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.

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

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Amplitude</th>
<th>Frequency</th>
<th>Relaxation</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>A_a := 1</td>
<td>ν_a := 1 Hz</td>
<td>T_a := 10 sec</td>
</tr>
<tr>
<td>b</td>
<td>A_b := 1</td>
<td>ν_b := 2 Hz</td>
<td>T_b := 10 sec</td>
</tr>
</tbody>
</table>

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 := 0.1 sec

Noise Level:
- Noise noise := 0.1

Calculated Parameters: The parameters above determine the following variables.

- Acquisition Time \( AT := DW \cdot N \) \( AT = 25.6 \text{ sec} \)
- Spectral Window \( SW := \frac{1}{2 \cdot DW} \) \( SW = 5 \text{ Hz} \)
- Digital Resolution Resolution := \( \frac{1}{AT} \) Resolution = 0.039 \( \text{Hz} \)
- Angular Frequency Wave a \( \omega_a := 2 \cdot \pi \cdot ν_a \) \( \omega_a = 6.283 \text{ rad/sec}^{-1} \)
  - Wave b \( \omega_b := 2 \cdot \pi \cdot ν_b \) \( \omega_b = 12.566 \text{ rad/sec}^{-1} \)

Index: These Indexes are used for various calculations.

\[
\begin{align*}
  i_a & := 0, 1, .. (N - 1) \\
  j_a & := 0, 1, \lfloor \frac{N}{2} - 1 \rfloor \\
  t_i.a & := i_a \cdot DW \\
  \text{frequency} & := \frac{j_a}{N \cdot DW}
\end{align*}
\]
**Calculate Observed Signal Waveform:** Calculate the FID from the above information.

**Signal Waveform**

\[ W_{\text{Signal}} := A_a \cos(t_{1a} \omega_a) e^{-\frac{t_{1a}}{T_a}} + A_b \cos(t_{1b} \omega_b) e^{-\frac{t_{1b}}{T_b}} \]

**Random Distribution**

\[ \text{NORM}(\sigma_n) := \sigma_n \sqrt{-2 \cdot \ln(\text{rnd}(1))} \cdot \cos(2\pi \cdot \text{rnd}(1)) \]

**Random Noise**

\[ \text{Noise}_{1a} := \text{NORM}(\text{noise}) \]

**Observed Signal Waveform**

\[ W_{\text{Observe}} := \text{Noise} + W_{\text{Signal}} \]

**Observed Signal Waveform**

![Observed Signal Waveform](image)

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

\[ F_{\text{Observe}} := \text{fft}(W_{\text{Observe}}) \]

**Frequency Spectrum of Observed Signal**

![Frequency Spectrum of Observed Signal](image)
**Zero Fill**: Increase the digital resolution by adding null data to the FID, increasing the size of the data array.

Number of zero fills: \( ZF := 1 \)

Create zero array: \( k := 0, 1 \cdots (N - (2^{ZF} - 1)) \quad \text{zero}_k := 0 \)

Reset indexes and data array:

\[
N := N + (N - (2^{ZF} - 1)) \\
i_b := 0, 1 \cdots (N - 1) \\
j := 0, 1 \cdots \left(\frac{N}{2} - 1\right) \\
W_{ZF} := \text{stack}(W_{\text{Observe}}, \text{zero}) \quad F_{ZF} := \text{fft}(W_{ZF})
\]

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**Observed Signal Waveform**

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**Frequency Spectrum of Observed Signal**
Exponential Multiplication for S/N enhancement:

Line Broadening Factor: \( LB := 1 \)

Calculate Apodization Function:
\[
\text{Apodize } EM_{i,a} := e^{-\frac{t_i}{2 \pi \text{sec} \cdot LB}}
\]

Calculate Apodized Waveform:
\[
W_{EM_{i,a}} := W_{\text{Observe}_{i,a}} \cdot \text{Apodize } EM_{i,a}
\]
\[
W_{EM} := \text{stack}(W_{EM_{i,a}})
\]
\[
\text{Apodize } EM := \text{stack}(\text{Apodize } EM_{i,a})
\]

Fourier Transform:
\[
F_{EM} := \text{fft}(W_{EM})
\]
Gaussian Multiplication for S/N enhancement:

Line Broadening: \( \text{LB} := 1 \)

Calculate Apodization Function: \( \text{Apodize}_{\text{GM}} := e^{-\left(\frac{t_{ia}}{2 \times \text{sec}}\right)^2} \)

Calculate Apodized Waveform: \( \text{W}_{\text{GM}} := \text{W}_{\text{Observe}} \cdot \text{Apodize}_{\text{GM}} \)

\( \text{W}_{\text{GM}} := \text{stack}(\text{W}_{\text{GM}} \cdot \text{zero}) \)

\( \text{Apodize}_{\text{GM}} := \text{stack}(\text{Apodize}_{\text{GM}} \cdot \text{zero}) \)

Fourier Transform:

\( \text{F}_{\text{GM}} := \text{fft}(\text{W}_{\text{GM}}) \)
Double Exponential Multiplication for Resolution enhancement:

Line Broadening Factor: \[ \text{LB} := 1 \]

Gaussian Multiplication Factor: \[ \text{GM} := 0.2 \]

Calculate Apodization Function:

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

Calculate Apodized Waveform:

\[ W_{DE_{i_a}} := W_{\text{Observe}_{i_a}} \cdot \text{Apodize } DE_{i_a} \]

\[ W_{DE} := \text{stack} \left( W_{DE \cdot \text{zero}} \right) \]

\[ \text{Apodize } DE := \text{stack} \left( \text{Apodize } DE, \text{zero} \right) \]

Fourier Transform:

\[ F_{DE} := \text{fft} \left( W_{DE} \right) \]
**TRAF Function for Resolution Enhancement:**

Line Broadening Factor: \( \text{LB} := 0.4 \)

Calculate Apodization Function:

\[
\text{Apodize TRAF}_{i_a} := \left( -\left( \frac{t_{i_a}}{2 \pi \text{sec}} \right)^2 \text{LB} \right) + \left( -\left( \frac{t_{i_a}}{2 \pi \text{sec}} \right)^3 \text{LB} \right)^3
\]

Calculate Apodized Waveform:

\[
W \ \text{TRAF}_{i_a} := W \ \text{Observe}_{i_a} ; \text{Apodize TRAF}_{i_a}
\]

\[
W \ \text{TRAF} := \text{stack} \left( W \ \text{TRAF} ; \text{zero} \right)
\]

\[
\text{Apodize TRAF} := \text{stack} \left( \text{Apodize TRAF} ; \text{zero} \right)
\]

Fourier Transform:

\[
F \ \text{TRAF} := \text{fft} \left( W \ \text{TRAF} \right)
\]
Comparison of Apodization Functions

$F_{ZF}$ + 4
$F_{EM}$ + 3
$F_{GM}$ + 2
$F_{DE}$ + 1
$F_{TRAF}$ / 3

frequency

0 1 2 3 4 5 6
0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6

0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6

0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6

0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5 6
Questions.

1. Make the following changes and observe their effect on the FID and the spectra.
   a. Change the number of zero fills.
   b. Change the line broadening factor for Exponential Multiplication.
   c. Change the line broadening factor for Gaussian Multiplication.
   d. Change the line broadening factor and the GM factor for Double Exponential Multiplication.
   e. Change the line broadening factor for the TRAF Function.

2. Change the Relaxation constant for one of the Nuclei and repeat question 1. How does the natural linewidth effect the spectrum.

3. Change the number of data points sampled and repeat question 1 and 2. How does the acquisition time change, and how does this effect the S/N?

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