Numerical Considerations

The true relationships between the wave function in x-space and the amplitude function is the Fourier transform. By using discrete numerical techniques, we have changed the infinite integral to a finite sum. Since we only summed over a finite number of complex harmonics, we have implied that the x-space representation is periodic! This periodicity can come back to haunt us if we are not careful.

Because we estimated the Fourier transform by making the x-space function periodic, it also means that the reciprocal space amplitude function will be discrete, and harmonically related. Using this information, we can determine that the values for $\vec{q}$ should be separated by

$$\delta q = \frac{2\pi}{N \delta x}$$

where **N** is the number of points in $\vec{x}$, and is chosen to be odd to simplify matters. Furthermore, the maximum (most positive) and minimum (most negative) values of $\vec{q}$ should be

$$q_{\substack{\max \\ \min}} = \pm \frac{\pi}{\delta x} \frac{N-1}{N}$$

Note, to take into account larger values of **q** (``higher frequencies"), we should decrease $\delta x$ (``increase the sampling frequency"). To decrease δq (without increasing δx) we should make our maximum value of **x** larger, and keep N the same.

In 6.011 you will learn more about the numerical issues concerning the Discrete Fourier Transform. You will also learn how to accelerate its computation by a method known as the Fast Fourier Transform (FFT).