# An Introduction to the Fourier Transform

by

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**Abstract**

The Fourier Transform is used in many instrumental techniques, including infrared spectroscopy, NMR, and mass spectrometry. Although most instruments perform this mathematical technique transparently, understanding how it works is important. This understanding will help instrument users set appropriate parameters, appreciate the limitations of an instrument, and obtain better spectra. This document introduces students to both how the Fourier Transform works, and how various instrument parameters affect the results of the Fourier Transform.  Waveforms are produced and integrated using sine waves, cosine waves, and simple functions.  The fast Fourier transform is used with simulated data to introduce students to the relationship between the signal waveform and the signal frequency of a spectrum. Students are then led to the concepts of dwell time and resolution through a series of interactive exercises. The document ends with an introduction to the Fourier transform of decaying signals. This document may be used by students and teachers as written, or teachers may remove some graphs to increase discovery learning and class discussion. The document includes substantial student interaction by changing variables and written reflection exercises.  The companion document, LectureIntroFT.mcd, designed for instructors to use interactively during lecture, is the abbreviated version of IntroFourierTransform.mcd. These Mathcad documents build on previously published work, "Using Mathcad to Teach Instrumental techniques" J. Chem. Educ. 75, 1998, pp 375-378.

**Goal**

To show how the Fourier Transform is performed and explain the effect of important experimental parameters.

## Prerequisites

This document is written with the assumption that students are familiar with Mathcad functions, graphs, and arrays.

**Performance Objectives:** after studying the material in this document you should be able to:

1. Graph the time and frequency domain signals and explain how they are related.
2. Graph the time and frequency domain signals with different phase shifts.
3. Explain how the phase shift relates to the real and imaginary spectra.
4. Predict the position of folded signals based upon the Nyquist sampling theorem.
5. Explain the significance of the dwell time, sampling rate, number of data points, and acquisition time.
6. Simulate a decaying signal in the time domain and relate the decay rate to spectral features in the frequency spectrum.

## Getting started, a signal with one frequency:

In this section, you will simulate a signal that contains a single frequency component. Start with a cosine wave with a frequency of 2 Hz.

The signal frequency ($\nu$) in Hz. $\nu := 2 \cdot Hz$ $\nu \equiv 2 \cdot Hz$

Active local variable
Equation toggled on

Inactive global variable. (The global variable can be moved to any location in the document and toggled on for experiments with this variable. Toggle the local variable off if you do this. )

The radial frequency ($\omega$), typically given in radians/sec, is used for the trigonometry calculations in Mathcad. The frequency above is in Hertz, which is cycles per second. Now define the radial frequency of the signal.

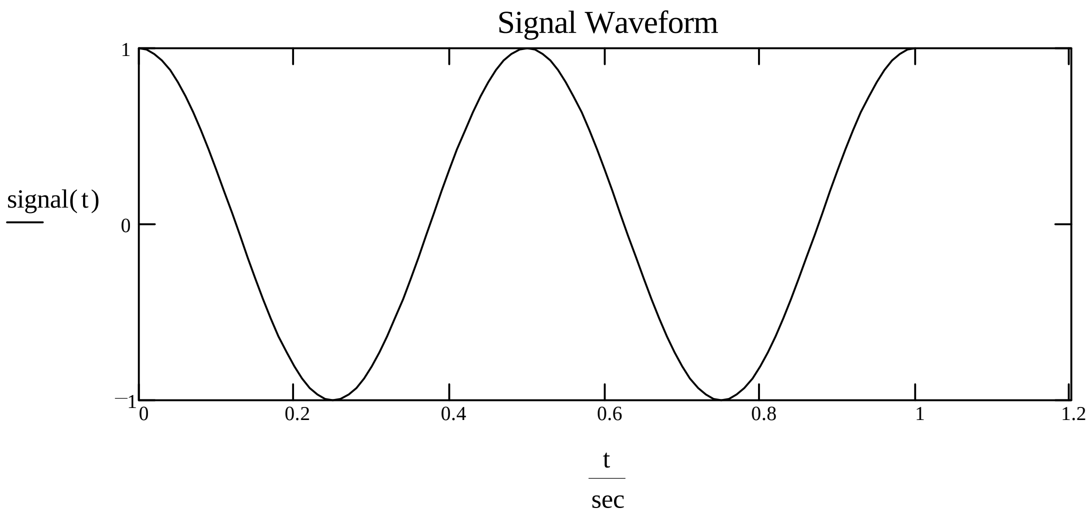
The radial signal frequency ($\omega$) in radians per second. $\omega := 2 \cdot \pi \cdot \nu$

Now plot the signal as a function of time. First define the points for the time axis. One hundred points between 0 and 1 second should work well for now. Define function for the signal as a cosine function with a frequency $\omega$.

Time Range (t) $t := 0 \cdot sec, 0.01 \cdot sec .. 1 \cdot sec$

Equation for signal as a function of time (signal(t)). $signal(t) := \cos(\omega \cdot t)$

Graph the signal waveform as a function of time.




**Exercises:**

1. Try changing the signal frequency. What do you expect will happen?
2. Try a noninteger value for the frequency.
3. Try large values for the frequency like 20, 40, 50, 60, 100 and 200 Hz. Now what happens?.
4. At what signal frequency does the graph stop looking like you expect?
5. Try some frequencies just above and below this value.
6. How many data points are graphed in the above plot?
7. What is time between data points?
8. What is the frequency of the data points?

Now go back and change the step size to 0.02 seconds and repeat the above exercise. After you do this, write a brief statement that summarizes your observations.

Use the index of any Instrumental Analysis textbook and look up Nyquist.  Compare your statement to the Nyquist sampling theorem.  This theorem has important implications in how data is acquired for FT instruments.  We'll come back to this again, but keep these observations in mind as you set different variables below.

After this brief detour to examine sampling theory, we return to the Fourier Transform.  First reset the signal frequency to 2 Hz and the time array to 0.01 second steps.

## The Test Waveform

The Fourier Transform is performed by multiplying the signal waveform by a test waveform.  So, now create this test waveform.  Specify the frequency of the test waveform (1 Hz), calculate the radial frequency, and define the function for the test waveform (just like the signal above).

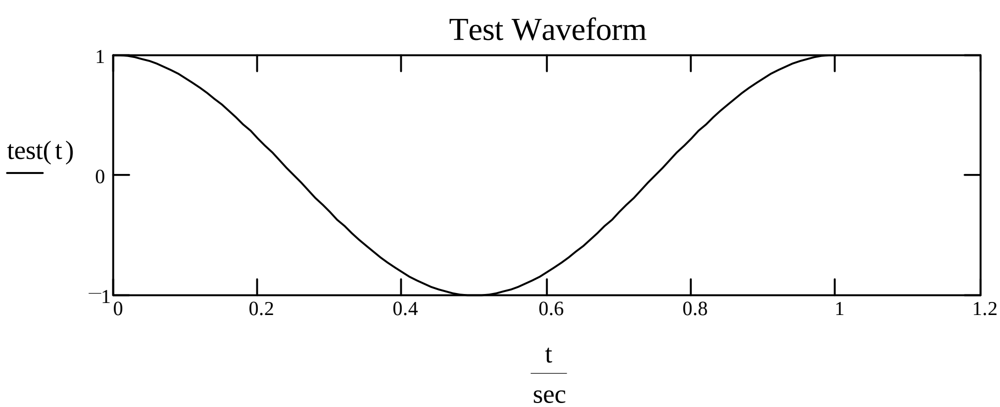
The test frequency ($\nu_{test}$) in Hz. $\nu_{test} := 1 \cdot Hz$ $\nu_{test} \equiv 1 \cdot Hz$

The radial test frequency ($\omega_{test}$) in rad/sec. $\omega_{test} := 2 \cdot \pi \cdot \nu_{test}$

The test function (test(t)). $test(t) := \cos(\omega_{test} \cdot t)$

**Mathcad Note**:
If $\nu_{test}$ is set here as a global variable. You can move it to other places in the document to facilitate variable testing. Only the global variable or local variable can be toggled on at one time.

Plot the test waveform as a function of time:

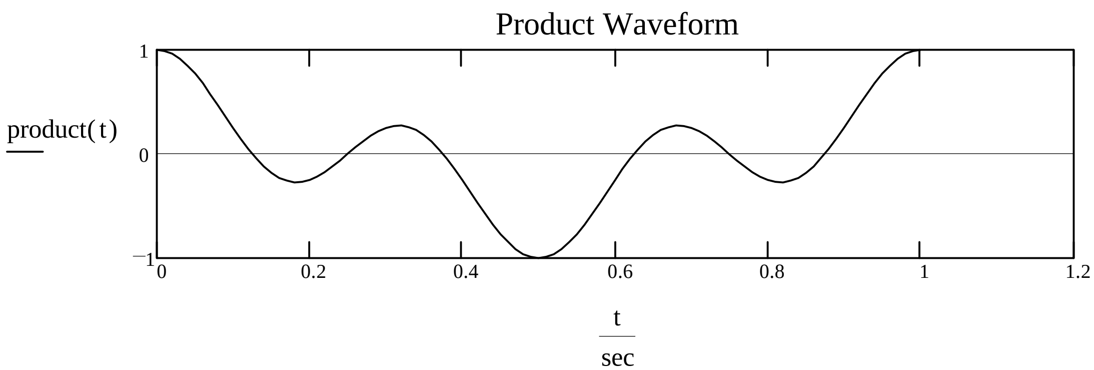


## The Product Waveform

Here we multiply the test waveform by the sample waveform.  This new function is the product waveform (product(t)).

$$\text{product}(t) := \text{test}(t)\cdot\text{signal}(t)$$

Graph the product waveform as a function of time.




The Fourier Transform determines the intensity of the signal at the test frequency by integrating this product waveform.  For a simple waveform, just inspect the graph shown above.  What is the area of this function?

A computer can integrate this waveform numerically by adding the product wave at each point.  This is done in Mathcad by creating an array of data points and then finding the sum of this array.  Define an index for the array (i) as a range from 0 to 99.  Define the array using the product function and this index (i).  Divide each point by 100 to produce 100 points between 0 and 1 second.  Then calculate the sum of the array.

$$i := 0, 1 .. 99$$

$$\text{array}_i := \text{product}\left(\frac{i}{100}\cdot\text{sec}\right)$$

$$\sum_i \text{array}_i = 0$$

This may also be done using the calculus functions in Mathcad.  Integrate the function product(t) with respect to time from 0 to 1 seconds.

$$\int_{0\cdot\text{sec}}^{1\cdot\text{sec}} \text{product}(t)\,dt = 0\cdot\text{sec}$$

## The Frequency Spectrum

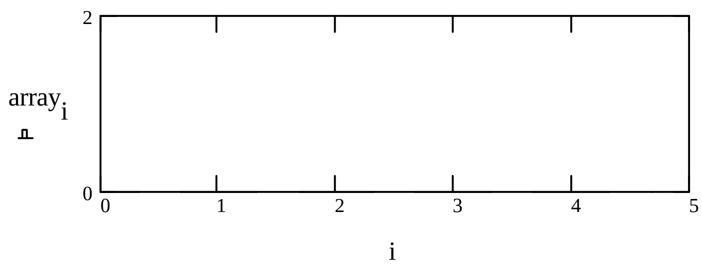
Ask the computer to run through a series of test frequencies to determine the signal intensity at each of these frequencies. Change the test frequency above ( you may move the global definition here to facilitate your exploration), and record the integration results for test frequencies of 0, 1, 2, 3, 4, and 5 Hz. Tabulate these results in the array below. The entries are all 0.0 at this time. After you enter your own results the bar graph will change. Explain what happened to the bar graph. What is the significance of this result?

$i := 0, 1 .. 5$

**Note**: set the lower limit of the y axis range in this graph to zero if necessary.

$array_i :=$

| |
|---|
| 0.0 |
| 0.0 |
| 0.0 |
| 0.0 |
| 0.0 |
| 0.0 |




**Exercise**: Go back and change the signal frequency to 4 Hz and repeat the above exercise. What conclusion can you draw from this new calculation?

So far we have met three basic components of the Fourier Transform.

- Start with a signal waveform
- Multiply it by a test waveform
- Integrate the product

The bar graphs of the frequencies shown above are the spectra produced by the Fourier transform. There are many important details yet to come, but first look at the document **LectureIntroFT.mcd** to clarify the ideas introduced so far. This document displays the signal, test and product waveforms on a single screen while you adjust the test frequency.

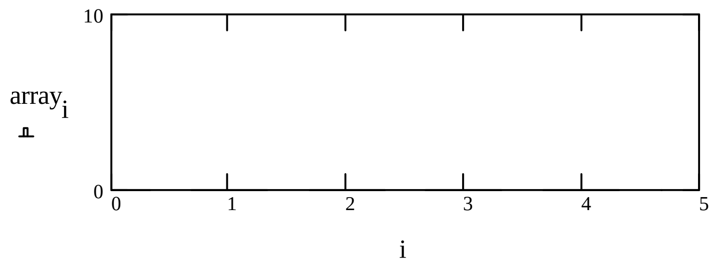
## The intensity of the signal:

The intensity of the signal is equivalent to the amplitude of the sine wave. Go back to the section above and change the amplitude of the signal wave to 10. Change the test frequency and produce a bar graph of the frequency spectrum. What changes in this spectrum?

$array_i :=$

| |
|---|
| 0.0 |
| 0.0 |
| 0.0 |
| 0.0 |
| 0.0 |
| 0.0 |
| |

**Note**: set the lower limit of the y axis to 0 if necessary




## But experimental signals are not always cosine waves.

Now it is time to introduce you to how the Fourier Transform accommodates waves that are not simple cosine functions. In addition to frequency, what other variables are used to describe a waveform?

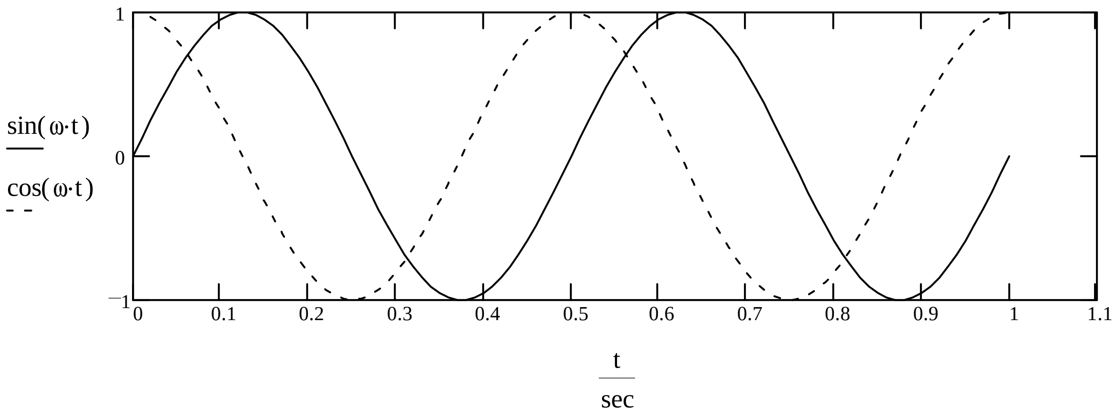
In this section, you will learn how the Fourier Transform interprets the phase of a signal. Understanding this concept explains many important ideas in Fourier Transform spectroscopy. Benchtop FTIR instruments usually handle this transparently, but research grade FTIR instruments, FT-NMR and FT-MS instruments all require the user to correct the phase of the spectrum. If you understand how this works, it is easier to correct the phase without blindly relying upon the computer. This section will help you produce better looking spectra with better integration.

Let's start by recalling a bit of trigonometry. Using the Mathcad functions, graph a 2 Hz cosine wave and a 2 Hz sine wave. Go back and reset the frequency of the signal to 2 Hz.

Check the current frequency setting: $\nu = 2 \cdot Hz$

## Sine and Cosine Waves

Graph of sin(ω*t) and cos(ω*t) as a function of time.

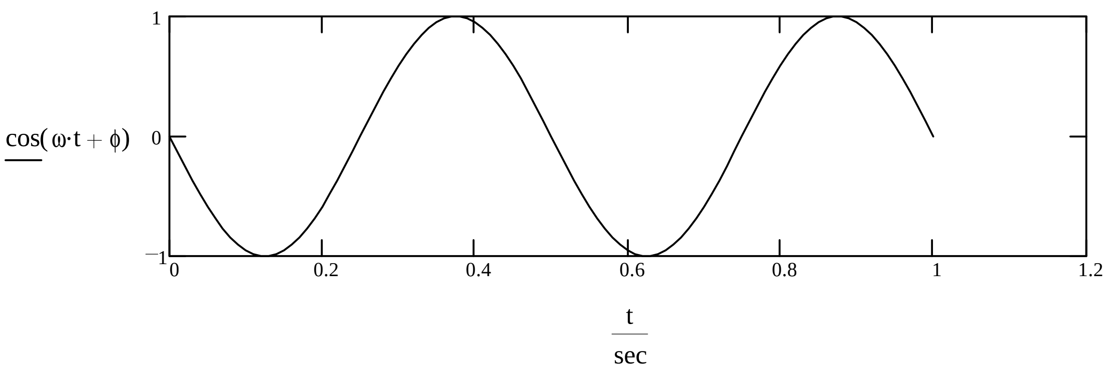



Looking at these two waves, the difference between a sine wave and a cosine wave is the shift along the x-axis. This shift is the phase. Now, make another graph that displays a cosine wave with a variable phase (ϕ).

## Phase Shift

The phase shift (ϕ) in degrees or radians. $\phi := 90\cdot deg$

Graph of cos(ω*t+ϕ) as a function of time.

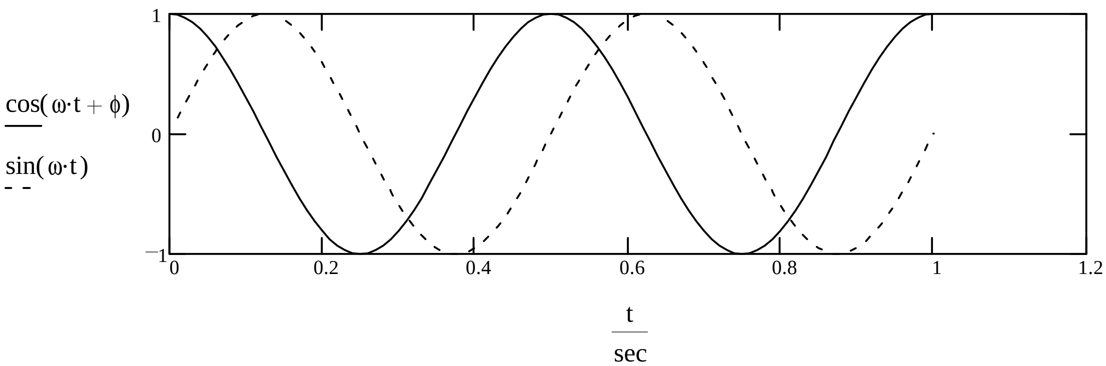



Now, try some different values of f and observe how that changes the waveform. 0, +/-30, +/-45, +/-60, +/-90, and +/-180 degrees are a good place to start. What happens to the waveform? If you are confused by this, you should review your trigonometry.

Next, graph a sine wave and a cosine wave with the phase shift on one graph.  Adjust the phase until the sine and cosine waves overlap.  Does the required phase shift fit with your expectations?

Set the phase shift here: $\phi := 0 \cdot deg$

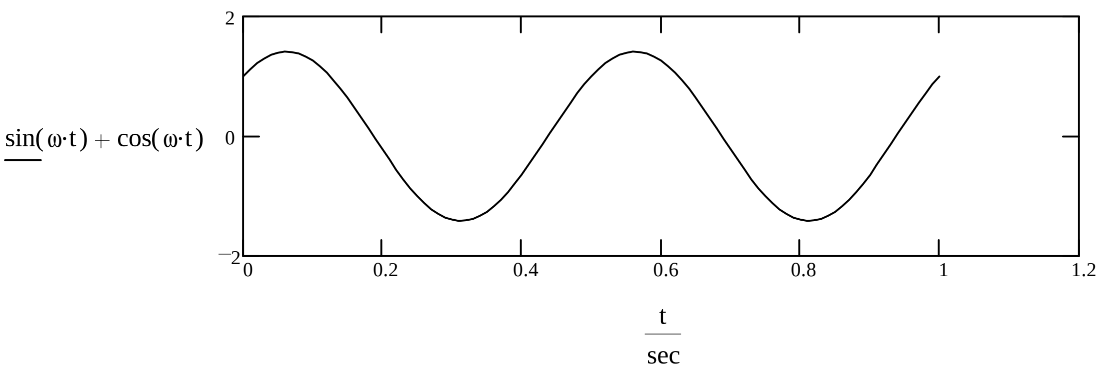
Graph of cos(ω*t+ϕ)  and sin(ω*t) as a function of time.




## Adding waves together

Now that you have explored the phase relationship between sine and cosine functions, what happens when you add sine and cosine waves together.

Graph of sin(ω*t) + cos(ω*t) as a function of time:

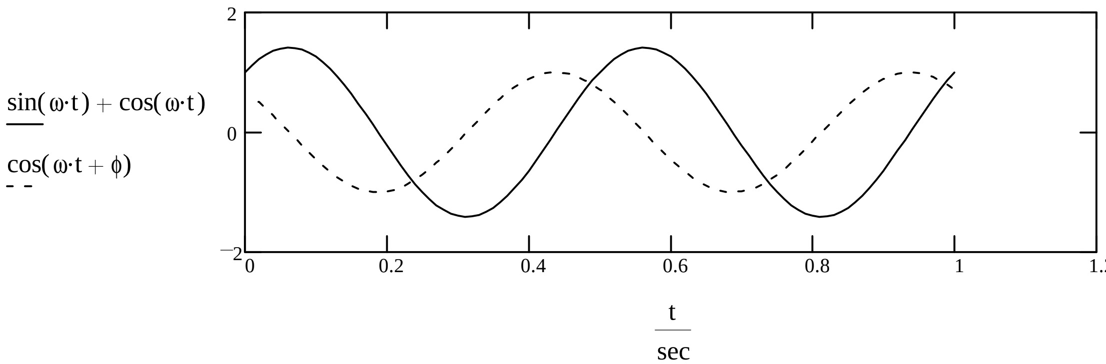



This new waveform is the sum wave.  It looks like a cosine wave with a phase shift.  This observation leads to a very important idea.  A wave with any phase can be described as a mixture of a cosine wave and a sine wave.  In this example, the wave is one part sine wave and one part cosine.  The phase of this sum wave is the angle where the sine and cosine are equal.

Verify this idea by creating a graph with the sum wave and a cosine wave with a phase shift. Compare the phase and frequency of these two waveforms.

phase shift: $\phi := 45\cdot deg$ Insert your own phase shift angle here.

Graph of sin(ω*t) + cos(ω*t) and cos(ω*t+ϕ) as a function of time:




Did you guess the phase of the sum wave correctly? If not, change the phase until the two waves are in phase.

The two waves above have the same frequency and phase, but different amplitudes. The cosine wave has an amplitude of one. But what is the amplitude of the sum wave? From the phase shift, you can determine the angle that corresponds to the maximum of the sum wave. Use the trigonometry functions in Mathcad to calculate the values for cosine and sine at this angle. How are these values related to the amplitude of the sum wave?

$$\cos(45\cdot deg) = 0.707$$

$$\sin(45\cdot deg) = 0.707$$

$$\cos(45\cdot deg) + \sin(45\cdot deg) = 1.414$$

Next create a new graph like the one immediately above. Show the sum wave and the cosine wave with a phase shift. Adjust the amplitude of the phase shifted wave to match the amplitude of the sum wave. Space has been left here for you to place your graph. What is your conclusion from this?

Graph of $\sin(\omega^*t) + \cos(\omega^*t)$ and $\cos(\omega^*t+\phi)$ as a function of time:

If you completed the exercise correctly you should observe that a waveform may either be described as a cosine wave with a phase shift or as a combination of a sine wave and a cosine wave.

To test your understanding of this concept create a graph with a cosine wave that has a phase shift of -60 degrees. Use what you learned above to calculate the amplitude of the cosine and sine components for this wave. Graph these waves to show that they overlap. Place your graph in the space left here for you.

In spectroscopy, the cosine component of a waveform is called the real spectrum. The sine component of a waveform is called the imaginary spectrum. Although this may be somewhat confusing, it will become clearer. The first time you need to phase correct an NMR spectrum, understanding this will allow you to understand what is happening rather than letting the computer do everything. *NOTE: The imaginary spectrum is not a figment of your imagination, it is just the term used for the sine component of the waveform. This terminology comes from the mathematics for complex numbers that contain a real and imaginary component (remember i in math and j in physics?).*

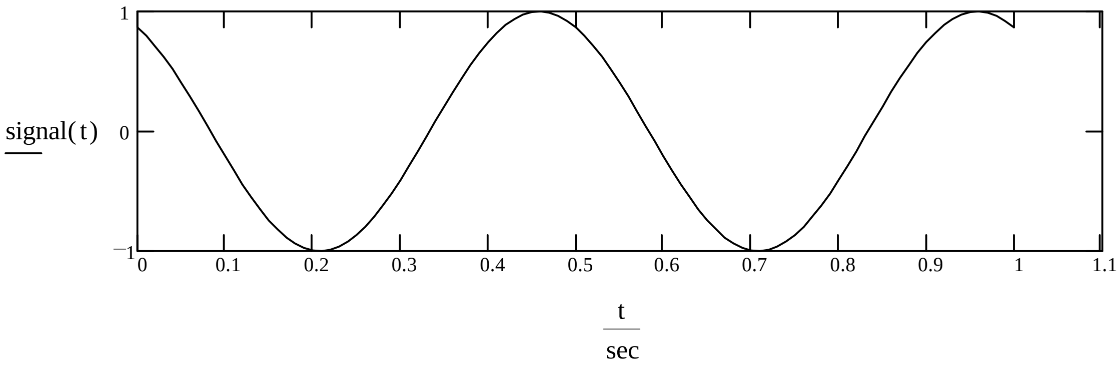
## Fourier Transform with sine and cosine components

Now, let's look at how the Fourier Transform determines the size of the real and imaginary components in a waveform using a sine test wave and a cosine test wave.

Check that the signal frequency is 2 Hz and redefine the phase shift ($\phi$) as 30 degrees. Be careful if you used global variables in your work with this document. Given:

| | |
|---|---|
| Frequency of signal | $\nu = 2 \cdot Hz$ |
| Phase shift of signal | $\phi := 30 \cdot deg$ |
| Signal as a function of time | $signal(t) := \cos(\omega \cdot t + \phi)$ |

The graph of the signal waveform as a function of time is:



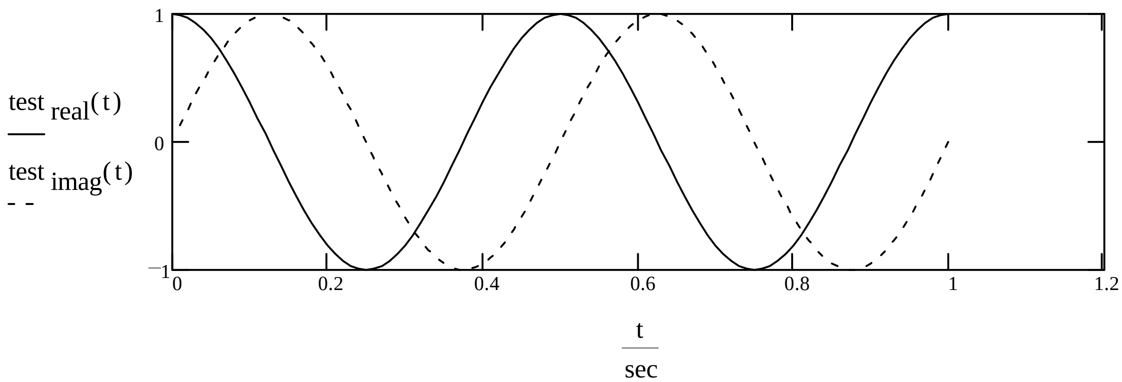
Now make two test waveforms. Redefine the radial frequency ($\omega_{test}$), as $4\pi$ rad/sec. The function $test_{real}$ is a cosine wave and $test_{imag}$ is a sine wave.

Define the radial test frequency: $\omega_{test} := 4\cdot\pi\cdot rad\cdot sec^{-1}$

Define the real and imaginary test waveforms:

| | Real | Imaginary |
|---|---|---|
| Test Wave | $test_{real}(t) := \cos(\omega_{test}\cdot t)$ | $test_{imag}(t) := \sin(\omega_{test}\cdot t)$ |

Graph the real and imaginary test waveforms as a function of time:

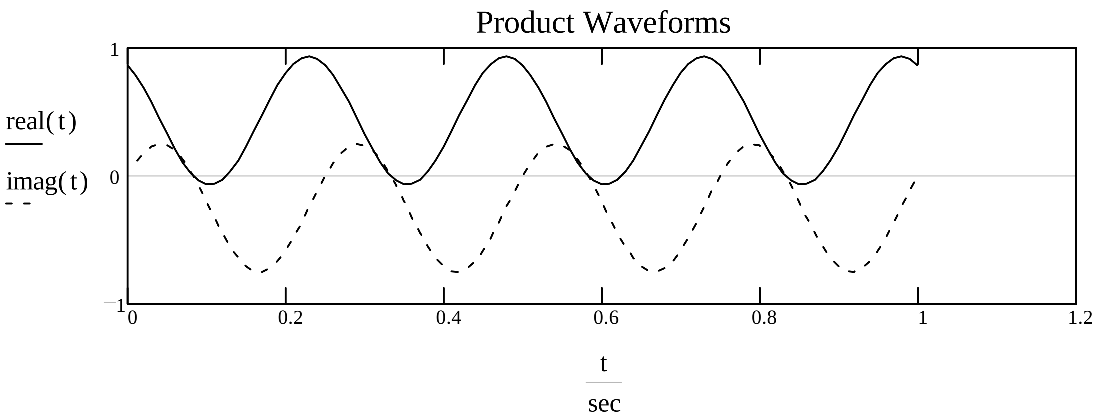



Define the real and imaginary product waves:

Real product wave $real(t) := test_{real}(t)\cdot signal(t)$

Imaginary product wave $imag(t) := test_{imag}(t)\cdot signal(t)$

Graph the real and imaginary product waves as a function of time.




Integrate the real and imaginary product waveforms from 0 to 1 sec.

Integrate $\int_{0\cdot sec}^{1\cdot sec} real(t)\,dt = 0.433\cdot sec$ $\int_{0\cdot sec}^{1\cdot sec} imag(t)\,dt = -0.25\cdot sec$

Recall that for the single cosine wave in the first part, the integration was related to the intensity of the peak at the frequency of the test waveform. The integration for the cosine wave gives the intensity of the cosine, or real, component of the signal at the frequency of the test waveform. The integration of the sine wave gives the intensity of the sine, or imaginary, component of the signal at the frequency of the test waveform.

Exercise: Change the phase angle and observe what happens. What is the integration when the phase angle is 0, 30, 60, 90, 180, 270, and 360 degrees? Write a trigonometric expression that will calculate the real and imaginary integration for different phase angles. Test it with different phase angles. What can you conclude from the experiment with phase angles? (Hint: you may wish to make the phase angle on page 12 a global variable and move it here.)

Real $0.5\cdot\cos(\phi) = 0.433$

Imaginary $0.5\cdot\sin(\phi) = 0.25$

## Data Acquisition Parameters for the Fourier Transform:

Now that you have an understanding of how the test function is used for the Fourier Transform we will use Mathcad's fast Fourier transform (FFT) function for the rest of this document. This function uses an algorithm that significantly enhances the speed for calculating the Fourier Transform. For this fast transform to work properly the number of data points must be a power of 2 (i.e.: 2, 4, 8, 16, 32, 64, etc.).

Note: Mathcad includes two functions (FFT and fft). Either of these functions will work but they use different normalization factors to calculate the amplitude of the wave. The FFT function is consistent with our usage.

For this function to work, the time domain data must be in an array. To do all this requires some new variables. Start with $2^8$ data points and 10 second acquisition:

The Number of Data points

exponent (x): $x := 10$

number of data points (N) $N := 2^x$

$N = 1.024 \cdot 10^3$

**Mathcad note**: x can be converted to a global variable and moved below to permit easier exploration with varying this parameter.

The total acquisition time ($t_{acquire}$) $t_{acquire} := 10 \cdot sec$

Together the number of data points and the acquisition time specify the dwell time. This is the time between data points. The dwell time is also frequently referred to as the sampling frequency (in Hz). On an FTIR instrument, this dwell time is equivalent to the distance traveled by the moving mirror between HeNe fringes. On an FT-NMR or FT-MS instrument, this is the time delay between each data point collected by the analog to digital converter.

Calculate the dwell time for N data points over the acquisition time t. Remember that for N data points, there are N-1 delays.

Define the dwell time (DW) $DW := \dfrac{t_{acquire}}{N - 1}$

Current value of DW $DW = 9.775 \cdot 10^{-3} \cdot sec$

Sampling Frequency: $\dfrac{1}{DW} = 102.3 \cdot sec^{-1}$

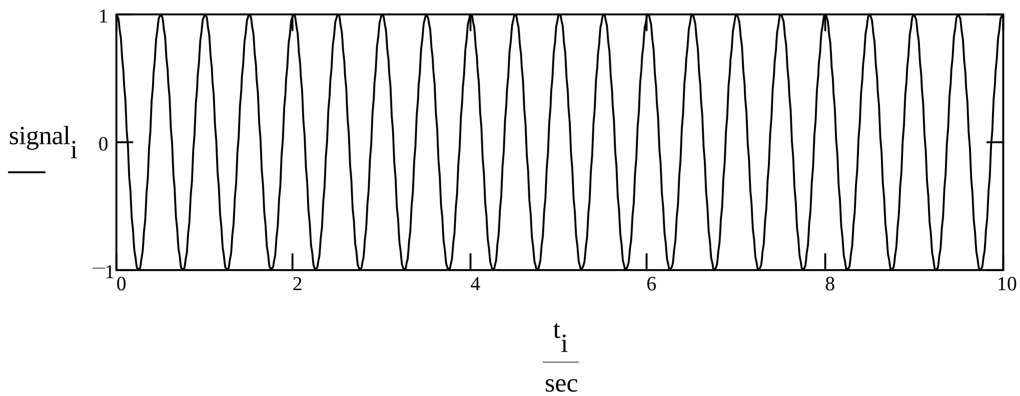
For Mathcad to calculate the FFT of the signal, the signal must be a vector instead of a function. This vector will have N points. Use i as the index for this vector array.

Index (i) from 0 to N-1 to contain N points $i := 0, 1 .. N - 1$

The time vector ($t_i$) defined using the index i and the dwell time. $t_i := i \cdot DW$

The signal vector defining a cosine wave with a radial frequency $\omega$, at each delay time in the vector $t_i$ $signal_i := \cos(\omega \cdot t_i)$

Graph $signal_i$ vs $t_i$.




Now Mathcad can calculate the Fourier Transform of this signal using the FFT function. Take a look at the help menu and look at the Mathcad resource center for an example to get you started. Now produce an array for the frequency data by taking the Fourier Transform of the signal.

The frequency array (F) $F := FFT(signal)$

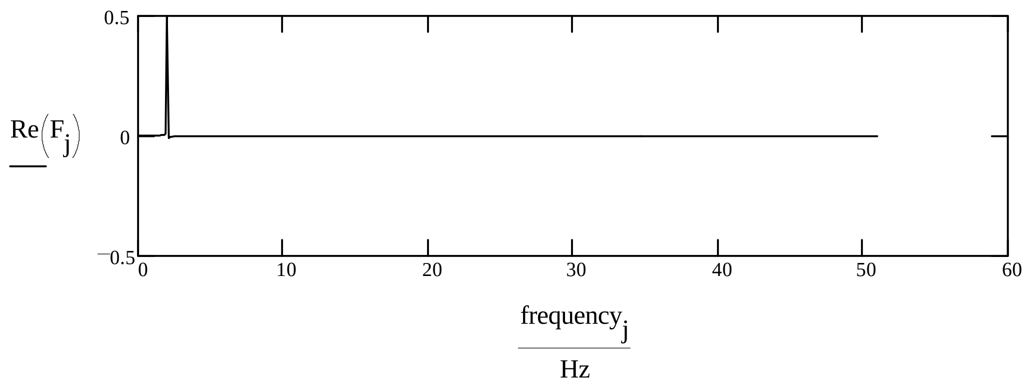
The FFT returns a complex (real and imaginary) number that gives the real and imaginary spectra. However, it only returns half as many points so we need a new array index. To explain why there are half as many data points, remember that the dwell time and acquisition time determine the sampling rate and spectral window. The Nyquist sampling theorem results in half as many points in the frequency domain. Create an index j from 0 to $\frac{N}{2} - 1$

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

Using the Mathcad help menu, find out how to calculate the frequency for the points in F. Create a new vector "frequency" with j points for the x axis.

The vector (frequency): $$frequency_j := \frac{j}{t_{acquire}}$$

Graph the real component of F vs. frequency. The FFT produces a complex number in the form a+bi, use the Mathcad function (Re) to extract the real component of this complex number.




Using this graph, observe the effect of the number of data points on the spectrum. Try several other values for N and observe how the spectrum changes with both smaller and larger numbers. Explain your results.

How does the number of data points effect the dwell time (time between data points) and sampling frequency (rate of data acquisition in Hz)?

Dwell time $$\frac{t_{acquire}}{N} = 9.766 \cdot 10^{-3} \cdot sec$$

Sampling frequency $$\frac{N}{t_{acquire}} = 102.4 \cdot sec^{-1}$$

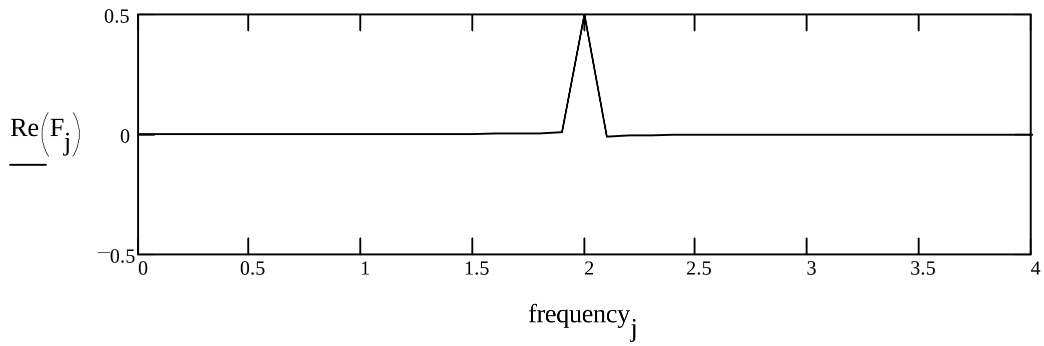
How is the sampling frequency related to the spectral window (the range of frequencies observed in the spectrum)?

Now, review the information about the Nyquist sampling theorem from the beginning of this document. Does this fit with what you just found?

When you acquire data on an FT instrument, you can specify the number of data points and the total acquisition time. These two variables determine the sampling frequency. When the acquisition time is constant, changing the number of data points changes the sampling frequency. This is what was observed above. Next, we will look at how the acquisition time effects the spectrum. To reduce the confusion, we will hold the sampling frequency constant.

Based upon your experience, select appropriate values for N and $t_{acquire}$ to change the acquisition time. The sampling rate should remain constant. For the easiest way to do this, double both the acquisition time and the number of data points set above. To clearly observe the effect of this, you will need to zoom in on a part of the spectrum to observe the changes. This is readily accomplished by adding another graph and setting the X-axis scale to go from 0 to 4 Hz.

Graph of Re(F) vs. frequency, zoomed in on the peak.




Here we have a set of equations that use the acquisition time and the number of data points to calculate the sampling rate, spectral window, and resolution:

Sampling Rate $SR := \frac{N}{t_{acquire}}$ $SR = 102.4 \cdot Hz$

Spectral window $SW := \frac{N}{2 \cdot t_{acquire}}$ $SW = 51.2 \cdot Hz$

Resolution $resolution := \frac{1}{t_{acquire}}$ $resolution = 0.1 \cdot sec^{-1}$

## Fourier Transform of Decaying Signals.

The signal from most FT instruments decays with time. The physical reason for the signal decay depends upon the type of experiment. For all instruments, the decay has a significant affect on the spectrum. Based upon your experience with the effect of the acquisition time, how do you expect a decaying signal to effect the spectrum?

Here we create a new equation for the signal waveform with a radial frequency ω (check above that the signal frequency is still 2 Hz). In the expressions below redefine the phase shift (ϕ) as 0 degrees, the acquisition time to 10 sec, and the number of data points to $2^{12}$. Set a time constant (τ) for the exponential decay to 1 second (you must set the parameters yourself):

| | |
|---|---|
| Radial Frequency of signal (ω) | $\omega = 12.566 \cdot sec^{-1}$ |
| Phase Shift (ϕ) | $\phi := 90 \cdot deg$ |
| Exponential Decay time constant (T) (start with a value of 1 second) | $\tau := 5 \cdot sec$ |
| Exponent for number of data points (x) | $x := 8$ $\quad N := 2^x \quad N = 256$ |
| Acquisition time ($t_{acquire}$) | $t_{acquire} := 20 \cdot sec$ |
| Vectors | $i := 0, 1 .. N - 1$ |

$$j := 0, 1 .. \frac{N}{2} - 1$$

$$t_i := i \cdot \frac{t_{acquire}}{N - 1}$$

The the signal array with an exponential decay and a phase shift.

$$signal_i := \cos\left(t_i \cdot \omega + \phi\right) \cdot e^{\frac{-t_i}{\tau}}$$

**Exercise:** In the space provided here prepare a graph of the signal vector vs. the time vector. Include a plot of the equation for the exponential decay of the signal on this graph.

**Exercise:** Change the time constant for the exponential decay and observe the effect on the signal. Try 0.5, 2 and 5 seconds.

Here we Fourier Transform the signal vector into the frequency vector (F), and redefine the frequency array.

$$F := \mathrm{FFT}(signal) \qquad frequency_j := \frac{j}{t_{acquire}}$$

**Exercise:** Below in the space provided plot the real, Re(F), and imaginary, Im(F), spectra. You may want to make a second graph to provide a zoom view. Adjust the frequency axis to provide an optimal view.

**Exercises:**

Notice the shape of the real and of the imaginary spectrum. You may want to adjust the acquisition time and the number of data points to provide a smooth curve.

Change the phase shift and observe the affect on the real and imaginary spectra.
Change the relaxation time and observe the affect on the spectra.
Record your observations in your notebook.

Here we Integrate the real and imaginary spectra by calculating the sum of the array:

$$\sum_{j} \mathrm{Re}\left(F_j\right) = 0.028 \qquad\qquad \sum_{j} \mathrm{Im}\left(F_j\right) = 0.322$$

Explain the significance of the sums of the arrays.

## Closing Comments

After working through this document you should have mastered several important aspects of the Fourier Transform that will help you set parameters for data acquisition on FT instruments. The significance of the number of data points, the acquisition time, the decay rate of the signal, and the sampling rate should all be clear. In addition, you should appreciate how the Fourier transform is performed. When you begin to adjust the phase of an NMR peak, think about the real and imaginary spectra.

Now let's look at some experiments.....

## References and suggested reading

R. R. Williams *Spectroscopy and the Fourier Transform* Wiley: New York, 1995

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