := 0 \cdot rad$	$\theta_b := 0 \cdot rad$
Relaxation Constant	$T_a := 4 \cdot sec$	$T_b := 4 \cdot sec$

Sampling Parameters:

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

Dwell Time $DW := 0.08 \cdot sec$

Non-Ideal Problems:

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

Imbalance in Imaginary Amplifier Gain $G_e := 0 \cdot \%$

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

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

Calculated Values:

Phase Shift Error $\phi = 0 \cdot deg$

Receiver Gain Mismatch $G_I := (1 + G_e)$ $G_I = 1$

DC offset, Real Channel $DC_R := DC_{R\_e} \cdot (A_a + A_b)$ $DC_R = 0$

DC offset, Imaginary Channel $DC_I := DC_{I\_e} \cdot (A_a + A_b)$ $DC_I = 0$

Radial Frequency:

$\omega_a := 2 \cdot \pi \cdot \nu_a$ $\omega_b := 2 \cdot \pi \cdot \nu_b$

Index and Miscellaneous Calculations:

$i := 0, 1 .. (N - 1)$ $t_i := i \cdot DW$

$j := 0, 1 .. \left(\frac{N}{2} - 1\right)$ $frequency_j := \frac{j}{N \cdot DW}$ $frequency\ quad_i := \left(\frac{i}{N \cdot DW}\right) - \frac{N - 1}{2 \cdot N \cdot DW}$

First Step

Generation of the first step is shown in detail. Subsequent cycles are shown in an abbreviated format. For the first step, the transmitter phase is at 0 degrees. For additional information on quadrature detection, see the worksheet on *Quadrature Detection in NMR*.

Real Channel. These equations generate the FID signal and the spectrum for the real channel (The cosine signal).

The FID $$W_{R1_i} := \left(A_a \cdot \cos\left(t_i \cdot \omega_a + \theta_a\right) \cdot e^{-\frac{t_i}{T_a}} + DC_R\right) + \left(A_b \cdot \cos\left(t_i \cdot \omega_b + \theta_b\right) \cdot e^{-\frac{t_i}{T_b}} + DC_I\right)$$

The Spectrum $$F_{R1} := \mathrm{fft}\left(W_{R1}\right)$$

Imaginary Channel. The imaginary channel is rotated 90 degrees from the real channel (so it corresponds to the sine signal).

The FID $$W_{I1_i} := \left(G_I \cdot A_a \cdot \sin\left(t_i \cdot \omega_a + \theta_a + \phi\right) \cdot e^{-\frac{t_i}{T_a}} + DC_R\right) + \left(G_I \cdot A_b \cdot \sin\left(t_i \cdot \omega_b + \theta_b + \phi\right) \cdot e^{-\frac{t_i}{T_b}} + DC_I\right)$$

The Spectrum $$F_{I1} := \mathrm{fft}\left(W_{I1}\right)$$

Quadrature Manipulation. The real and imaginary spectra from the real and imaginary channels are manipulated to produce the real and imaginary quadrature spectra for this step. This notation is a bit confusing, but hold on. It gets more interesting.

Generating the Real. The real quadrature spectrum is generated from the real of the real and the imaginary of the imaginary. These are added to produce the right half of the spectrum and subtracted (then inverted) to produce the left half of the spectrum.

$$Real_{left1} := \mathrm{Re}\left(F_{R1}\right) - \mathrm{Im}\left(F_{I1}\right) \qquad Real_{right1} := \mathrm{Re}\left(F_{R1}\right) + \mathrm{Im}\left(F_{I1}\right)$$

$$Real_{1_j} := Real_{left1_{\left(\frac{N}{2}-1\right)-j}} \qquad Real_{1_{\left(\frac{N}{2}+j\right)}} := Real_{right1_j}$$

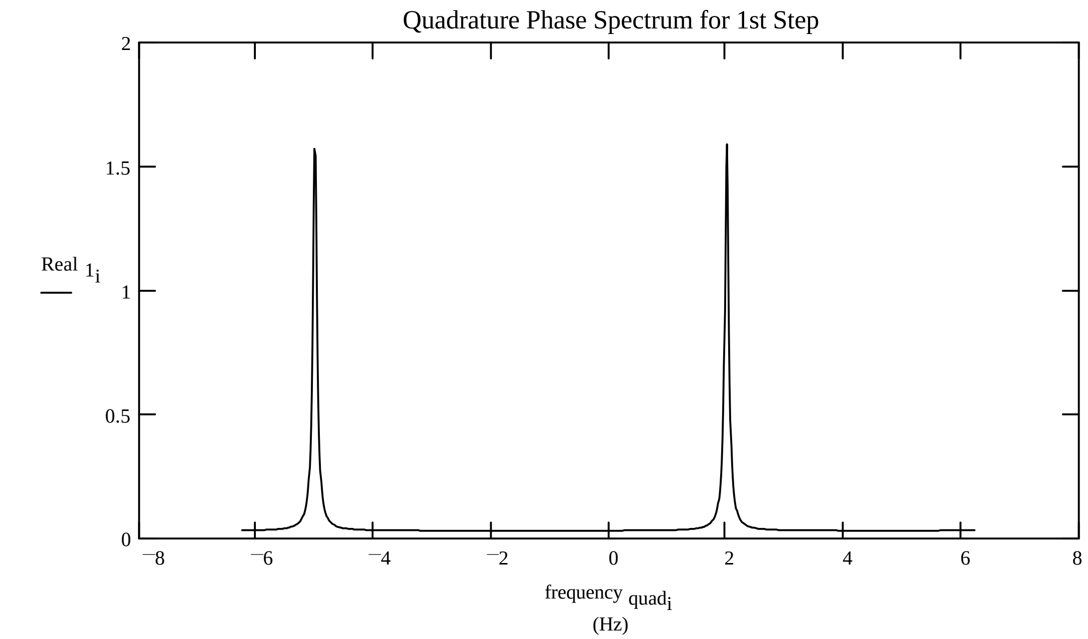
Generating the Imaginary. Similarly, the imaginary quadrature spectrum is generated from the imaginary of the real, and the real of the imaginary.

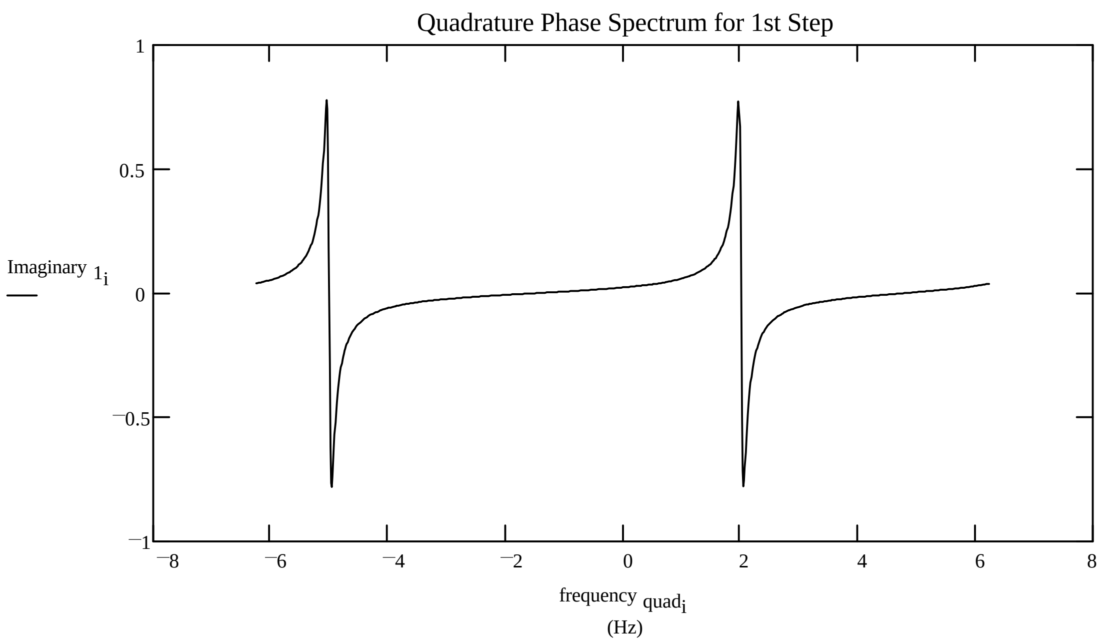
$$Imaginary_{left1} := \mathrm{Re}\left(F_{I1}\right) + \mathrm{Im}\left(F_{R1}\right) \qquad Imaginary_{right1} := \mathrm{Re}\left(F_{I1}\right) - \mathrm{Im}\left(F_{R1}\right)$$

$$Imaginary_{1_j} := Imaginary_{left1_{\left(\frac{N}{2}-1\right)-j}} \qquad Imaginary_{1_{\left(\frac{N}{2}+j\right)}} := Imaginary_{right1_j}$$

The Spectrum for the First Step.

These manipulations give the real and imaginary spectra from the first step of the phase cycle routine. Pay close attention to the phase of the signal peaks, and the phase of the various spectral artifacts (the spike at 0 Hz from the DC offset, and the ghost peaks from phase and gain imperfections. The phase cycling will cancel the artifacts, and add the signal.





Second Step 90°.

In the Second step of the phase cycle the transmitter phase is rotated 90 degrees (π/2 radians) from the first step.

Real Channel.

FID $$W_{R2_i} := \left(A_a \cdot \cos\left(t_i \cdot \omega_a + \theta_a + \frac{\pi}{2}\right) \cdot e^{\frac{-t_i}{T_a}} + DC_R\right) + \left(A_b \cdot \cos\left(t_i \cdot \omega_b + \theta_b + \frac{\pi}{2}\right) \cdot e^{\frac{-t_i}{T_b}} + DC_I\right)$$

Spectrum $$F_{R2} := \mathrm{fft}(W_{R2})$$

Imaginary Channel.

FID $$W_{I2_i} := \left(G_I \cdot A_a \cdot \sin\left(t_i \cdot \omega_a + \theta_a + \phi + \frac{\pi}{2}\right) \cdot e^{\frac{-t_i}{T_a}} + DC_I\right) + \left(G_I \cdot A_b \cdot \sin\left(t_i \cdot \omega_b + \theta_b + \phi + \frac{\pi}{2}\right) \cdot e^{\frac{-t_i}{T_b}} + DC_I\right)$$

Spectrum $$F_{I2} := \mathrm{fft}(W_{I2})$$

Quadrature Manipulation:

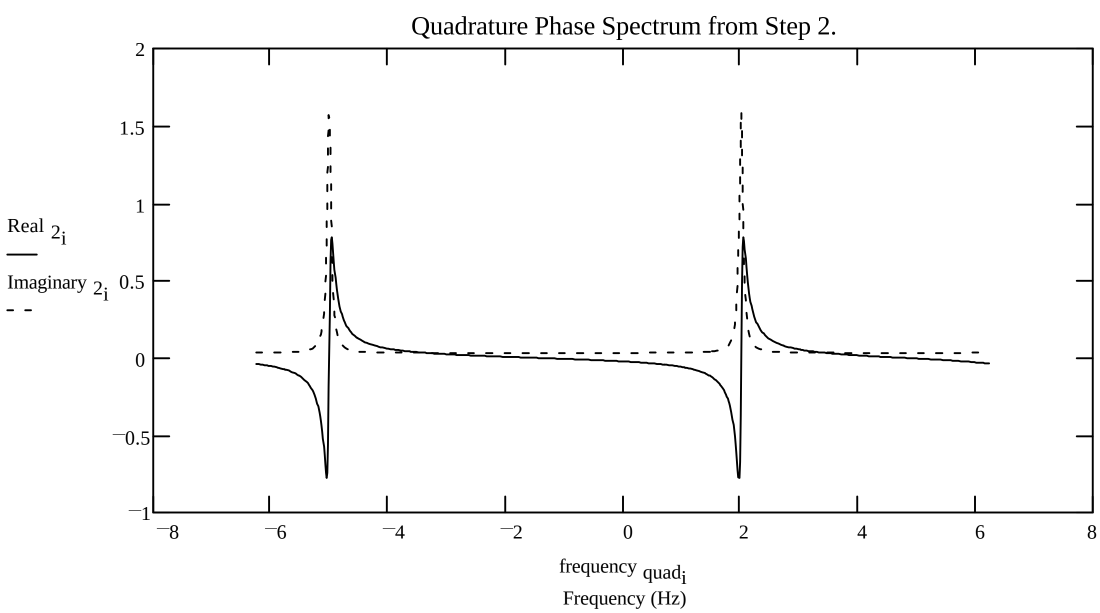
Generating the Real and Imaginary.

$$Real_{left2} := \mathrm{Re}(F_{R2}) - \mathrm{Im}(F_{I2}) \qquad Real_{right2} := \mathrm{Re}(F_{R2}) + \mathrm{Im}(F_{I2})$$

$$Real_{2_j} := Real_{left2_{\left(\frac{N}{2}-1\right)-j}} \qquad Real_{2_{\left(\frac{N}{2}+j\right)}} := Real_{right2_j}$$

$$Imaginary_{left2} := \mathrm{Re}(F_{I2}) + \mathrm{Im}(F_{R2}) \qquad Imaginary_{right2} := \mathrm{Re}(F_{I2}) - \mathrm{Im}(F_{R2})$$

$$Imaginary_{2_j} := Imaginary_{left2_{\left(\frac{N}{2}-1\right)-j}} \qquad Imaginary_{2_{\left(\frac{N}{2}+j\right)}} := Imaginary_{right2_j}$$



Third Step 180°. In the third step of the phase cycle the transmitter phase is at 180 degrees (π rad) relative to the first step.

Real Channel.

$$W_{R3_i} := \left(A_a \cdot \cos\left(t_i \cdot \omega_a + \theta_a + \pi\right) \cdot e^{\frac{-t_i}{T_a}} + DC_R\right) + \left(A_b \cdot \cos\left(t_i \cdot \omega_b + \theta_b + \pi\right) \cdot e^{\frac{-t_i}{T_b}} + DC_R\right)$$

$$F_{R3} := \mathrm{fft}\left(W_{R3}\right)$$

Imaginary Channel.

$$W_{I3_i} := G_I \cdot A_a \cdot \sin\left(t_i \cdot \omega_a + \theta_a + \phi + \pi\right) \cdot e^{\frac{-t_i}{T_a}} + DC_I + G_I \cdot A_b \cdot \sin\left(t_i \cdot \omega_b + \theta_b + \phi + \pi\right) \cdot e^{-\frac{t_i}{T_b}} + DC_I$$

$$F_{I3} := \mathrm{fft}\left(W_{I3}\right)$$

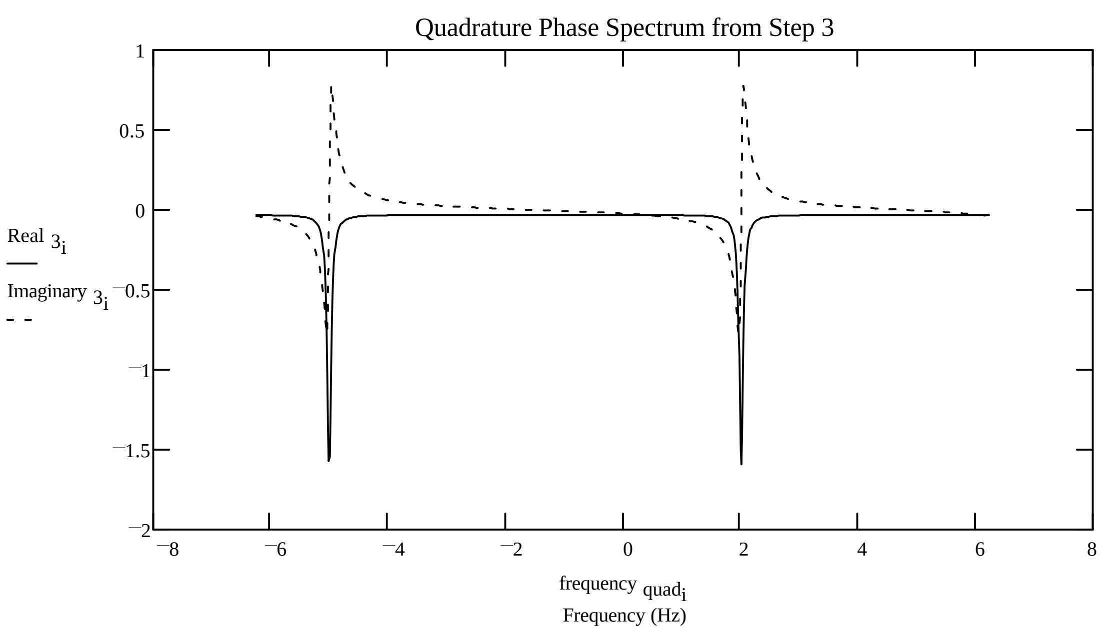
Quadrature Manipulation: Generating the Real and Imaginary.

$$Real_{left3} := \mathrm{Re}\left(F_{R3}\right) - \mathrm{Im}\left(F_{I3}\right) \qquad Real_{right3} := \mathrm{Re}\left(F_{R3}\right) + \mathrm{Im}\left(F_{I3}\right)$$

$$Real_{3_j} := Real_{left3_{\left(\frac{N}{2}-1\right)-j}} \qquad Real_{3_{\left(\frac{N}{2}+j\right)}} := Real_{right3_j}$$

$$Imaginary_{left3} := \mathrm{Re}\left(F_{I3}\right) + \mathrm{Im}\left(F_{R3}\right) \qquad Imaginary_{right3} := \mathrm{Re}\left(F_{I3}\right) - \mathrm{Im}\left(F_{R3}\right)$$

$$Imaginary_{3_j} := Imaginary_{left3_{\left(\frac{N}{2}-1\right)-j}} \qquad Imaginary_{3_{\left(\frac{N}{2}+j\right)}} := Imaginary_{right3_j}$$



Fourth Step 270º.

In the fourth step of the phase the transmitter phase is at 270 degrees (3/2 π radian) relative to the first step.

Real Channel.

$$W_{R4_i} := \left(A_a\cdot\cos\left(t_i\cdot\omega_a+\theta_a+\frac{3\cdot\pi}{2}\right)\cdot e^{\frac{-t_i}{T_a}}+DC_R\right)+\left(A_b\cdot\cos\left(t_i\cdot\omega_b+\theta_b+\frac{3\cdot\pi}{2}\right)\cdot e^{-\frac{t_i}{T_b}}+DC_R\right)$$

$$F_{R4} := \mathrm{fft}\left(W_{R4}\right)$$

Imaginary Channel.

$$W_{I4_i} := A_a\cdot\sin\left(t_i\cdot\omega_a+\theta_a+\phi+\frac{3\cdot\pi}{2}\right)\cdot e^{\frac{-t_i}{T_a}}+DC_I+G_I\cdot A_b\cdot\sin\left(t_i\cdot\omega_b+\theta_b+\phi+\frac{3\cdot\pi}{2}\right)\cdot e^{-\frac{t_i}{T_b}}+DC_I$$

$$F_{I4} := \mathrm{fft}\left(W_{I4}\right)$$

Quadrature Manipulation:

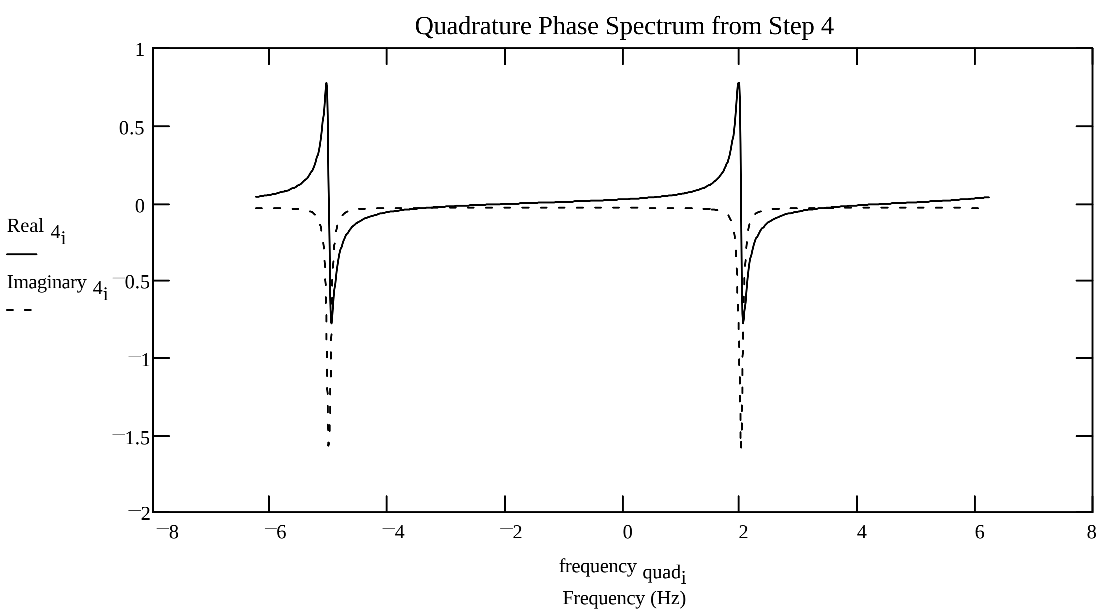
Generating the Real and Imaginary.

$$Real_{left4} := Re\left(F_{R4}\right)-Im\left(F_{I4}\right) \qquad Real_{right4} := Re\left(F_{R4}\right)+Im\left(F_{I4}\right)$$

$$Real_{4_j} := Real_{left4_{\left(\frac{N}{2}-1\right)-j}} \qquad Real_{4_{\left(\frac{N}{2}+j\right)}} := Real_{right4_j}$$

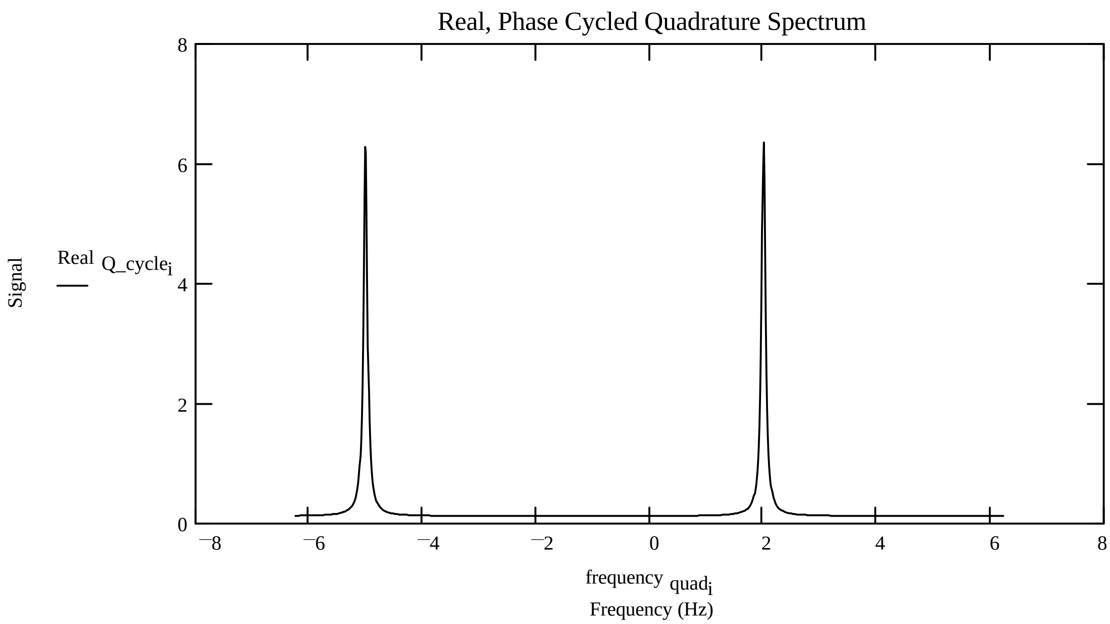
$$Imaginary_{left4} := Re\left(F_{I4}\right)+Im\left(F_{R4}\right) \qquad Imaginary_{right4} := Re\left(F_{I4}\right)-Im\left(F_{R4}\right)$$

$$Imaginary_{4_j} := Imaginary_{left4_{\left(\frac{N}{2}-1\right)-j}} \qquad Imaginary_{4_{\left(\frac{N}{2}+j\right)}} := Imaginary_{right4_j}$$

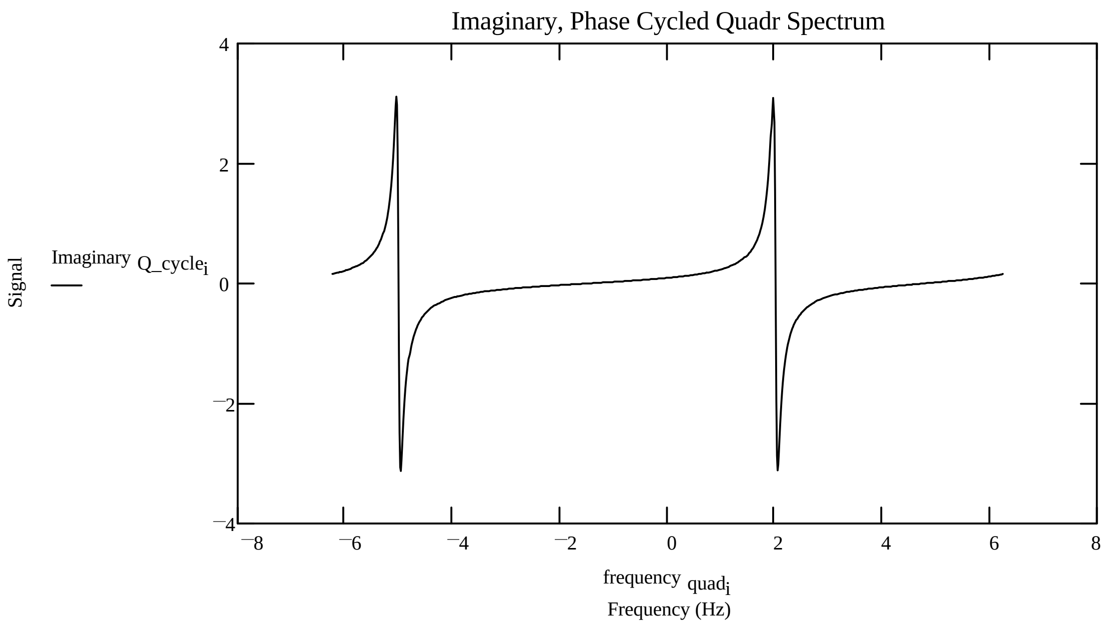


Phase Cycling Effect. Finally the spectra collected from each step of the phase cycle are combined to produce the quadrature phase cycled spectrum. Notice that the signals add, but the artifacts have a different phase relationship so they cancel.

$$\text{Real}_{\text{Q\_cycle}_i} := \text{Real}_{1_i} + \text{Imaginary}_{2_i} - \text{Real}_{3_i} - \text{Imaginary}_{4_i}$$



$$\text{Imaginary}_{\text{Q\_cycle}_i} := \text{Imaginary}_{1_i} - \text{Real}_{2_i} - \text{Imaginary}_{3_i} + \text{Real}_{4_i}$$



Questions.

1. Closely observe the phase relationship for the intermediate spectra from each step of the phase cycle. How do these intermediate spectra add together to produce the final spectra.

2. Adjusting the Non-Ideal problems.
   a. How does this effect the intermediate spectra?
   b. How does this effect the final phase cycled spectrum?
   c. Look closely at the phase relationships for all these spectra to find how the artifacts cancel.

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