NMR Part I, An Introduction

This worksheet is an introduction to how a FID is produced and then transformed to the frequency domain. It is interactive, so you can change the variables and see how they effect the signal.

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

	Nucleus a	*Nucleus b*
Amplitude	$A_a := 1$	$A_b := 1$
Frequency	$\nu_a := 1 \cdot Hz$	$\nu_b := 2 \cdot Hz$
Relaxation	$T_a := 10 \cdot sec$	$T_b := 10 \cdot sec$

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

Number of Data Points Sampled (binary number.) $N := 2^9$ $N = 512$

Dwell Time $DW := 0.10 \cdot sec$

Calculated Parameters:

Acquisition Time	$AT := DW \cdot N$	$AT = 51.2 \cdot sec$
Spectral Window	$SW := \frac{1}{2 \cdot DW}$	$SW = 5 \cdot Hz$
Digital Resolution	$Resolution := \frac{1}{AT}$	$Resolution = 0.02 \cdot Hz$
Angular Frequency Nucleus a	$\omega_a := 2 \cdot \pi \cdot \nu_a$	$\omega_a = 6.283 \cdot rad \cdot sec^{-1}$
Nucleus b	$\omega_b := 2 \cdot \pi \cdot \nu_b$	$\omega_b = 12.566 \cdot rad \cdot sec^{-1}$

Index: These Indexes are used for calculations.

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

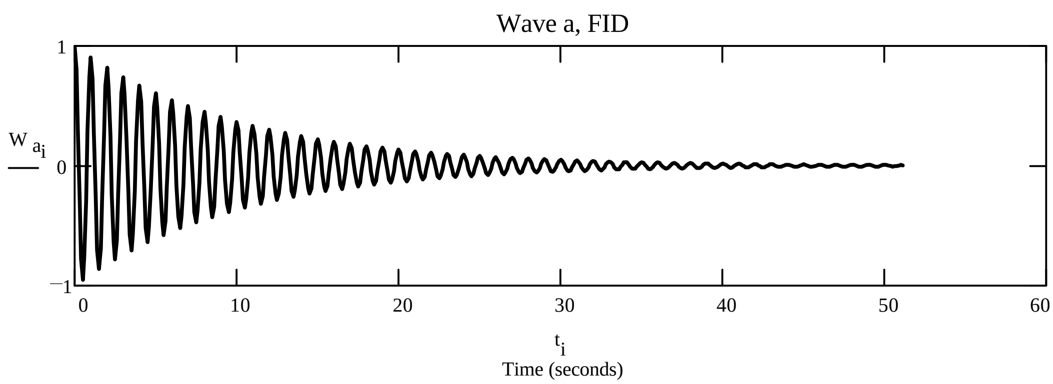
$j := 0, 1 .. \left(\frac{N}{2} - 1\right)$ $frequency_j := \frac{j}{N \cdot DW}$ Frequency index

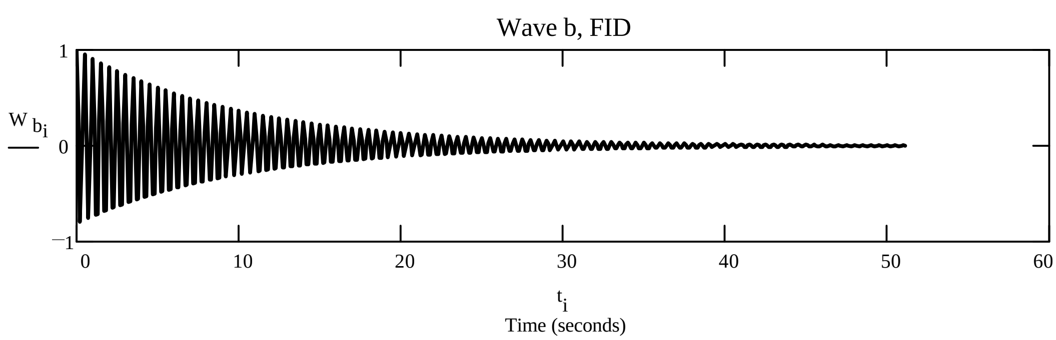
Calculate Waveforms: Calculate the FID from the above information.

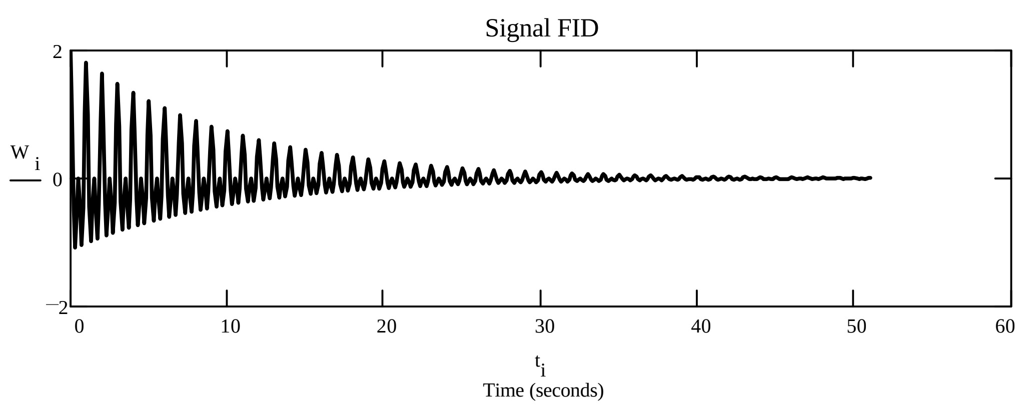
Wave a $$W_{a_i} := A_a \cdot \cos\left(t_i \cdot \omega_a\right) \cdot e^{-\frac{t_i}{T_a}}$$

Wave b $$W_{b_i} := A_b \cdot \cos\left(t_i \cdot \omega_b\right) \cdot e^{-\frac{t_i}{T_b}}$$

Signal $$W := W_a + W_b$$





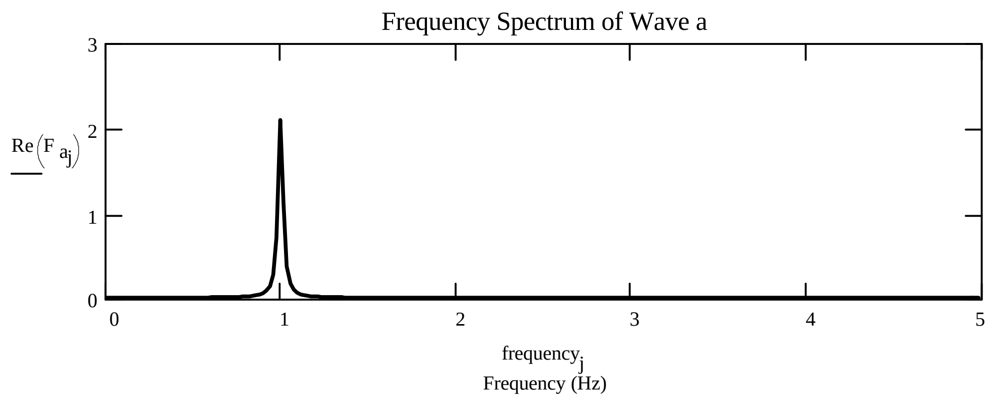


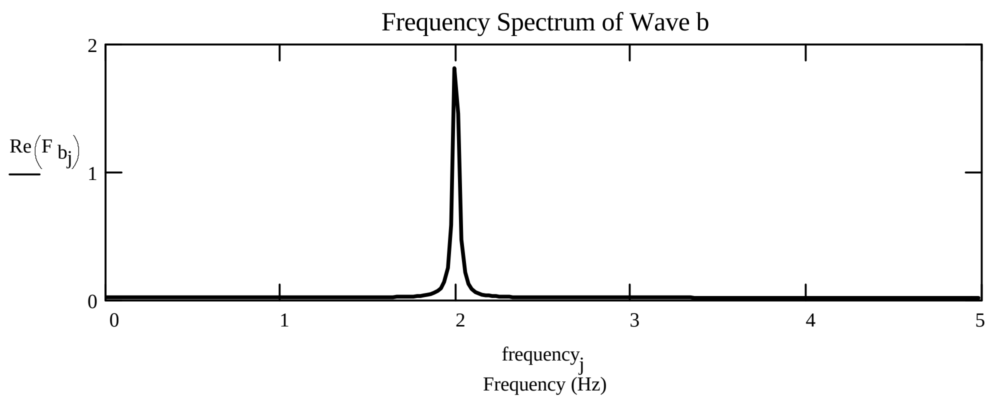
Fourier Transforms: Fourier transform FID to produce frequency domain signal (spectrum).

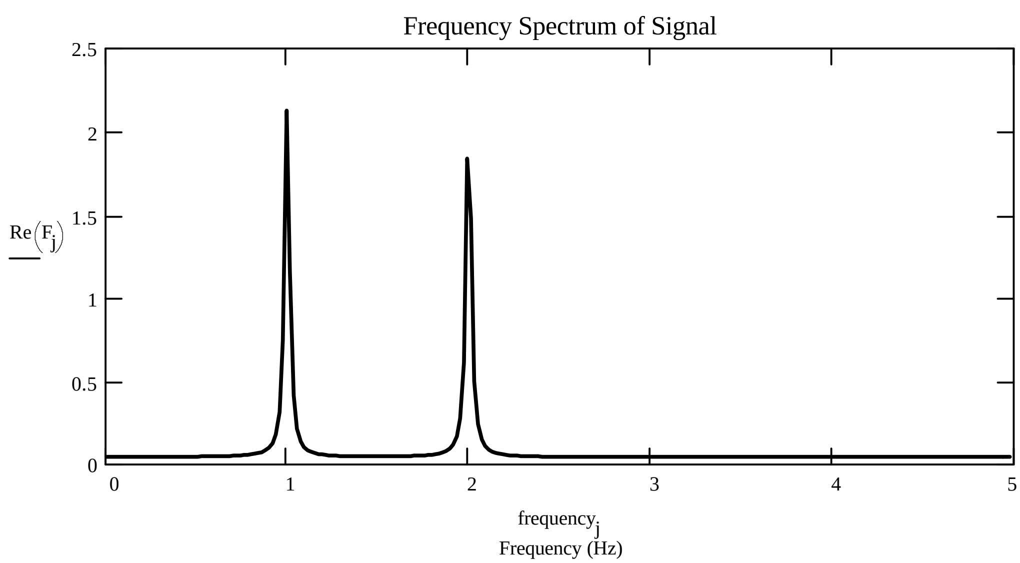
FFT Wave a $F_a := \mathrm{fft}(W_a)$

FFT Wave b $F_b := \mathrm{fft}(W_b)$

FFT sum of a and b $F := \mathrm{fft}(W)$







Questions

1. Change the signal frequency and observe how this changes the FID and the spectrum. Change the frequency so that it is greater than the spectral window. What happens? Enter a negative frequency. What happens?

2. Change the signal amplitude to observe how this effects the spectrum. If one wave is very large and the other is very small, what happens.

3. Change the relaxation time constant and observe how this effects the FID and the spectrum. What happens if the relaxation rate is very long? What happens if it is very short?

4. Change the sampling parameters and see how this effects the spectrum. First reduce the dwell time and notice what happens to the calculated parameters (the resolution, acquisition time, and spectral window) and the axis on the graphs (the FID and the spectrum). Then change the number of data points and notice what happens to all these parameters (And how long the calculations take).

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