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 $\tilde{q}$ should be separated by

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

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

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

Note, to take into account larger values of $q$ ("higher frequencies"), we should decrease $\delta x$ ("increase the sampling frequency"). To decrease $\delta q$ (without increasing $\delta x$) 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).