# NMR Part IV, Apodization and Zero Filling

This worksheet is an introduction to how apodization and zero filling enhance S/N and resolution. It is interactive, so you can change the variables and see how they effect the signal.

**Noise Level**:

Noise $noise := 0.2$

**Sampling Parameters:** This section defines the spectrometer sampling parameters. These will effect the resolution, spectral window, and acquisition time.

Number of Data Points Sampled (binary.) $N := 2^8$ $N = 256$

Dwell Time $DW := 0.01 \cdot sec$ $AT := DW \cdot N$

**Signals Generated:** This section defines the observed signals. You can change the amplitude, frequency and relaxation constants for each nucleus.

| | *Nucleus a* | *Nucleus b* |
|---|---|---|
| Amplitude | $A_a := 1$ | $A_b := 1$ |
| Frequency | $\nu_a := 10 \cdot Hz$ | $\nu_b := 20 \cdot Hz$ |
| Relaxation | $T_a := 1 \cdot sec$ | $T_b := 1 \cdot sec$ |
| Angular Frequency | $\omega_a := 2 \cdot \pi \cdot \nu_a$ | $\omega_b := 2 \cdot \pi \cdot \nu_b$ |

**Index:** These Indexes are used for various calculations.

$i_a := 0, 1 .. (N - 1)$ $t_{i_a} := i_a \cdot DW$

$j_a := 0, 1 .. \left(\frac{N}{2} - 1\right)$ $frequency\ a_{j_a} := \frac{j_a}{N \cdot DW}$

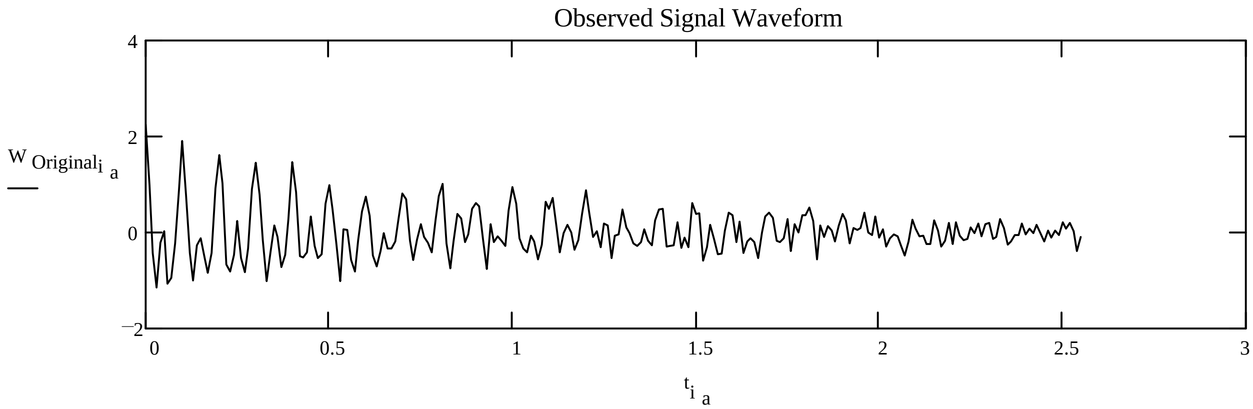
**Calculate Observed Signal Waveform:** Calculate the FID from the above information.

Signal Waveform $$W_{Signal_{i_a}} := A_a \cdot \cos\left(t_{i_a} \cdot \omega_a\right) \cdot e^{-\frac{t_{i_a}}{T_a}} + A_b \cdot \cos\left(t_{i_a} \cdot \omega_b\right) \cdot e^{-\frac{t_{i_a}}{T_b}}$$

Random Distribution $$NORM\left(\sigma_n\right) := \sigma_n \cdot \sqrt{-2 \cdot \ln(rnd(1))} \cdot \cos(2 \cdot \pi \cdot rnd(1))$$

Random Noise $$Noise_{i_a} := NORM(noise)$$

Original Signal Waveform $$W_{Original} := Noise + W_{Signal}$$



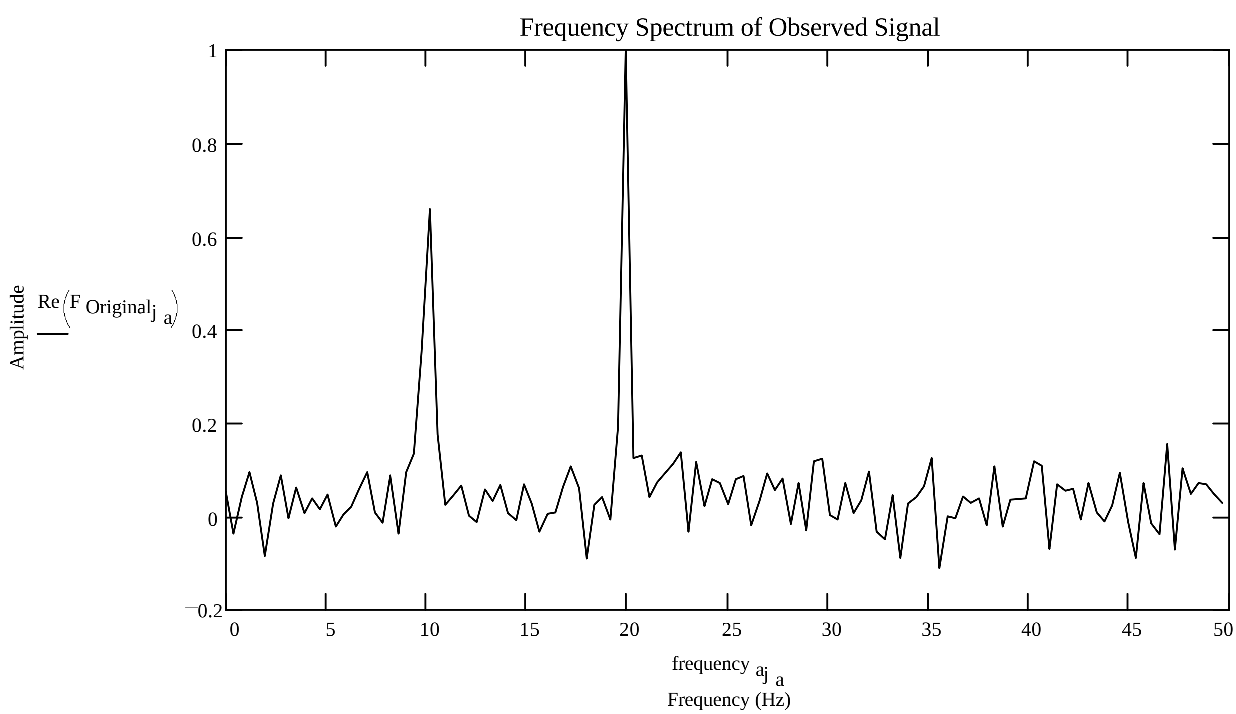

**Fourier Transforms:** Fourier transform of FID to generate a frequency domain signal (spectrum) and normalize..

$$F_{Original} := \frac{fft(W_{Original})}{max(Re(fft(W_{Original})))}$$

**Signal to Noise Ratio**:

$$SN_{Original} := \frac{1}{stdev\left[submatrix\left[F_{Original}, \frac{N}{4}, \left(\frac{N}{2} - 1\right), 0, 0\right]\right]}$$

$SN_{Original} = 13.1$



**Zero Fill**: Increase the digital resolution by adding null data to the FID, increasing the size of the data array.

Number of zero fills: $ZF := 2$

Create zero array: $k := 0, 1 .. (N)\cdot\left(2^{ZF} - 1\right) - 1$ $zero_k := 0$

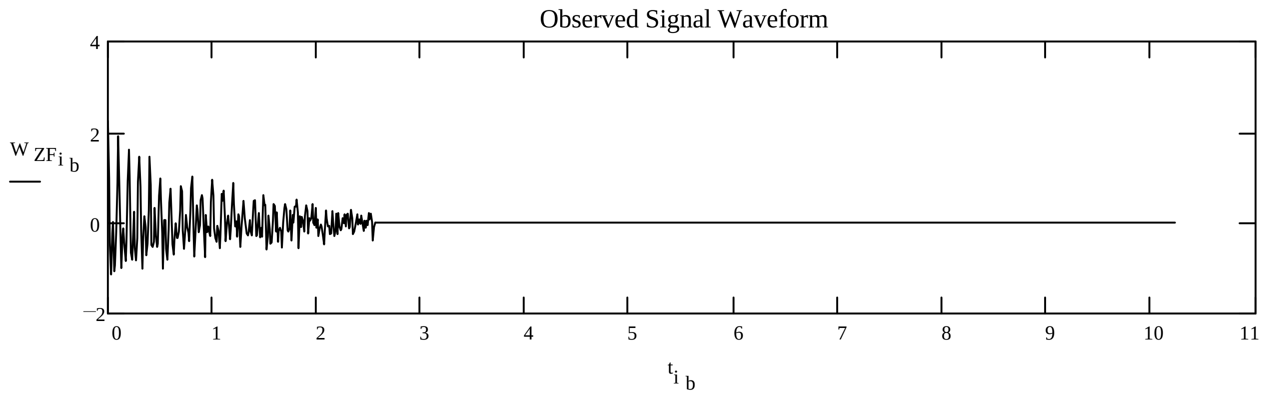
Reset indexes and data array:

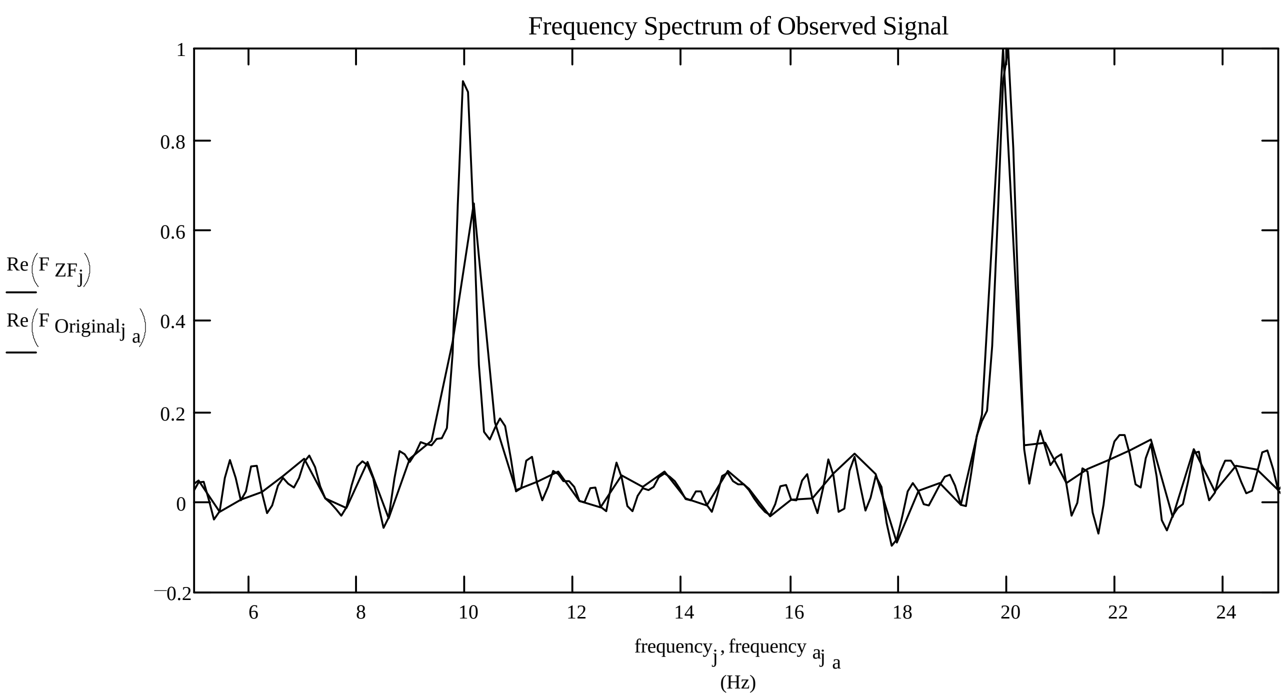
$N := N + (N)\cdot\left(2^{ZF} - 1\right)$ $i_b := 0, 1 .. (N - 1)$ $j := 0, 1 .. \left(\frac{N}{2} - 1\right)$ $t_{i_b} := i_b \cdot DW$ $frequency_j := \frac{j}{N\cdot DW}$

$W_{ZF} := stack\left(W_{Original}, zero\right)$

$$SN(X) := \frac{1}{stdev\left[submatrix\left[X, \frac{N}{4}, \left(\frac{N}{2} - 1\right), 0, 0\right]\right]}$$

$$F_{ZF} := \frac{fft\left(W_{ZF}\right)}{max\left(Re\left(fft\left(W_{ZF}\right)\right)\right)}$$




$SN\left(F_{ZF}\right) = 14.2$ $SN_{Original} = 13.1$

**Exponential Multiplication for S/N enhancement:**

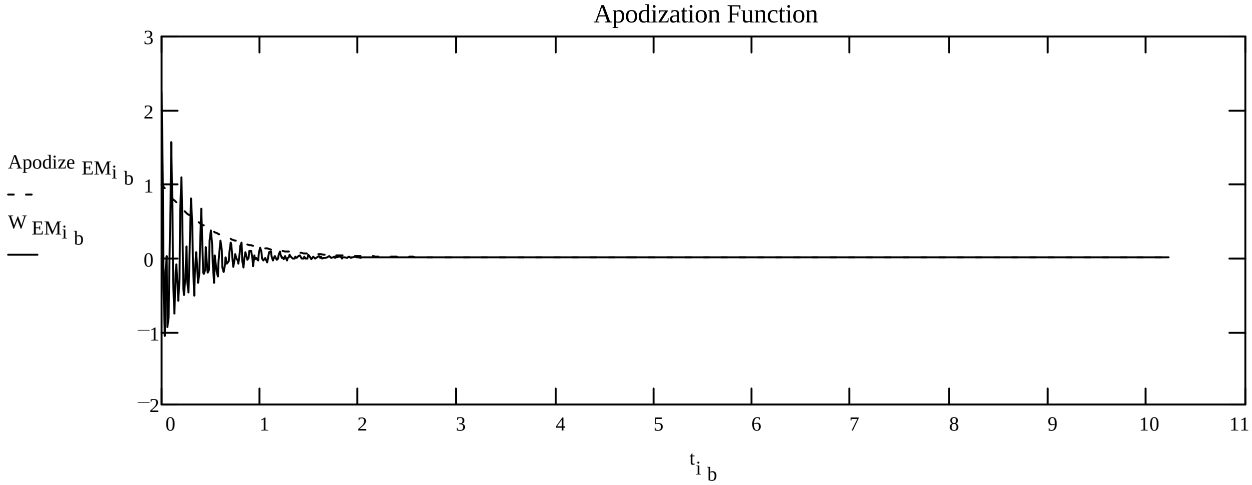
Line Broadening Factor $LB := 2 \cdot Hz$

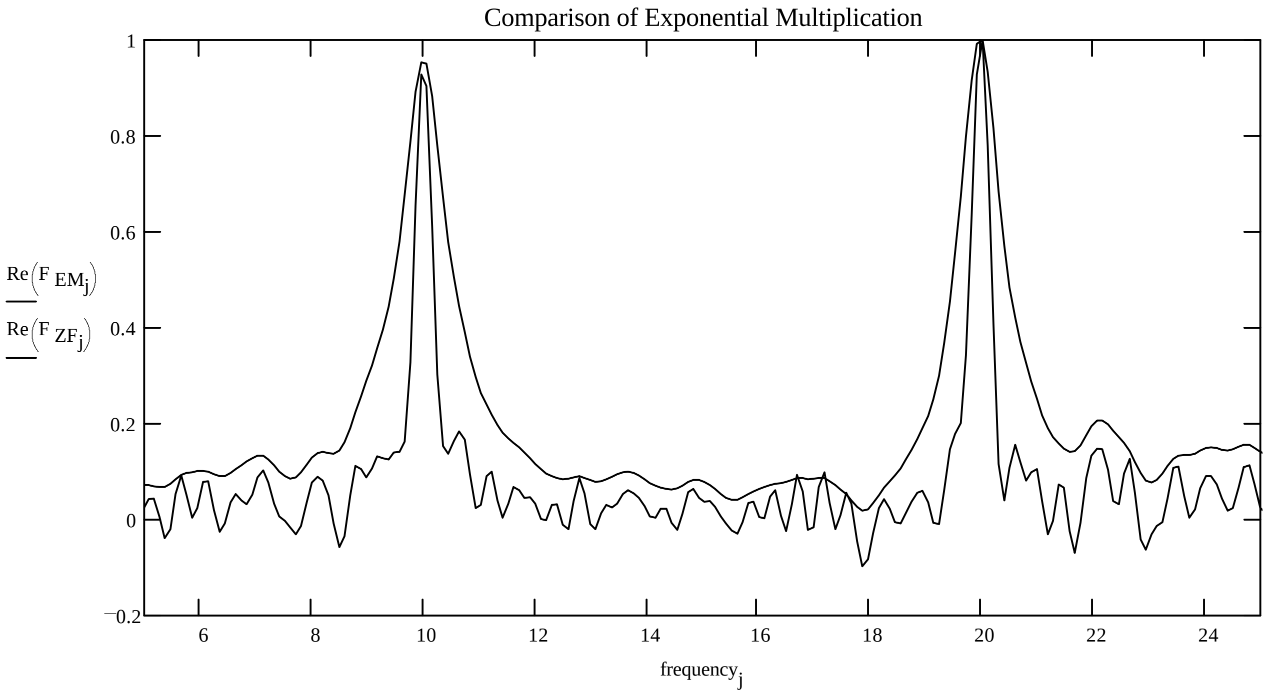
Calculate Apodization Function: $Apodize_{EM_{i_a}} := e^{-t_{i_a} \cdot LB}$

Calculate and Transform Apodized Waveform:

$W_{EM_{i_a}} := W_{Original_{i_a}} \cdot Apodize_{EM_{i_a}}$ $W_{EM} := stack(W_{EM}, zero)$

$Apodize_{EM} := stack(Apodize_{EM}, zero)$ $F_{EM} := \dfrac{fft(W_{EM})}{max(Re(fft(W_{EM})))}$




$SN(F_{EM}) = 14.083$ $SN(F_{ZF}) = 14.178$

**Gaussian Multiplication for S/N enhancement:**

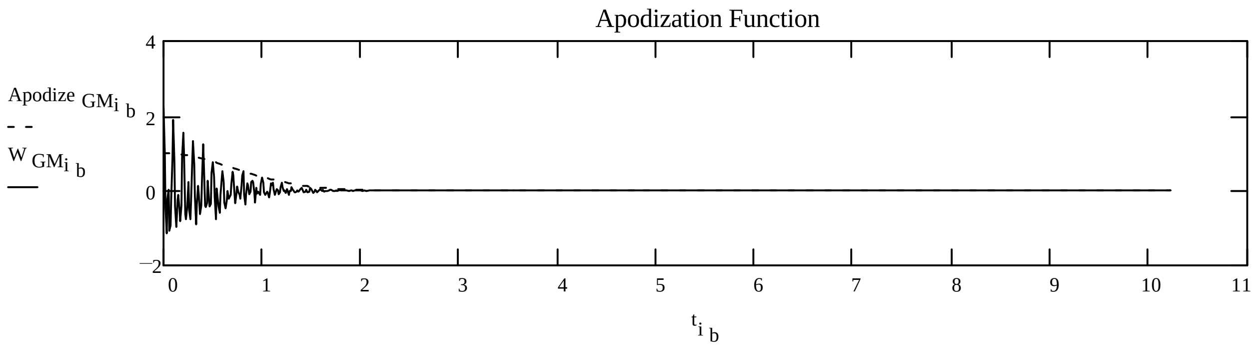
Line Broadening: $LB := 1 \cdot Hz$

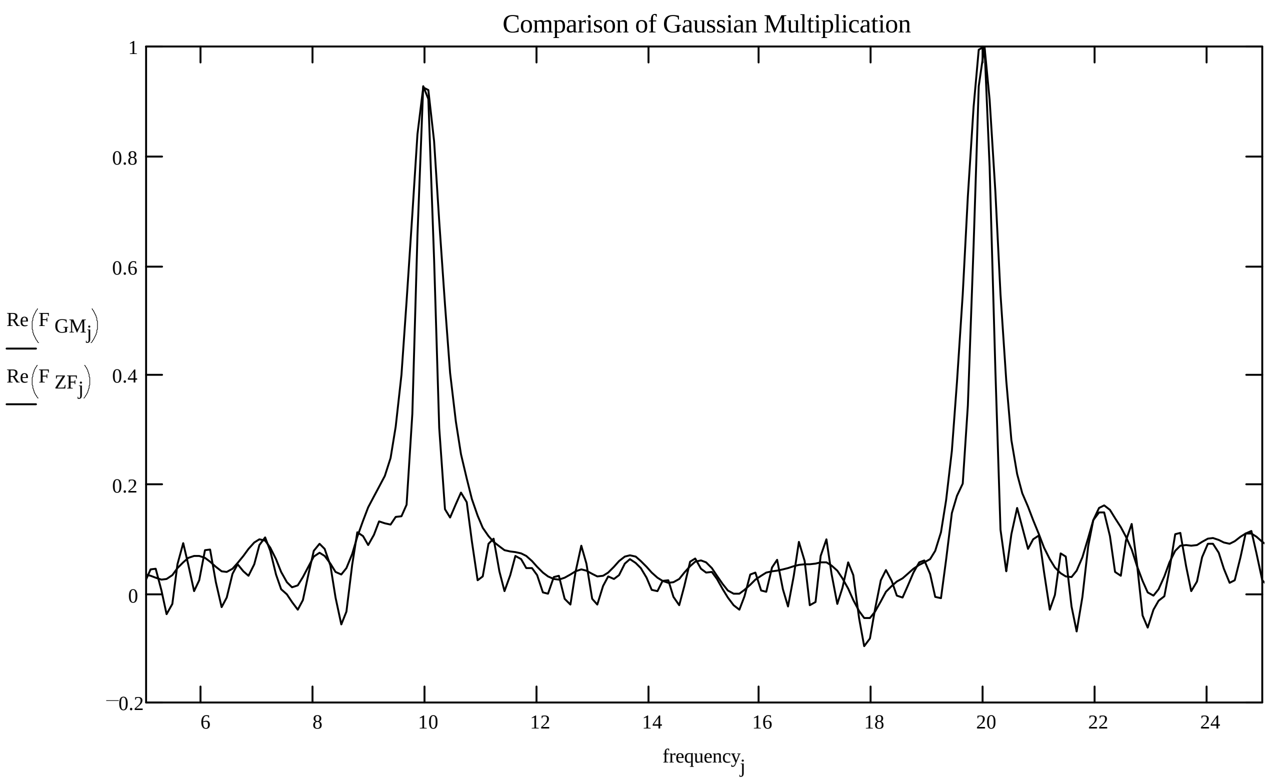
Calculate Apodization Function: $Apodize_{GM_{i_a}} := e^{-\left[\left(t_{i_a}\right) \cdot LB\right]^2}$

Calculate Apodized Waveform:

$W_{GM_{i_a}} := W_{Original_{i_a}} \cdot Apodize_{GM_{i_a}}$ $W_{GM} := stack\left(W_{GM}, zero\right)$

$Apodize_{GM} := stack\left(Apodize_{GM}, zero\right)$ $F_{GM} := \frac{fft\left(W_{GM}\right)}{max\left(Re\left(fft\left(W_{GM}\right)\right)\right)}$




$SN\left(F_{GM}\right) = 16.425$ $SN\left(F_{ZF}\right) = 14.178$

**Double Exponential Multiplication for Resolution enhancement:**

Line Broadening Factor: $LB := 0.5 \cdot Hz$

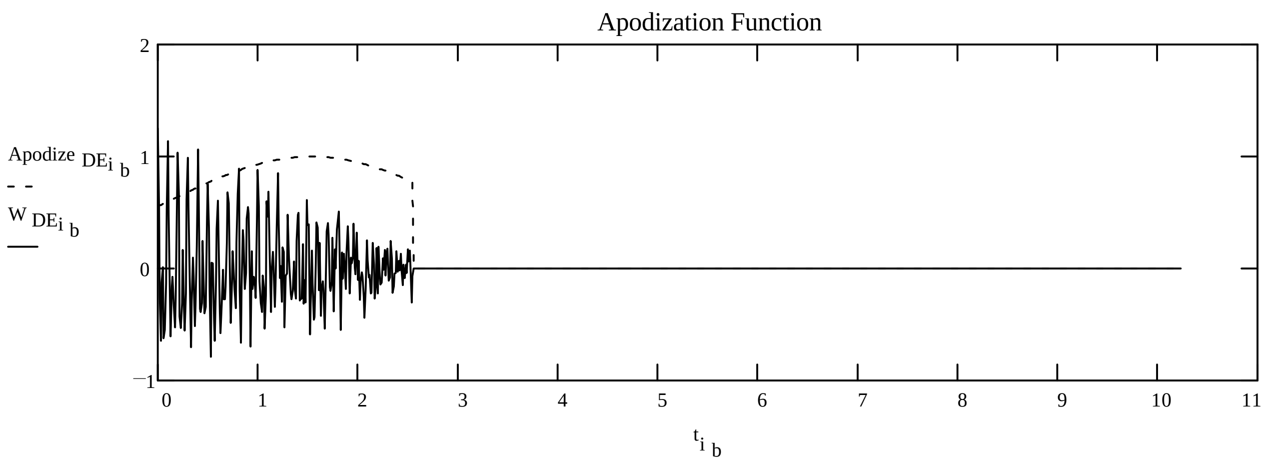
Gaussian Multiplication Factor: $GM := 0.3 \cdot Hz$

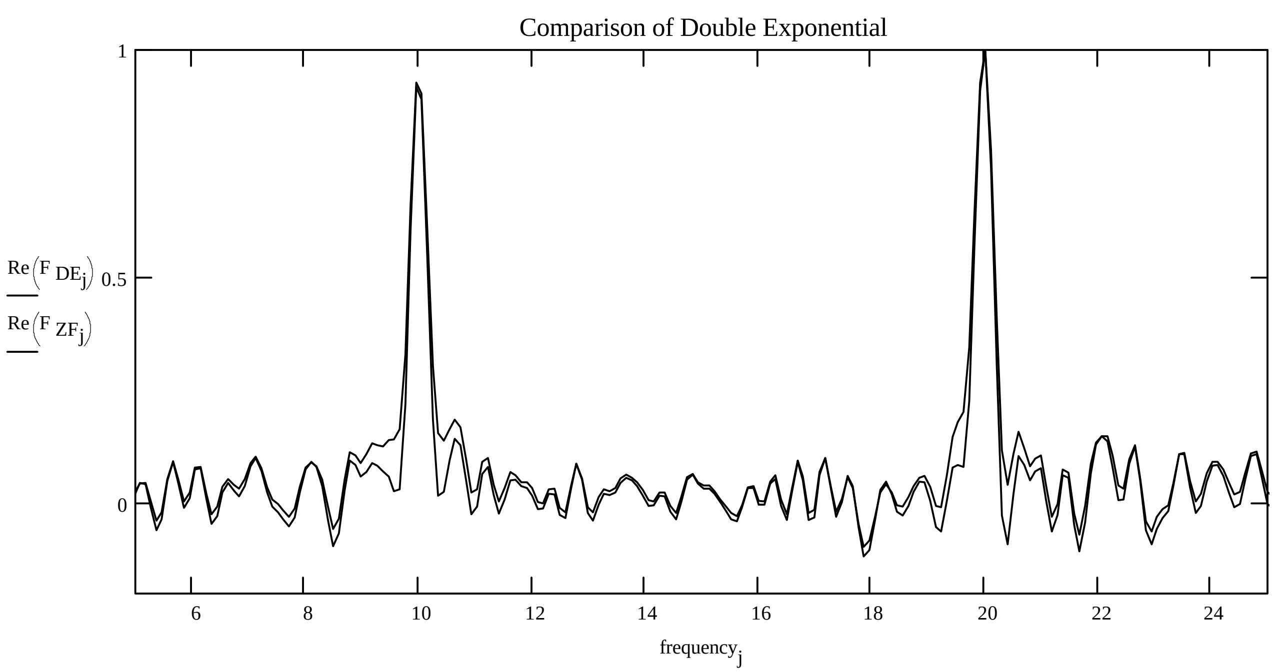
Calculate Apodization Function: $Apodize_{DE_{i_a}} := e^{-\left[\left[\left(t_{i_a}\right)\cdot LB\right] - GM\cdot AT\right]^2}$

Calculate Apodized Waveform and FT:

$W_{DE_{i_a}} := W_{Original_{i_a}} \cdot Apodize_{DE_{i_a}}$ $\quad W_{DE} := stack\left(W_{DE}, zero\right)$

$Apodize_{DE} := stack\left(Apodize_{DE}, zero\right)$ $\quad F_{DE} := \dfrac{fft\left(W_{DE}\right)}{max\left(Re\left(fft\left(W_{DE}\right)\right)\right)}$




$SN\left(F_{DE}\right) = 12.885$ $\quad SN\left(F_{ZF}\right) = 14.178$

**TRAF Function for Resolution Enhancement:**

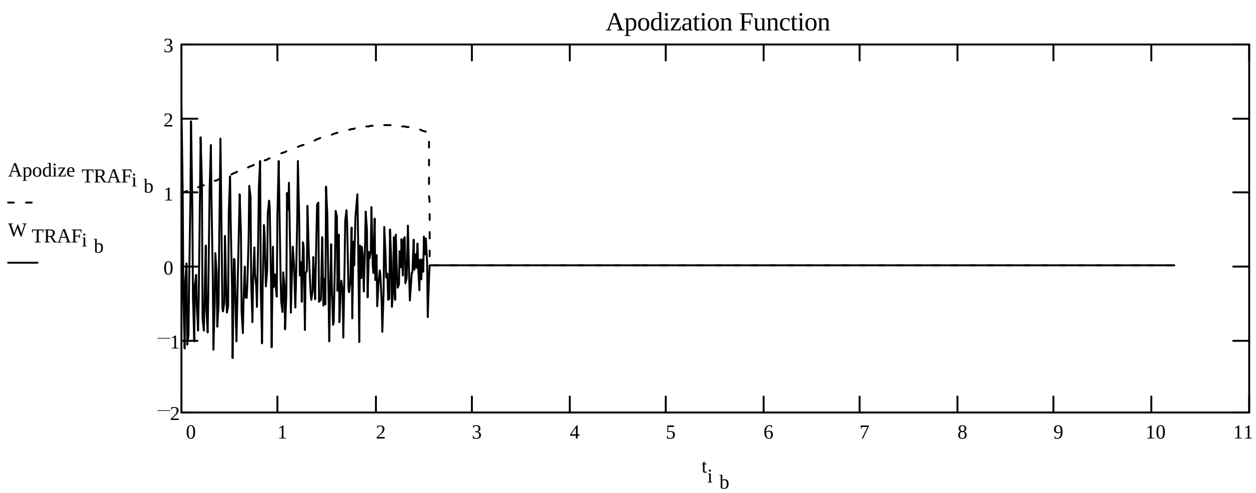
Line Broadening Factor: $LB := 0.5 \cdot Hz$

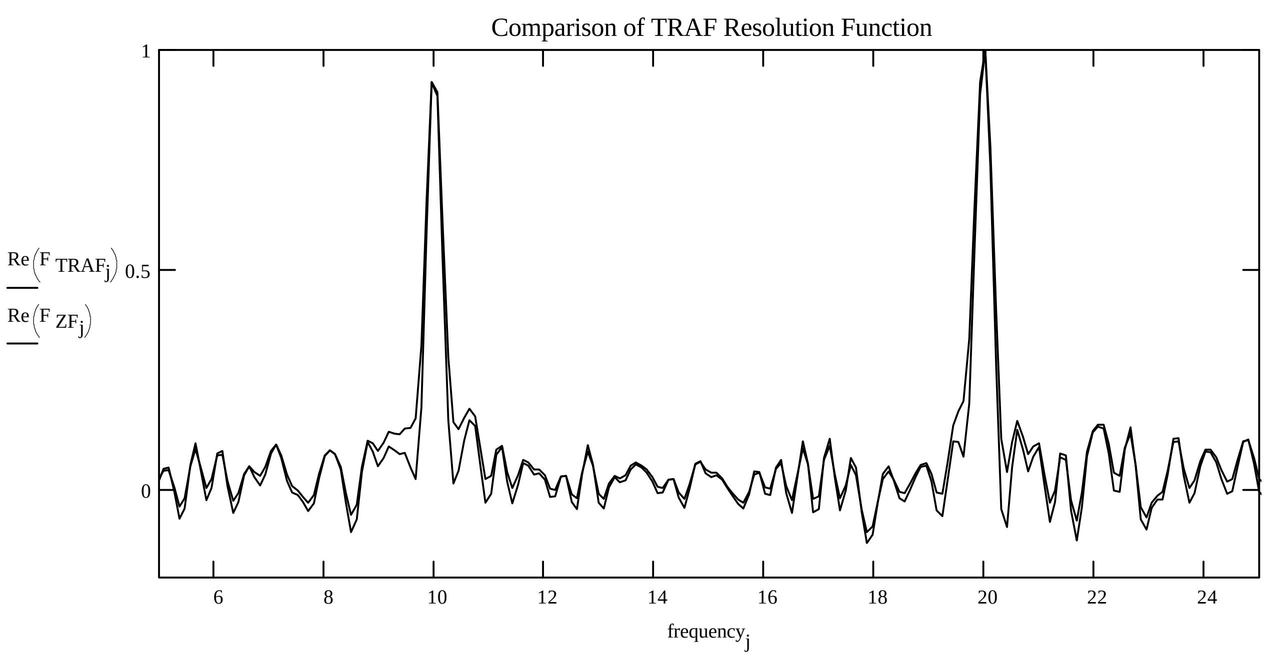
Calculate Apodization Function: $$Apodize_{TRAF_{i_a}} := \frac{\left[e^{-\left(t_{i_a}\right)\cdot LB}\right]^2}{\left[e^{-\left(t_{i_a}\right)\cdot LB}\right]^3 + \left[e^{-(AT)\cdot LB}\right]^3}$$

Calculate Apodized Waveform and FT:

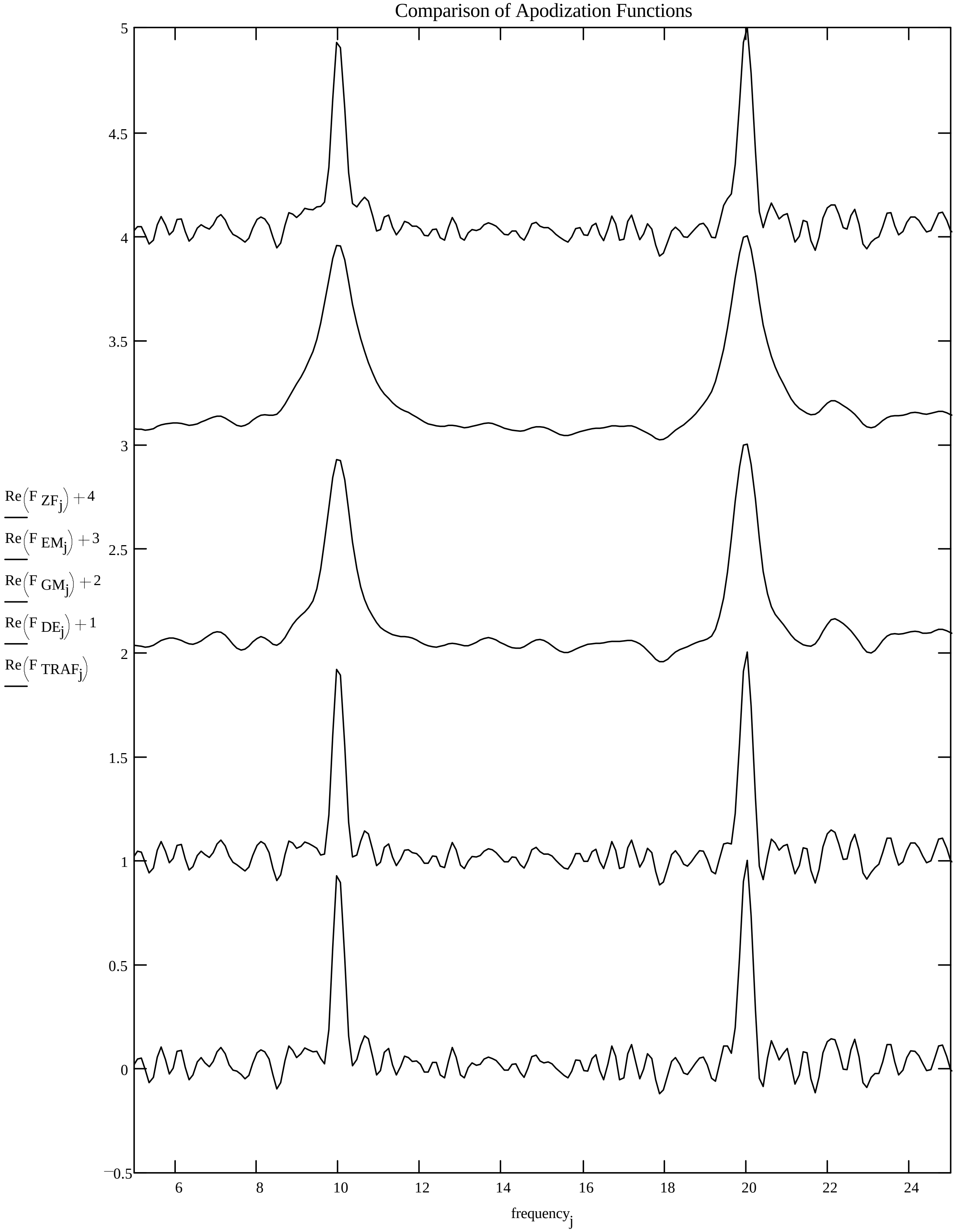
$$W_{TRAF_{i_a}} := W_{Original_{i_a}} \cdot Apodize_{TRAF_{i_a}} \qquad W_{TRAF} := stack\left(W_{TRAF}, zero\right)$$

$$Apodize_{TRAF} := stack\left(Apodize_{TRAF}, zero\right) \qquad F_{TRAF} := \frac{fft\left(W_{TRAF}\right)}{max\left(Re\left(fft\left(W_{TRAF}\right)\right)\right)}$$




$SN\left(F_{TRAF}\right) = 12.051 \qquad SN\left(F_{ZF}\right) = 14.178$




$SN(F_{ZF}) = 14.2$ $SN(F_{EM}) = 14.1$ $SN(F_{GM}) = 16.4$ $SN(F_{DE}) = 12.9$ $SN(F_{TRAF}) = 12.1$

Questions.

1. Determine the effect of zero filling the FID by comparing the original spectrum to the zero filled spectrum. Change the number of zero fills to see what occurs. Are there any tradeoffs involved with zero filling?

2. Determine the effect of Exponential Multiplication by comparing the spectrum for the zero filled spectrum to the exponential multiplied spectrum. Change the line broadening and see what occurs. Are there any tradeoffs with exponential multiplication?

3. Determine the effect of Gaussian Multiplication by comparing the spectrum for the zero filled spectrum to the gaussian multiplied spectrum. Change the line broadening and see what occurs. Are there any tradeoffs with gaussian multiplication?

4. Determine the effect of Double Exponential Multiplication by comparing the spectrum for the zero filled spectrum to the double exponential multiplied spectrum. Change the line broadening and the gaussian multiplication factor, see what occurs. Are there any tradeoffs with double exponential multiplication?

5. Determine the effect of the TRAF function by comparing the spectrum for the zero filled spectrum to the TRAF spectrum. Change the line broadening and see what occurs. Are there any tradeoffs with the TRAF function?

6. Change the number of data points sampled and observe how this effects the S/N?

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