Introduction to FT-IR

Fourier Transform Infrared Spectroscopy (FTIR) uses an interferometer rather than a monochrometer to provide wavelength information. The interferometer has several different settings that effect the apperance of the final spectrum. This worksheet demonstrates these interactions and shows how these settings effect the final spectrum. To simplify the calculations, emission spectra are used for this simulation.

Signal: This section defines the observed signal. You can change the amplitude, frequency and natural linewidth of each peak.

	Band *a*	Band *b*
Amplitude	$A_a := 10$	$A_b := 10$
Frequency	$\nu_a := 400 \cdot cm^{-1}$	$\nu_b := 450 \cdot cm^{-1}$
Natural linewidth	$\Delta\nu_a := 10 \cdot cm^{-1}$	$\Delta\nu_b := 10 \cdot cm^{-1}$
Separation	$\Delta_{a\_b} := \left|\nu_a - \nu_b\right|$	$\Delta_{a\_b} = 50 \cdot cm^{-1}$

Interferometer Settings: This section defines the sampling parameters of the interferometer.

Number of data points: (this must be a binary number)	$N := 2^{12}$	$N = 4 \cdot k$
Number of HeNe fringes between data points: (this determins when the interferometer collects data)	$fringes := 2$	

Calculated Parameters: Based upon the parameters entered above, the spectrometer can calculate the following variables. (Note: the optical path distance is twice the mirror travel.)

Optical Path Delay between data points	$\Delta_{OPD} := fringes \cdot 690 \cdot nm$	$\Delta_{OPD} = 1.38 \cdot 10^{-6} \cdot m$
Max Optical Path Delay	$max_{OPD} := \Delta_{OPD} \cdot N$	$max_{OPD} = 0.565 \cdot cm$
Spectral Window	$SW := \frac{1}{2 \cdot \Delta_{OPD}}$	$SW = 3623 \cdot cm^{-1}$
Digital Resolution	$Resolution := \frac{1}{max_{OPD}}$	$Resolution = 1.769 \cdot cm^{-1}$

Index: These Indexes are used for various calculations.

$i := 0, 1 .. (N-1)$	$optical\_delay_i := i \cdot \Delta_{OPD} \cdot 1$	Interferometer step index
$j := 2, 3 .. \left(\frac{N}{2} - 1\right)$	$wavenumber_j := \frac{j}{N \cdot \Delta_{OPD}}$	Wavenumber calibration index

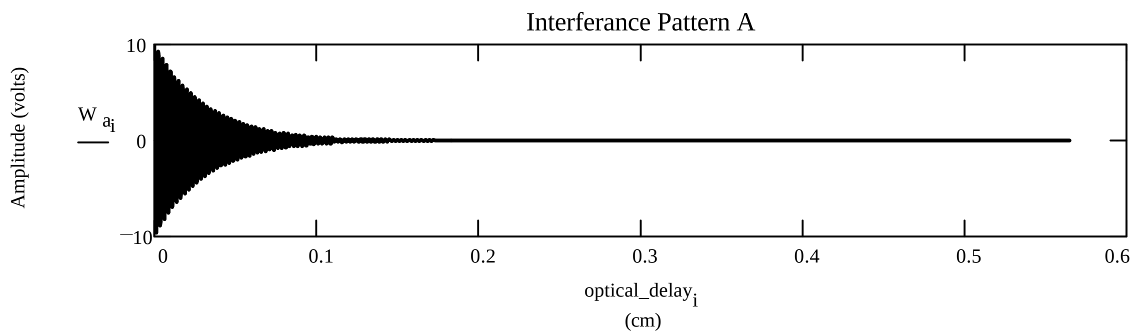
Calculate Interferogram: Calculate an Interferogram using the above information.

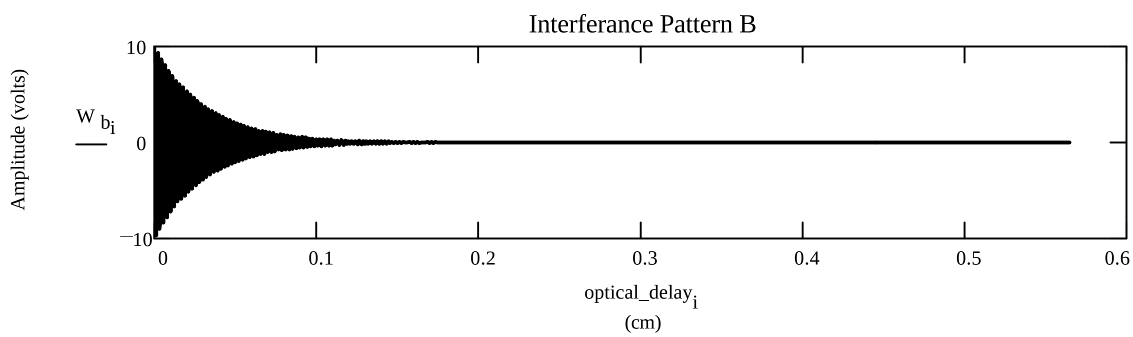
Wave a $$W_{a_i} := \left(A_a \cdot \cos\left(optical\_delay_i \cdot \nu_a \cdot 2 \cdot \pi\right)\right) \cdot e^{-\left(\left|optical\_delay_i\right| \cdot \Delta\nu_a \cdot \pi\right)}$$

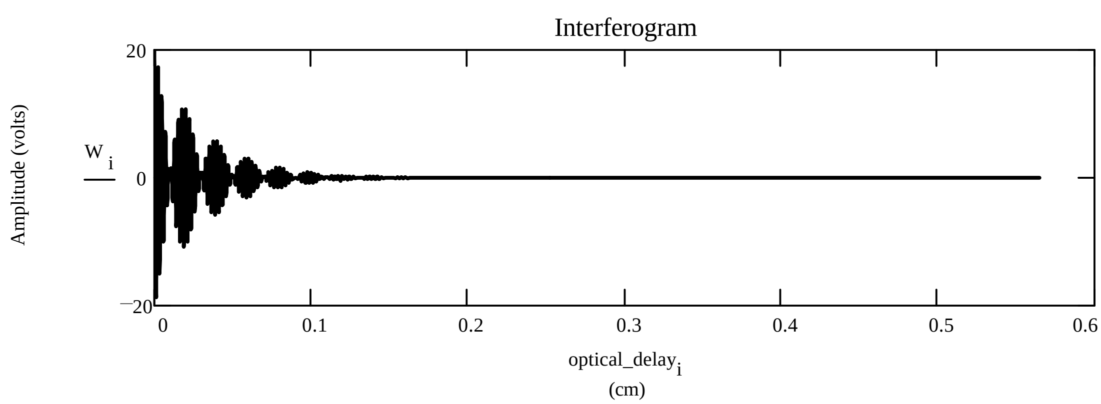
Wave b $$W_{b_i} := \left(A_b \cdot \cos\left(optical\_delay_i \cdot \nu_b \cdot 2 \cdot \pi\right)\right) \cdot e^{-\left(\left|optical\_delay_i\right| \cdot \Delta\nu_b \cdot \pi\right)}$$

Wave a and b $$W := W_a + W_b$$

Display Waveforms: Display the Interferogram signals for the above information.



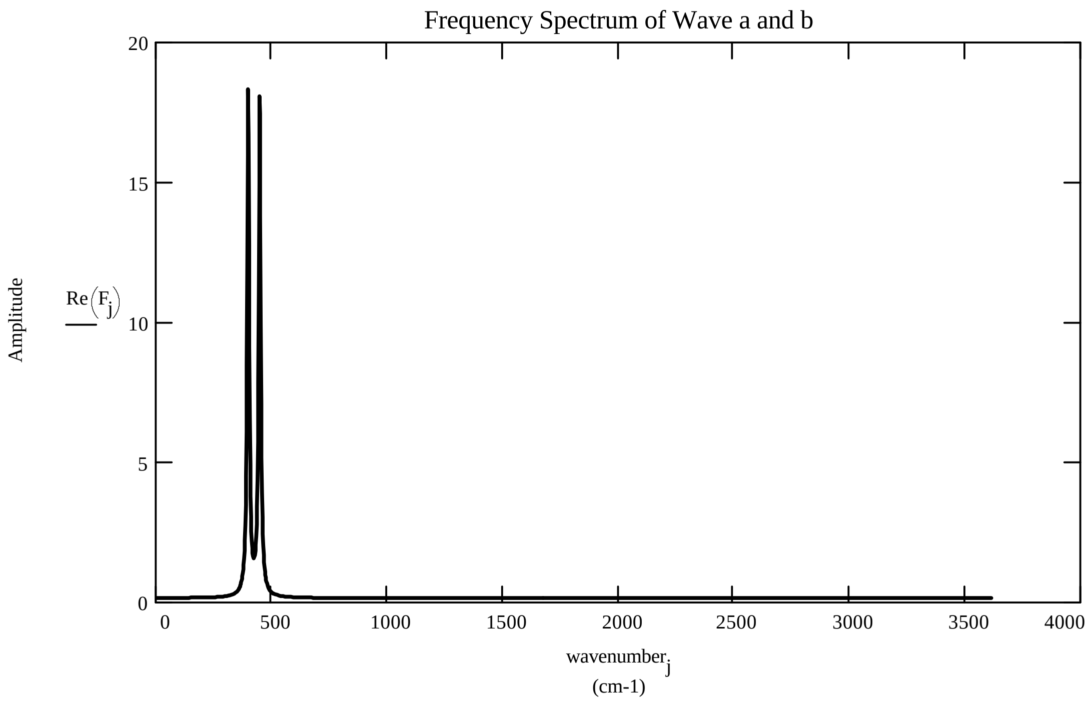


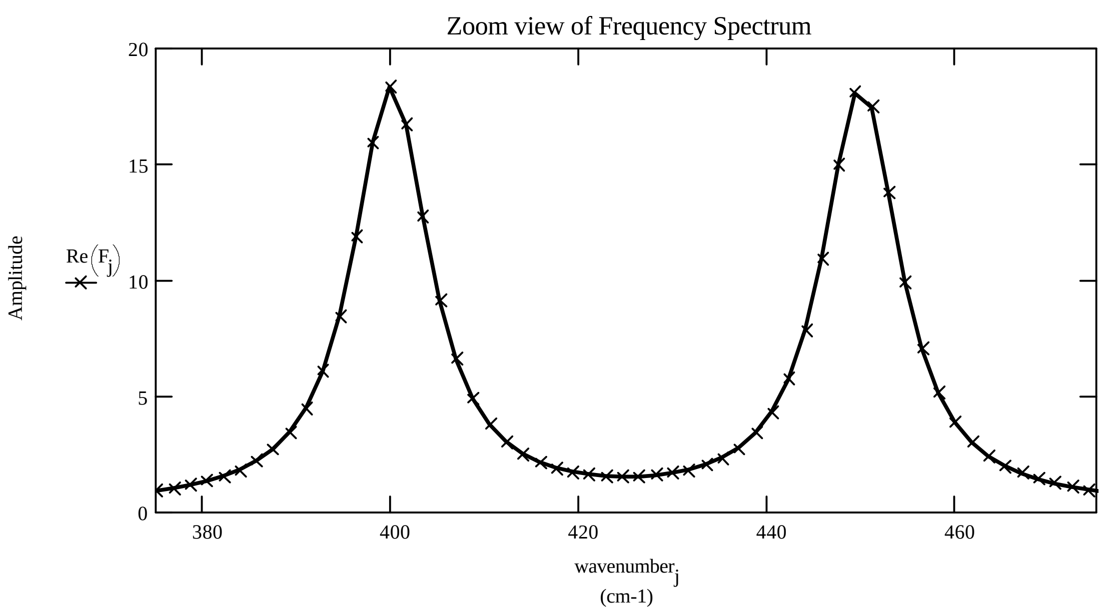


Fourier Transforms: Fourier transform of interferogram to produce frequency domain signal (spectrum).

FFT sum of a and b $F := \mathrm{fft}(W)$

Display Fourier Transforms of Waves:





Questions:

1. Determine how the number of data points effects the spectrum and the operation of the interferometer. Change the number of data points (it must be a power of two so change the exponent above) and record the values for the "Calculated Parameters". Also observe the apperance of the spectra. Prepare a table that summarizes your results and write a brief statement answering the question "What effect does the number of data points have on the observed spectrum?".

2. Determine how the number of HeNe fringes per acquisition effects the spectrum and the operation of the interferometer. Change the number of fringes (for most instruments this must be an integer value) and record the values for the "Calculated Paramters." Also observe the apperance of the spectra. Prepare a table that summarizes your results and write a brief statement answering the question "What effect does the number of fringes have on the observed spectrum?".

3. What happens if you change the absorbance frequency for υ_b so that it is outside the spectral window? Reload the worksheet (so the number of data points and fringes are set at the default values). Change υ_b to: 3000 cm^{-1}, 3600 cm^{-1}, 4000 cm^{-1}, 5000 cm^{-1}, 6000 cm^{-1}, and 7000 cm^{-1}. Prepare a table that summerizes your results and write a brief statement answering the question "What happens if the signal is outside the spectral window?"

4. Change the natural linewidth for a peak and observe the interferogram and the spectrum. What happens to the interferogram and the spectrum if the linewidth is wide? What happens if it is very narrow?

5. How would you set the instrument for the widest spectral window? How could you design an instrument to increase the spectral window? What advantage is there to a narrow spectral window?

6. How would you design an instrument to increase the resolution? What are the advantages and disadvantages of this?

Global Variables

$k \equiv 1024$

$nm \equiv 10^{-7} \cdot cm$

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