NMR, Lecture Version

Signals Generated:

	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:

Number of Data Points	$N := 2^8$
Dwell Time	$DW := 0.10 \cdot sec$

Calculated Parameters:

Acquisition Time	$AT := DW \cdot N$	$AT = 25.6 \cdot sec$
Spectral Window	$SW := \frac{1}{(2 \cdot DW)}$	$SW = 5 \cdot Hz$
Digital Resolution	$Resolution := \frac{1}{AT}$	$Resolution = 0.039 \cdot Hz$

Calculations:

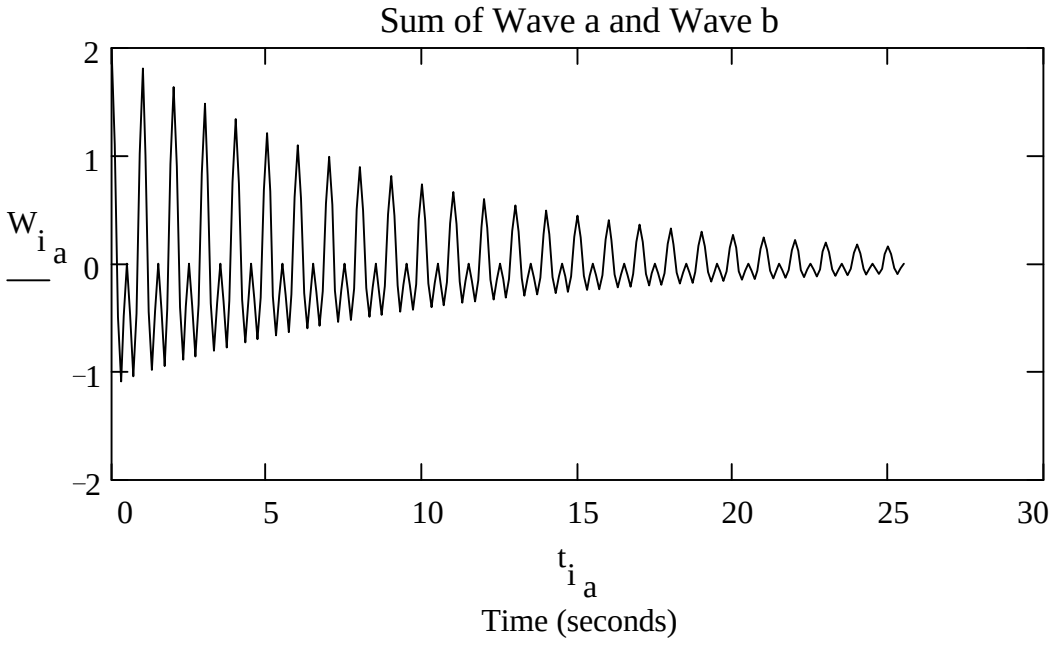
$\omega_a := 2 \cdot \pi \cdot \nu_a$ $\omega_b := 2 \cdot \pi \cdot \nu_b$

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

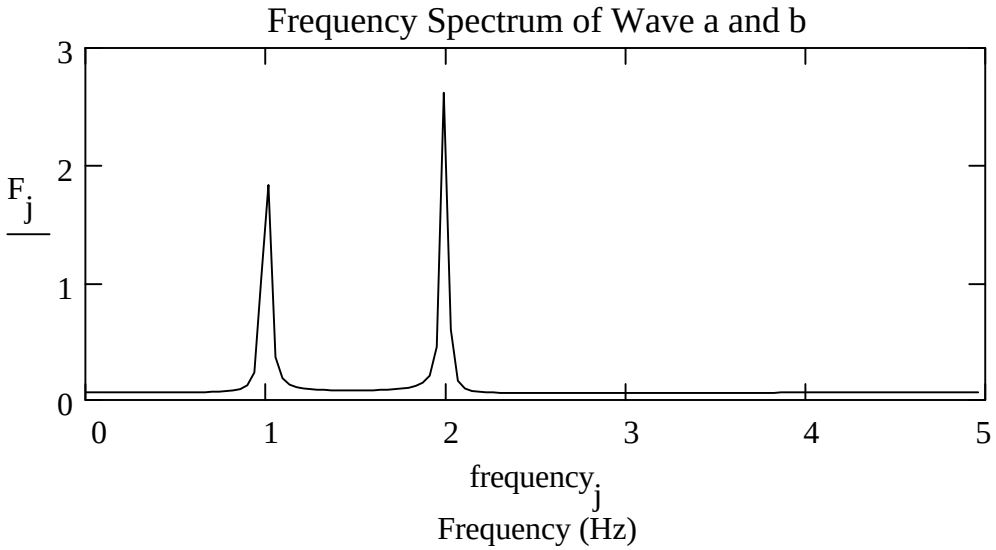
$j := 0, 1 .. \left(\frac{N}{2} - 1\right)$ $frequency_j := \frac{j}{N \cdot DW}$

Waveforms:

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



Fourier Transform: $F := \mathrm{fft}(W)$



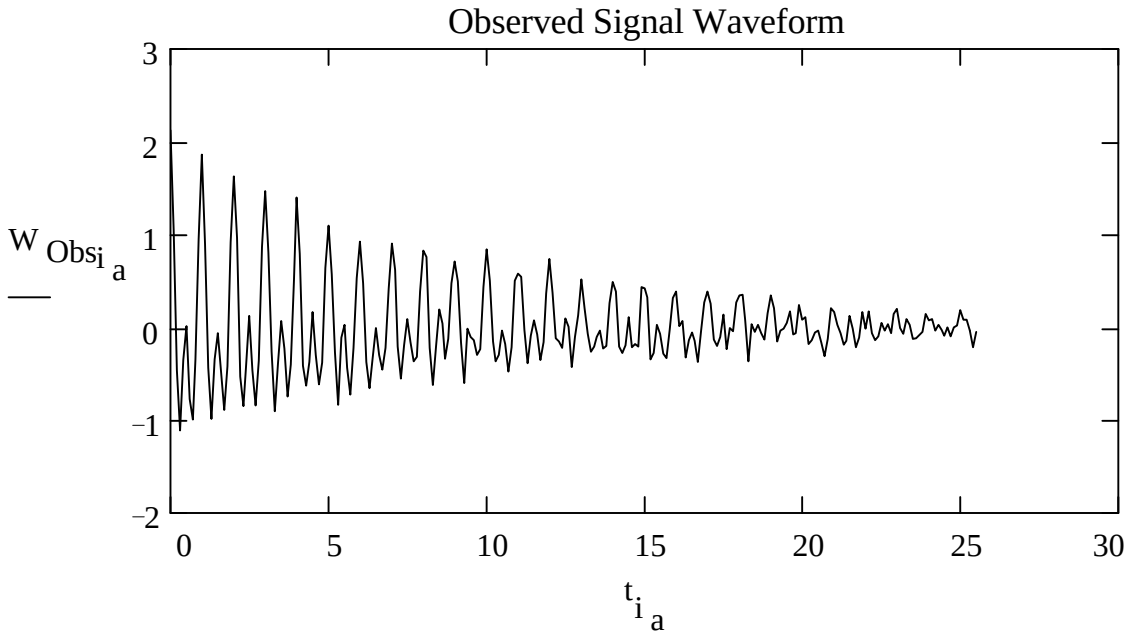
Apodization and Zero Filling

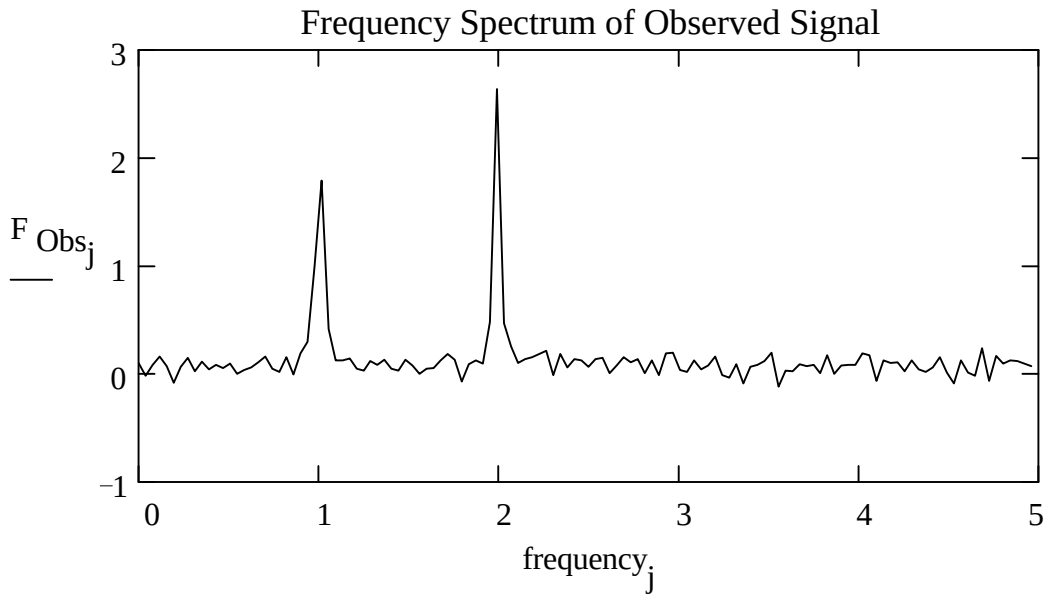
Noise Level: noise := 0.1

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

Random Noise $Noise_{i\,a} := NORM(noise)$

Observed Waveform $W_{Obs} := Noise + W$ $F_{Obs} := fft(W_{Obs})$





Zero Fill Calculations:

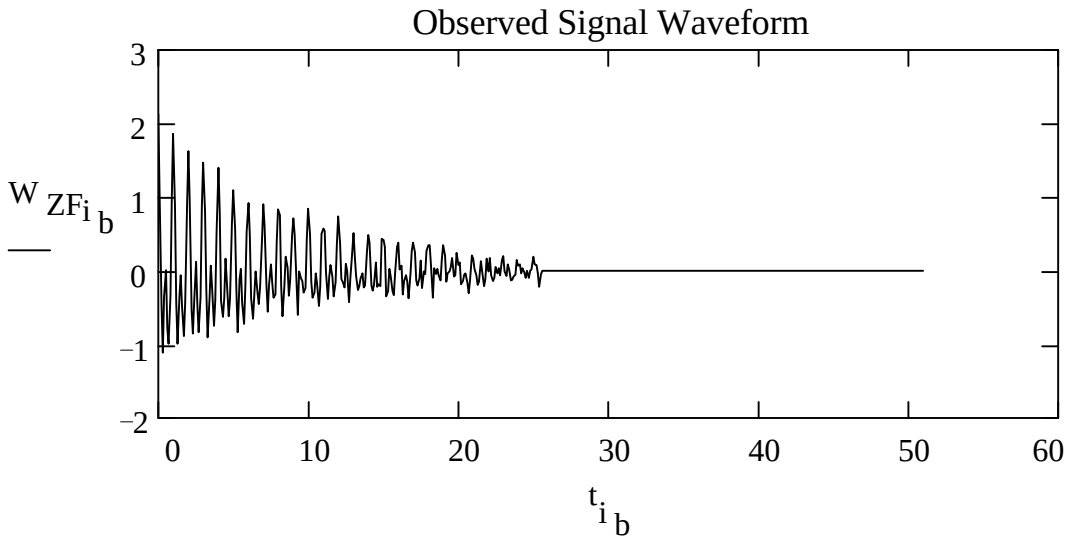
Number of zero fills: $ZF := 1$

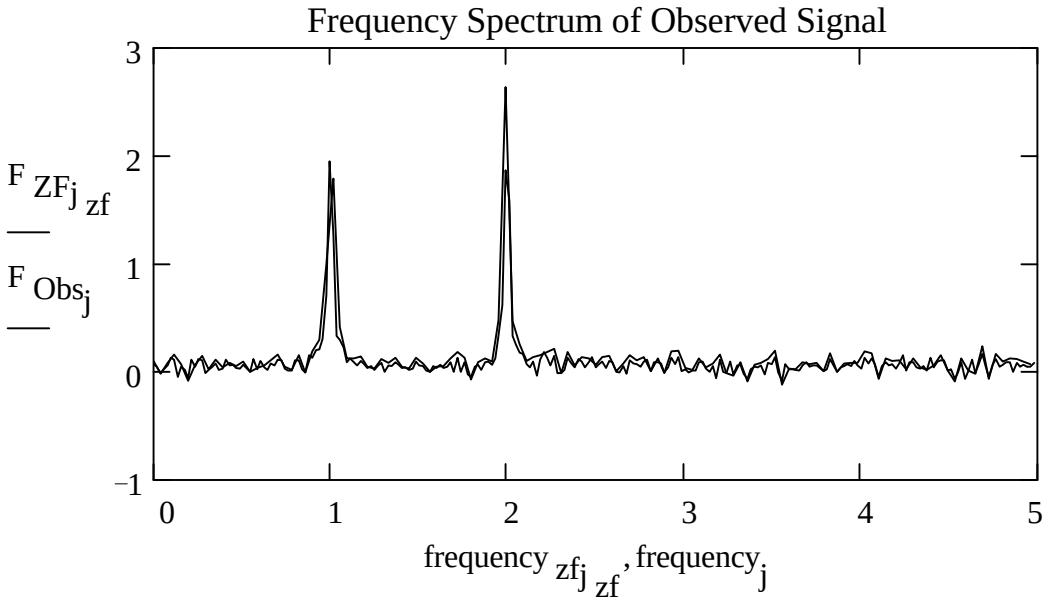
Create zero array: $k := 0, 1 .. (N)\cdot\left(2^{ZF} - 1\right) - 1 \qquad zero_k := 0$

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

$j_{zf} := 0, 1 .. \left(\frac{N}{2} - 1\right) \qquad frequency_{zf_{j_{zf}}} := \frac{j_{zf}}{N \cdot DW}$

$W_{ZF} := stack\left(W_{Obs}, zero\right) \qquad F_{ZF} := fft\left(W_{ZF}\right)$





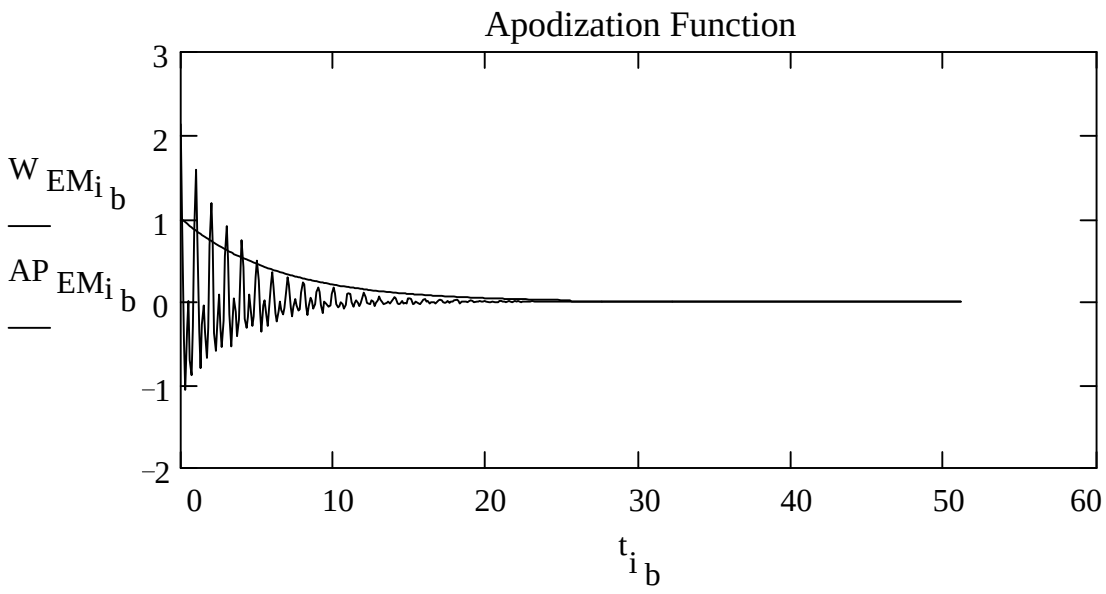
Exponential Multiplication for S/N enhancment:

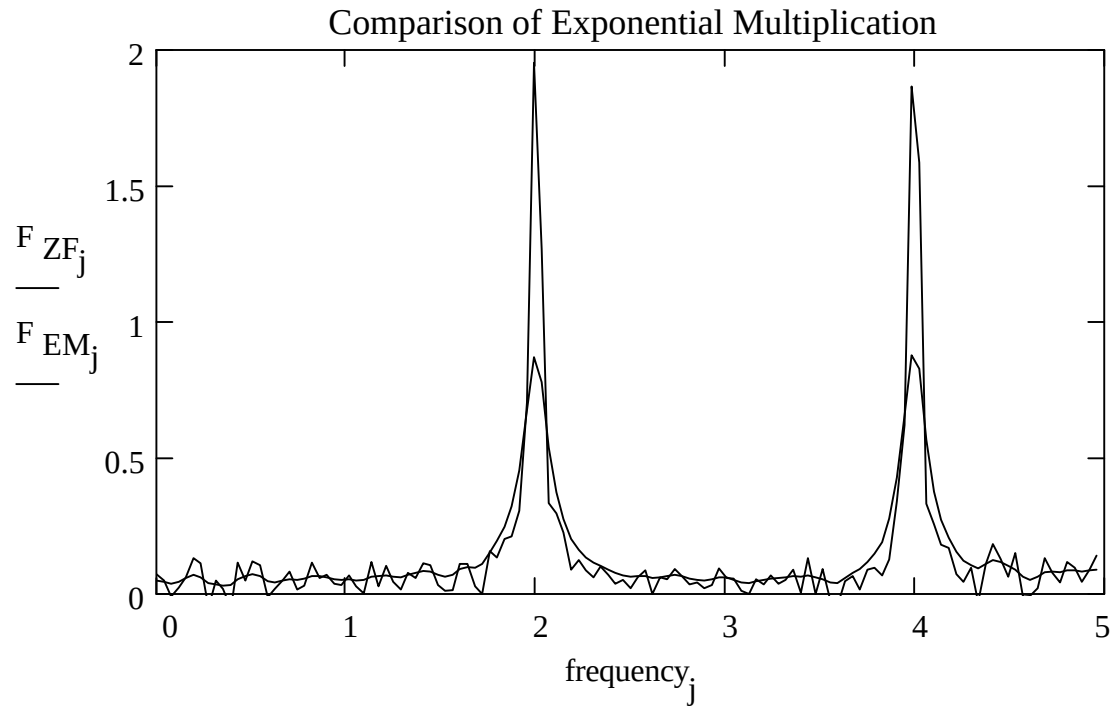
Line Broadening Factor $LB := 1$

$$AP_{EMi_a} := e^{-\frac{t_{i_a}}{2\cdot\pi\cdot sec}\cdot LB} \qquad W_{EMi_a} := W_{Obsi_a}\cdot AP_{EMi_a}$$

$$W_{EM} := stack\left(W_{EM}, zero\right) \qquad AP_{EM} := stack\left(AP_{EM}, zero\right)$$

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





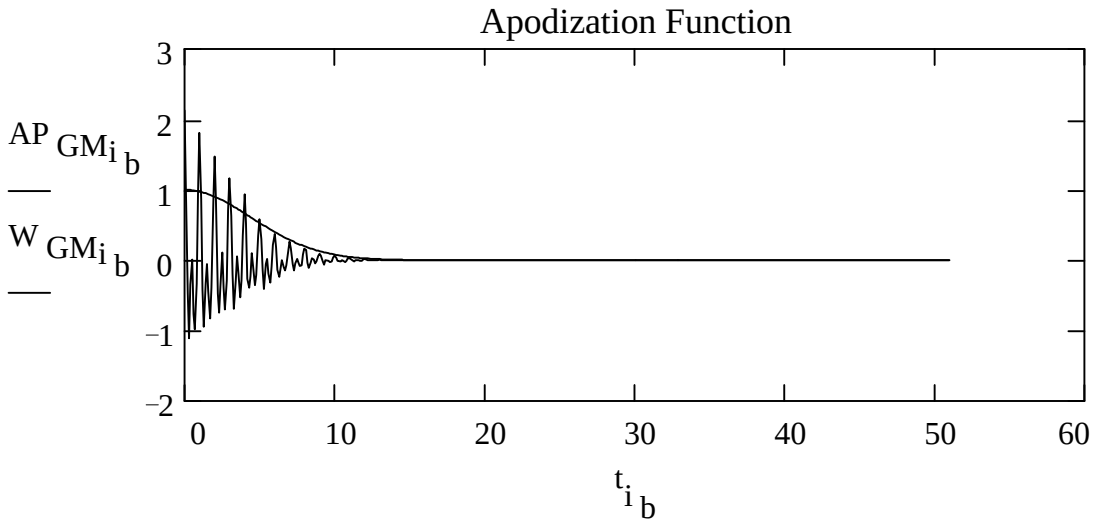
Gaussian Multiplication for S/N enhancment:

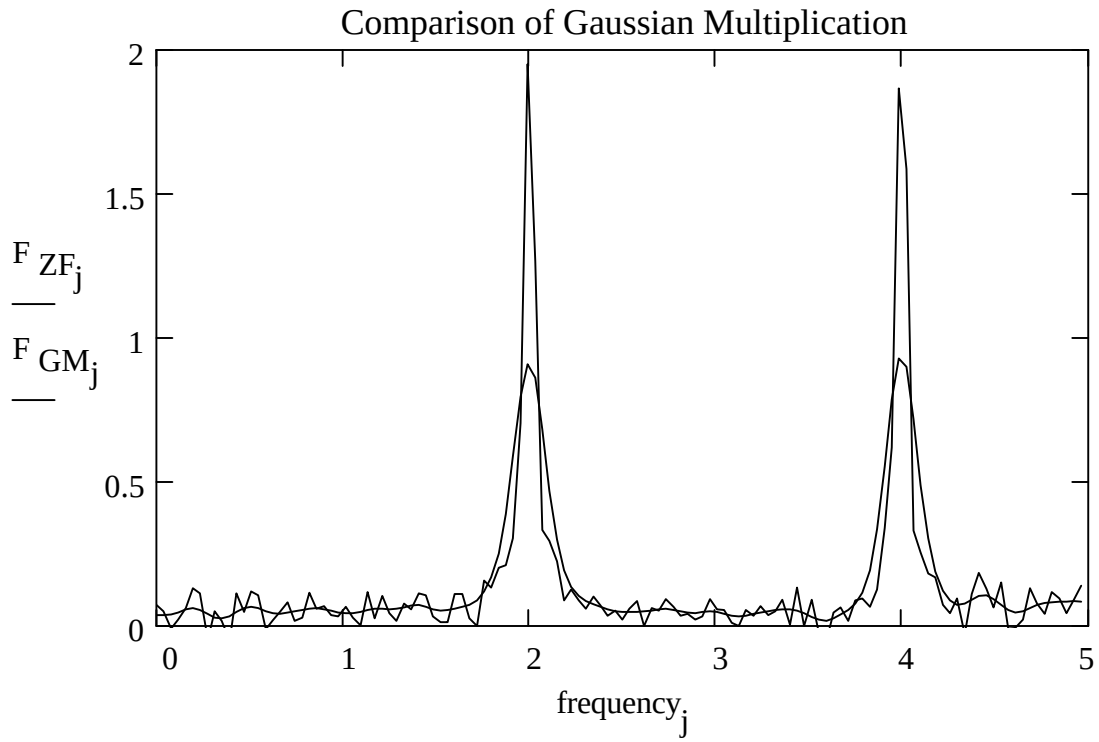
Line Broadening: $LB := 1$

$$AP_{GMi_a} := e^{-\left[\left(\frac{t_{i_a}}{2\cdot\pi\cdot sec}\right)\cdot LB\right]^2} \qquad W_{GMi_a} := W_{Obsi_a}\cdot AP_{GMi_a}$$

$$W_{GM} := stack\left(W_{GM}, zero\right) \qquad AP_{GM} := stack\left(AP_{GM}, zero\right)$$

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





Double Exponential Multiplication for Resolution enhancment:

Line Broadening Factor: $LB := 1$

Gaussian Multiplication Factor: $GM := 0.2$

$$AP_{DEi_a} := e^{-\left[\left[\left(\frac{t_{i_a}}{2\cdot\pi\cdot sec}\right)\cdot LB\right]-\frac{GM\cdot AT}{2\cdot\pi\cdot sec}\right]^2}$$

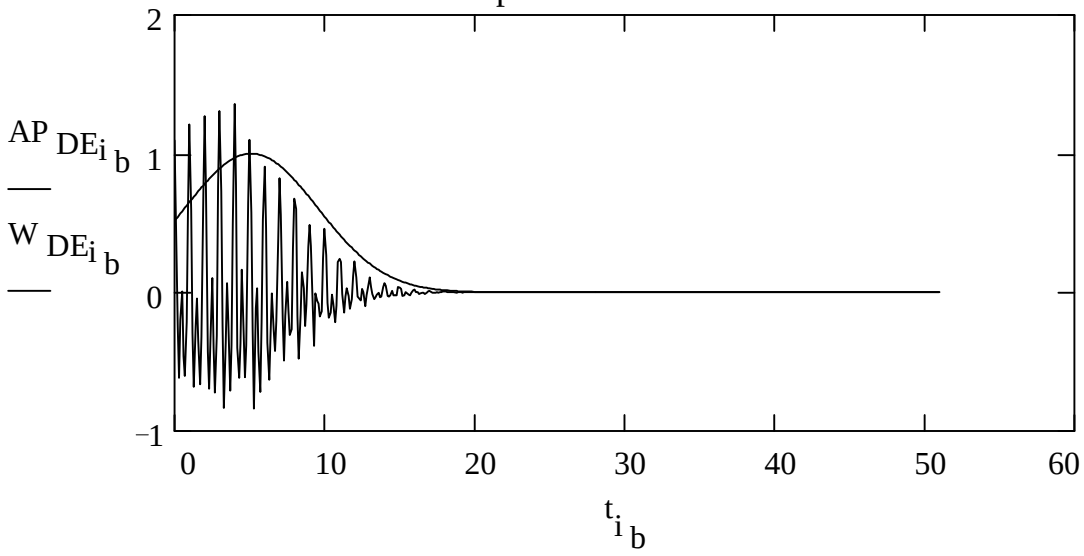
$$W_{DEi_a} := W_{Obsi_a}\cdot AP_{DEi_a}$$

$$AP_{DE} := stack\left(AP_{DE}, zero\right)$$

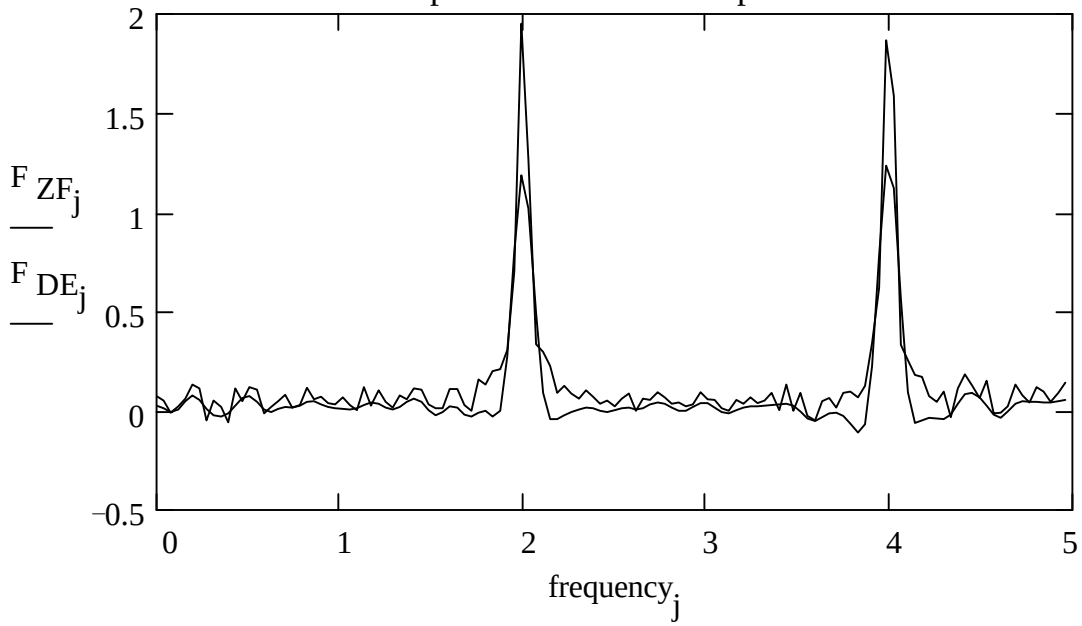
$$W_{DE} := stack\left(W_{DE}, zero\right)$$

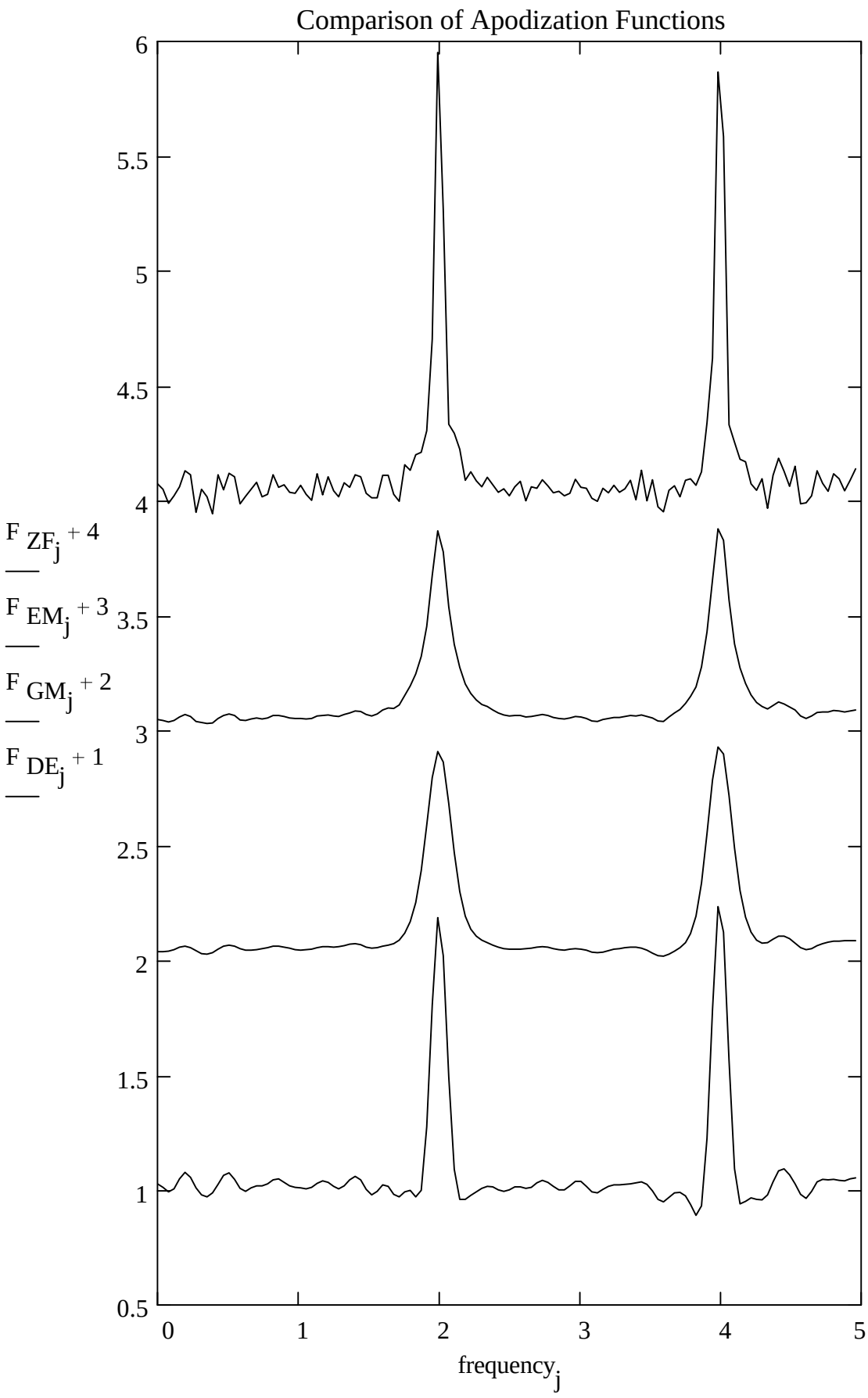
$$F_{DE} := fft\left(W_{DE}\right)$$

Apodization Function



Comparison of Double Exponential




Comparison of Apodization Functions
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1
2
3
4
5
frequency_j
F ZF_j + 4
F EM_j + 3
F GM_j + 2
F DE_j + 1

This Document Produced by:
Scott Van Bramer
Department of Chemistry
Widener University
Chester, PA 19013
svanbram@science.widener.edu
http://science.widener.edu/~svanbram