Exploring Fourier Transform Techniques with Mathcad
Document 4: Fourier Transform of a Free-induction Decay

by

Mark Iannone
Department of Chemistry
Millersville University
Millersville, PA 17551-0302

miannone@marauder.millersv.edu

Note: the Automatic Calculation option in the Math menu should NOT be checked.

Objectives:

Upon completing this exercise, the student should be able to

1. describe what the raw data in an FTNMR experiment looks like and what spectral information it contains;
2. explain the significance of T_2 times in an NMR experiment
3. calculate resolution and Nyquist frequency from data acquisition time and sampling interval.

Introduction

The sound of a bell's ringing after being struck contains several frequency components, each of which dies out at a characteristic rate. If the ringing is Fourier-transformed it gives a frequency spectrum of the bell.

FTNMR is analogous in that the sample is "struck" by a radio-frequency pulse, and each proton "resonates" at its nuclear magnetic resonance frequency. This ringing is called a free-induction decay (FID) . When the FID is Fourier transformed, the resonance frequency of each proton in the sample can be obtained. The difference between a proton's resonance frequency and that of TMS in parts per million is commonly given as δ. The decay time of the FID signal can also provide useful information, but we are usually more interested in the frequency spectrum.

In this document, a simulated FID is transformed to produce a simulated NMR spectrum. FTIntro.mcd demonstrated that the transform of a waveform is its frequency spectrum; FT3pulse.mcd showed that the frequency spectrum of a pulse is broadened as the pulse becomes shorter. Likewise, the FT of an FID is its frequency spectrum, but the decay of the FID, like pulse duration, limits sampling time and imposes a width on the spectral lines. To illustrate this point, the decay times used are far shorter in relation to the frequencies than is the case in FTNMR, so that the peaks in the FT in this document appear far broader than typical NMR peaks.

Part 1: Setup

$k := 9$

$m := 2^k$ m=number of data points in sample

$i := 0 .. m - 1$

$t_i := \frac{i}{m} \cdot A$ time of data points (s)

$j := 0 .. \frac{m}{2}$

$f_j := \frac{j}{t_{m-1}}$ frequency for each data point in the transform (s^{-1})

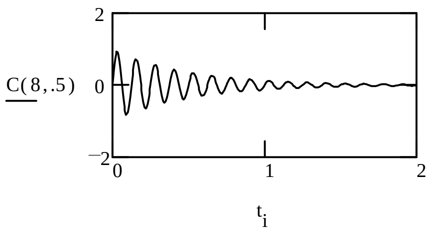
Part 2: Free-induction decay

A simulated FID will now be graphed. Each component is characterized by a frequency f and a decay time T_2, as implemented in the function C(f,T2). (In NMR literature, this decay time is called T_2*).

In an NMR experiment, T_2 times are often long enough to produce extremely sharp peaks in the spectrum. In the simulated data below, the T_2 times are relatively short in relation to the frequency.

$$C(f,T2) := \sin\left(2\cdot\pi\cdot f\cdot t_i\right)\cdot\exp\left(-\frac{t_i}{T2}\right)$$

contribution at frequency f with decay time T2



Graph 1: example of a free induction decay with only one frequency component. Note the exponential decay with time constant T2 of the oscillating signal with frequency f.

EXERCISE

4.1 Note that the entry to the left of the y-axis of Graph 1 is "C(8, .5)". This sets f equal to 8 s^{-1} and T2 equal to 0.5 s. Recalculate the graph with T2 set to 0.1, then 2. Comment on the precision with which the frequency could be measured from the FID in each case.

```
Click on ".5" in the expression C(8,.5) next to the graph.
Press F3 to delete; enter the new value for T2.
```

Part 3: Multicomponent FID and transform

The simulated free induction decay to be transformed, **y,** is the sum of 3 components, each with its own frequency f and decay time T_2. When graphed, this gives a sine-wave-like pattern, with beats, which dies away gradually. This pattern is sampled by recording data every A/m seconds for a total of A seconds.

This FID is analogous to the raw data in an FTNMR experiment. The transform is the frequency spectrum.

$y_i := C(80,1) + C(90,.5) + C(100,.25)$ Simulated 3-component free induction decay

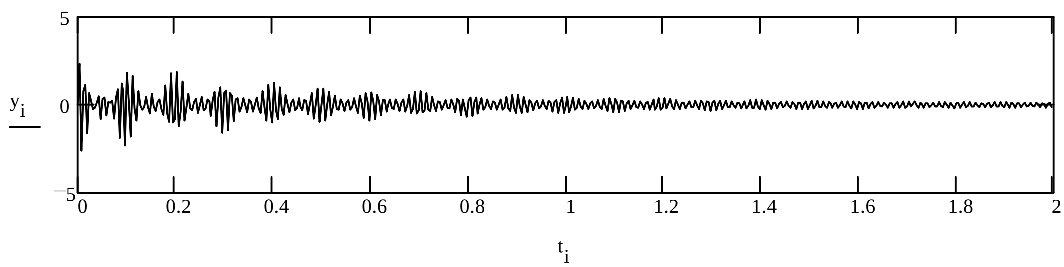
$A \equiv 2$ Total sampling time (s). This document is set up so that changing the number of data points, m (by changing k in setup above) will change the sampling interval but not the total data acquisition time. The sampling interval is given by A/m. (A can also be changed if desired.)

$\frac{A}{m} = 3.90625 \cdot 10^{-3}$ Sampling interval (s)

EXERCISE

4.2 Fixing A fixes the resolution, Nyquist frequency or both?

Graph 2: simulated FID

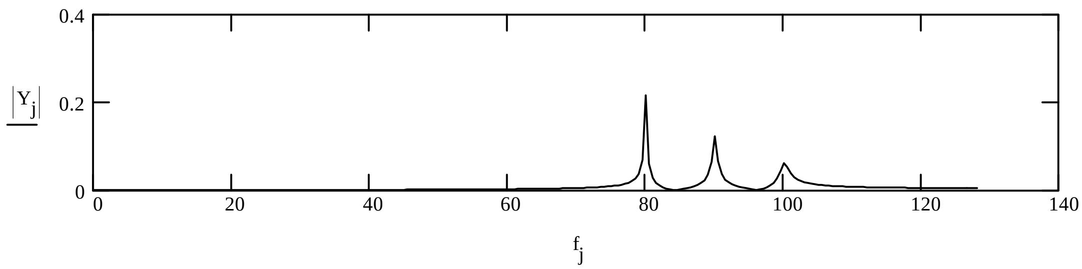


Part 4: Fourier transform

The graph of the Fourier transform of the FID gives a frequency spectrum of the source. However, peak heights and widths vary. This is investigated here in Part 4.

$Y := FFT(y)$ Fourier transform of y

Graph 3: frequency spectrum of FID



EXERCISES

4.3. Modify frequencies f in the "signal" y to verify that Y is the frequency spectrum of the FID.

4.4 Vary the values of T2 incorporated in the signal and determine the effect on the peaks in the spectrum. Explain how it is possible for frequency components contaned in the same decay to have different peak widths in the spectrum.

4.5 In this program, A, the total sample time, and m ($=2^k$), the number of samples, can be varied independently. Which of these determines the resolution of the spectrum? What limitation does the other impose? Include two closely-spaced frequencies in the signal and then experiment with A and k to answer this question.

4.6 Find the Nyquist frequency. Add frequency components higher than this to verify. Describe the result.

4.7 Each frequency component makes the same contribution to the FID, yet the peak heights are different. How is this explained? Hint: ^1H NMR signals are typically integrated.

Another way to determine the resonance frequencies of a bell would be to subject it to sound waves, varying the frequency until the bell resonates. Clearly this would be a much slower process. Early NMR spectrometers worked in this way, although in fact the magnetic field, not the RF frequency, was varied.

The Fourier transform is used to determine the frequency content of the FID. It also plays a role in the excitation process since all protons in the sample are excited by a short pulse from a monochromatic RF source.