Computer lab 4   Name_____

I.   Questions related to the FFT lab

1. After adding the noise to the Gaussian does the intensity still drop to zero at higher frequencies?

yes _____   no   _____

2. Do you still see the Gaussian in reciprocal space?

yes _____   no   _____

3. Where does the intensity at low frequencies come from

A. mostly from the Gaussian peak but some of it also from the noise

B. the Gaussian peak only

C. mostly from the noise but some of it also from the Gaussian peak

D. the noise only

4. Prior to World War II the technology of making movies was not advanced enough to take more than 16 frames per second or so. In old silent movies this is often visible when you see a wheel or a propeller starting to turn. At first it seems to start turning the right way but at some point the propeller seems to stand still and then start to turn backwards.

Why is this related to the Nyqvist frequency?

II. Numerical computations using Excel

II.A. Modeling NMR spectra

Using the FFT worksheet activated with the same methods used for the laboratory, let's create some Free Induction Decays (FIDs) that represent the kind of signals seen in NMR spectroscopy. In NMR a 90o pulse rotates the magnetization due to the nuclei into the x-y plane. Then this magnetization rotates at a characteristic frequency and relaxes back to the vertical configuration. The FID is a cosine (or sine) function multiplied by an exponential function.

1.   First type into C1 := COS(32*B1)*EXP(-B1). Fill the C column. Take the FFT

2. Determine the position and estimate the line width of the resulting spectral feature. To determine the line width find the full width at half maximum (FWHM). What is functional form of the line shape?
3. Next type into C1 := COS(32*B1)*EXP(-2*B1). Fill the C column. Take the FFT
4. Determine the position and estimate the line width of the resulting spectral feature. We can call the exponent the relaxation rate. For example, in the first part the relaxation rate, Γ, is $\Gamma = 1$ and in the second trial the relaxation rate is $\Gamma = 2$. What can you conclude about the relationship between the relaxation rate and the FWHM?
5. If there are two spins connected through a bonding pathway (H-C-C-H) then they can interact by a scalar coupling. In this case one spin's magnetic field will cause a splitting in the magnetic field of the connected spin. To model this effect type into C1 := 0.5*(COS(B1*30)+COS(B1*34))*EXP(-B1). Fill the C column. Take the FFT. Describe what you see. What is the scalar coupling J?
6. In the following aspect we will consider the appearance of the scalar coupling as the relaxation rate increases. To compare with the above scalar coupling type:
   A. C1 := 0.5*(COS(B1*30)+COS(B1*34))*EXP(-2*B1).
   B. C1 := 0.5*(COS(B1*30)+COS(B1*34))*EXP(-4*B1).
7. Describe the observed line shapes as the relaxation rate increases from $\Gamma = 1$ to $\Gamma = 4$. Can you state a general rule for the appearance of line shapes in terms of the relative magnitude of J and Γ?

II.B. Modeling crystal structures

Scattering, including X-ray diffraction is nothing but a Fourier transform of the electron density function of your sample, e.g. an ice crystal. Consider how the electron density (the local concentration of electrons) fluctuates inside an ice crystal. We shall pretend it is just a one dimensional row of ordered molecules and project all the electron density onto the x-axis.
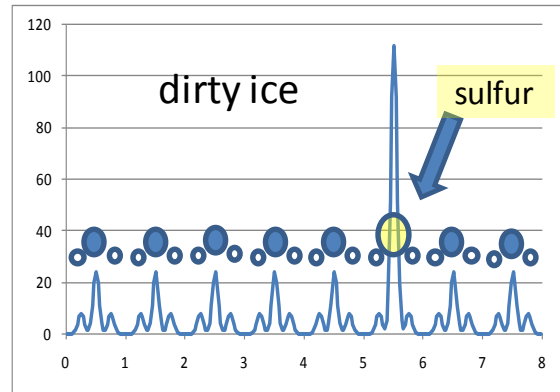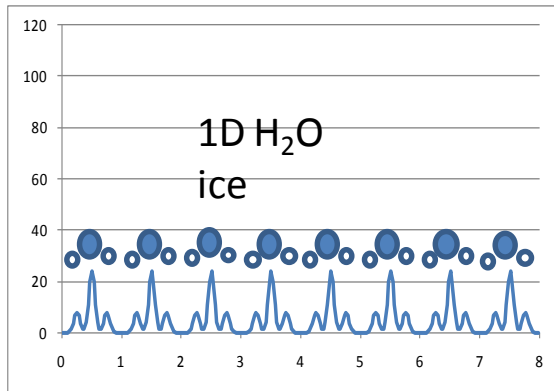
Simulated electron densities in four one dimensional solids.
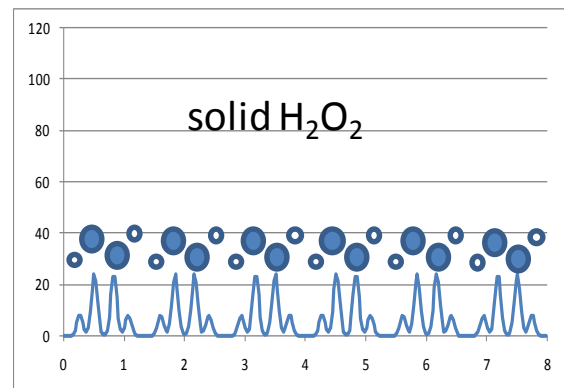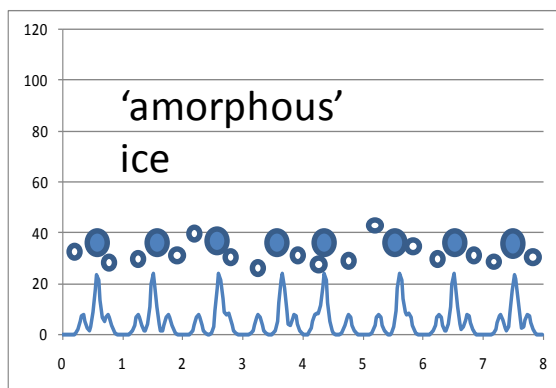
Open up spreadsheet: icefft.xls.   You will find the functions with and without S and a "liquid" (amorphous) one. Also a 1D crystal of hydrogen peroxide is simulated.

Make a graph of the four functions. They should look like above. You can think of the x-axis as Angstroms, although I did not adhere to ionic radii. Notice that the third function is not quite as regular as the others.

- How many molecules are there in 8 Angstroms?
- What is the repeat unit in Angstrom?

Now transform each of the functions by FFT.   You can transfer the data to the other sheet and use the button, but you can also go to the data analysis pack and invoke Fourier transform. There is a popup where you specify where your data are and where you want the result.

We will not consider the zeroth harmonic. In X-ray diffraction that corresponds to the incident beam passing straight through the sample and you cannot measure anything if there is no diffraction. Now make a plot of the intensity = $(IMABS)^2$.   The graph you get looks very much like a powder pattern, which you will encounter later in the demonstration portion of the course. However, here you may consider these peaks reciprocal space to be due to the periodicity of the structure. For example, the peak

at in reciprocal space represents the minimum periodic "wavelength" of 1 molecule per Angstrom. In that case how would you interpret "frequencies" of 1/2 or 1/4? Perhaps more challenging is to understand the meaning of the peak at 3/4. Plot your output in reciprocal space (i.e. using the $(IMABS)^2$ of the FFT and try to interpret the peaks that result.

The substitution of one molecule of H_2S in the lattice of H_2O is called dirty (or impure) ice. Interpret the $(IMABS)^2$ of the FFT of this structural file.
- Does the substitution of O by S affect the peak positions?
- Does it affect the peak intensities?
- What happens to the 'empty' harmonics between the peaks, when the strict translation order is broken in the dirty ice?

The amorphous ice structure has greater disorder. Take the FFT of this structural file and then plot the $(IMABS)^2$. Describe the change in structure. Can you account for this change?

In what ways is the hydrogen peroxide reciprocal lattice (given by the FFT) different from the ice reciprocal lattice?