Fall 2002. 10.34. Numerical Methods Applied to Chemical Engineering

Homework # 6. Fourier Transforms

Assigned Monday 10/28/02. Due Monday 11/4/02

Calculate an IR transmission spectrum from instrument data

We wish to measure the IR spectrum of an unknown sample. To obtain this data, we have a machine that provides pulses of infrared radiation of finite duration (see figure below). This radiation passes through the sample, where part of it is absorbed at specific frequencies that may be used to identify the sample. The radiation that is transmitted from the sample then is detected in the machine, and its intensity is recorded as a time-varying output voltage signal. This signal is sampled at times separated by a uniform interval Δt.

One might think to measure the IR spectrum by varying the frequency of the input radiation, and then to plot the intensity of the time-averaged output signal as a function of frequency. Of course the intensity of the IR source must be held constant. A quicker way to measure the spectrum is to input the IR radiation in a time-varying manner and then to use Fourier analysis to estimate the transmittance spectrum of the sample. This approach is known as *Fourier Transform Infrared spectroscopy*, or FTIR.

We must select the sampling interval Δt so that we can compute the frequency spectrum in the range of interest for IR experiments. Spectroscopists usually express frequencies in IR experiments as wave numbers in units of reciprocal centimeters, $k(cm^{-1})$. Typical values of wave numbers sampled in an IR experiment are 650 to 4,000 cm^{-1}. We can compute the corresponding angular frequencies in units of *radians/second* from the formula

$$\omega(\text{rad/s}) = k(cm^{-1}) \times 100(cm/m) \times c(m/s) \qquad \text{(EQ 1)}$$

where the speed of light is $c = 3 \times 10^8 \text{m/s}$. For our machine, we have selected the time interval so that the Nyquist critical frequency corresponds to a wave number of 4,000 cm^{-1}.

We then choose the number of data points to be sampled as the smallest power of 2 that provides a frequency resolution, expressed in wave numbers, of 1 cm^{-1}. We find that we have to acquire 8192 data points to achieve this resolution. For our time-varying input signal, we choose a number of square wave pulses (see figure below). The strength of the input signal as a function of time is stored in the ASCII file pulse_signal.dat.

To calibrate the machine, you first perform the experiment without a sample present to measure the response of the machine. The results of the output voltage signal from this experiment are also plotted in the figure below and are stored in the ASCII file calibration_signal.dat. We then place the sample in the instrument and perform again the same experiment, recording the results in the ASCII data file acquisition_signal.dat.

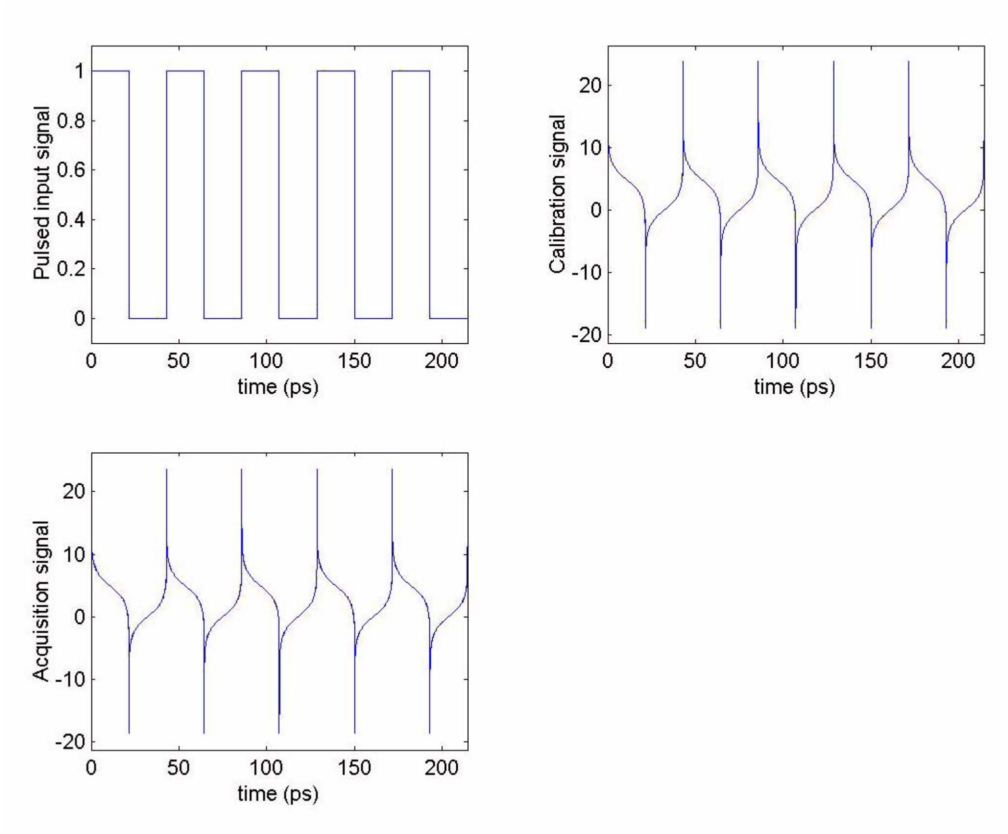

FIGURE 1. Time-varying input and output signals of IR experiment. (upper left) pulsed input signal of IR radiation into sample chamber. (upper right) Output voltage signal measured during a calibration experiment in which no sample is present. (lower left) Output voltage signal measured with sample present.

Your assignment is the following:

From this data, compute the transmittance spectrum of the sample. Plot the results as the percentage of IR radiation transmitted as a function of wave number, over the range 650 to 4,000 cm^{-1}.