Analysis of Complex Rotation Spectra

1. Fourier and All Poles transforms
2. Maximum Entropy spectral analysis
3. Time domain analysis versus frequency domain analysis
A dephasing effect will reduce the asymmetry of TF data if not enough groups are used:

\[ \text{Dephasing factor} = \frac{\sin(\pi/N)}{(\pi/N)} \]

<table>
<thead>
<tr>
<th>TF Groups</th>
<th>Dephasing Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>99 %</td>
</tr>
<tr>
<td>8</td>
<td>98 %</td>
</tr>
<tr>
<td>4</td>
<td>90 %</td>
</tr>
<tr>
<td>2</td>
<td>64 %</td>
</tr>
</tbody>
</table>

i.e. 8 TF groups are sufficient for most purposes
Fourier and All-Poles Transforms

FFT (Fast Fourier Transform) is the standard way to convert from time domain to frequency domain.

FFT assumes frequency spectrum is well represented by array of evenly spaced points, which works well for spectra containing broad spectral features.

However, if the spectrum contains very narrow features, other types of frequency transform can work better.

The All-Poles (maxent) method is one such method, which makes an expansion of the data in terms of a series of sharp frequencies.

See Press et al, Numerical Recipes, CUP for further details of the All-Poles transform.

All transform methods assume that the data error is independent of time, which is clearly not the case for μSR data.

Data filtering (apodization) is an important step before transforming.
Apodization involves multiplying the time data by a smooth cutoff function (e.g. a Gaussian or exponential decay) before making the transform into frequency space.

This addresses two problems:

1) Finite time window of the data (e.g. 0 to 32 μs at ISIS)
   - without apodization the instrument response in frequency space is a sinc function
   - with apodization the instrumental function becomes smooth without any troublesome lobes, however the frequency resolution is lowered

2) Decrease of signal to noise ratio at longer times
   - By weighting towards early time data and against long time data the S/N of the frequency spectrum is kept under control

*For narrow spectra one can turn off the apodization and directly model the instrumental function in frequency space*
Combining Groups: Power Spectra versus Phase-Corrected Cosine Spectra

Spectral intensity from power spectra

Advantages:
simplicity
copes with different $t_0$ for different components

Disadvantages:
broadened spectral tails
non-linear processing distorts errors

Spectral intensity from phase-corrected spectra

Advantages:
no extra broadening or tails
linear process

Disadvantages:
phase estimation step needed
problem if $t_0$ varies across spectrum
Fourier and All-Poles Transforms

Optimal filtering time constant for a single undamped test frequency
Fourier and All-Poles Transforms

A close pair of undamped test frequencies

Pair of undamped frequencies 0.95/1.05 MHz; 10 MEv test data

FFT

All-poles Maxent

Spectral Intensity

Spectral Intensity

Frequency (MHz)

Frequency (MHz)
The Maximum Entropy Method

Avoids the noise problem and need for filtering; takes data errors fully into account

Iterative procedure for constructing the frequency spectrum with the minimum structure (i.e. maximum entropy) that is consistent with the measured data

Entropy here is determined from the frequency spectrum $p_k$

$$S = - \sum_k \frac{p_k}{b} \log \frac{p_k}{b}$$

The procedure involves maximising $S - \lambda \chi^2$, where $\lambda$ is a Lagrange multiplier

A key point is that the model spectrum is being transformed rather than the data

See Rainford and Daniell, Hyperfine Interactions 87, 1129 (1994) for a detailed discussion of using Maximum Entropy in $\mu$SR

For a general reference see:

The Maximum Entropy Method

Demonstration of MaxEnt using the test data used for the transforms
Organic Superconductor Example

Characteristic field distribution due to vortex lattice

Maximum Entropy Spectra

Characteristic field distribution due to vortex lattice
## Time Domain Analysis versus Frequency Domain Analysis

### Single Frequency

<table>
<thead>
<tr>
<th></th>
<th>Freq (MHz)</th>
<th>Width (MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Data</td>
<td>1.0000</td>
<td>0.000</td>
</tr>
<tr>
<td>Time domain fit</td>
<td>0.9998(1)</td>
<td>0.001(1)</td>
</tr>
<tr>
<td>Maximum Entropy</td>
<td>1.006</td>
<td>0.003</td>
</tr>
</tbody>
</table>

### Pair of Frequencies

<table>
<thead>
<tr>
<th></th>
<th>Freq (MHz)</th>
<th>Width (MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Data</td>
<td>0.9500, 1.0500</td>
<td>0.000, 0.000</td>
</tr>
<tr>
<td>Time domain fit</td>
<td>0.9493(1), 1.0499(3)</td>
<td>0.003(3), 0.004(3)</td>
</tr>
<tr>
<td>Maximum Entropy</td>
<td>0.956, 1.054</td>
<td>0.002, 0.005</td>
</tr>
</tbody>
</table>
Time Domain Analysis versus Frequency Domain Analysis

Transforms are good for determining a qualitative picture of data:
- \text{FFT} best for spectra containing relatively broad features
- All-poles transform best for spectra composed of sharp features

Iterative Maximum Entropy Method gives an ‘unbiased’ view of the data
but Time Domain Fitting gives best ultimate accuracy, provided the correct model is being used.

CONCLUSION
A combination of Frequency Domain and Time Domain analysis usually works best in practice