Fourier Transformations & Understanding Uncertainty
Uncertainty Relation: Fourier Analysis of Wave Packets

Group 1: Brian Allgeier, Chris Browder, Brian Kim
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Introduction:

In Quantum Mechanics, wave functions offer statistical information about possible results, not the exact outcome of an experiment. Two wave functions of interest are the position wave function and the momentum wave function; these wave functions represent the components of a state vector in the position basis and the momentum basis, respectively. These two can be related through the Fourier Transform and the Inverse Fourier Transform. This demonstration application will allow the users to define their own momentum wave function and use the inverse Fourier transformation to find the position wave function. If the Fourier transform were to be used on the resulting wave function, the result would then be the original momentum wave function. Both wave functions visually show the wave packets in momentum and position space. The momentum wave packet is a Gaussian while the corresponding position wave packet is a Gaussian envelope which contains an internal oscillatory wave. The two wave packets are related by the uncertainty principle, which states that the more defined (i.e. more localized) the wave function is in one basis, the less defined the corresponding wave function will be in the other basis. The application will also create an interactive 3-dimensional model that relates the two wave functions through the inverse Fourier transformation, or more specifically, by visually decomposing a Gaussian wave packet (in momentum space) into a specified number of components waves (in position space). Using this application will give the user a stronger knowledge of the relationship between the Fourier transform, inverse Fourier transform, and the relationship between wave packets in momentum space and position space as determined by the Uncertainty Principle.

Concept:

Wavelength and Position

In Griffith's *Introduction to Quantum Mechanics*, Griffith brings up the following scenario: one steadily oscillates a long rope and generates a standing wave, proceeding to ask the odd question, "Where exactly is the wave?" This question is odd since the wave is not exactly anywhere; it is spread out over the length of the rope. A more reasonable question would be, "What is its wavelength?" However, if one were to give the same rope a sudden jerk to create a single, narrow bump travelling down the rope, then the situation is reversed: one could answer for the *location* of the wave, but it would be difficult to interpret what a *wavelength* would be. This is a very basic model of the uncertainty relationship; one is able to achieve a well-defined wavelength (localized in momentum space) *or* a well-defined position (localized in position space) but *not both* at the same time.

Wave Packet
The position wave function is a superposition of potentially infinite sinusoidal waves. The amplitude of a wave with a certain wave number k_0 is given by the momentum wave function evaluated at the corresponding point $\hbar k_0$ in momentum space. The position wave function will contain internal "ripples" whose peaks and troughs form the shape of an external Gaussian "envelope" or "group." This is known as the wave packet. By using the 3-dimensional model generated from the application, this relationship can be seen visually.

Uncertainty Principle
The uncertainty of measurements is related to the variance (σ^2) of the distribution. The general uncertainty principle is defined as

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2$$

where $\hat{A}$ and $\hat{B}$ are the A and B hermitian operators respectively. The term $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator of the two hermitian operators. When two operators commute, the commutator is zero. Mathematically, this allows the product of the two variances to equal zero. However, when the commutator is not zero, the two operators are incompatible observables. The uncertainty principle is the result of the statistical interpretation of quantum mechanics.

The demonstration application focuses on two vector spaces: the momentum space and the position space. By using the momentum and position operators, one is able to reproduce the Heisenberg uncertainty principle that states that the more defined (i.e. localized) the momentum or position wave function is in its respective basis, the less defined (i.e. more spread out) the corresponding wave function of the other basis. By the canonical commutation relation, $[\hat{x},\hat{p}] = i\hbar$, where $\hat{x}$ is the position operator and $\hat{p}$ is the momentum operator and $\hbar$ is the reduced Planck's constant.

$$\sigma_x^2 \sigma_p^2 \geq \left(\frac{1}{2i}\langle[\hat{x},\hat{p}]\rangle\right)^2 = \left(\frac{1}{2i}i\hbar\right)^2 = \left(\frac{\hbar}{2}\right)^2$$

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \qquad\qquad \text{Heisenberg Uncertainty Principle}$$

where σ is the standard deviation, defined as the uncertainty in the distributions.

Fourier Transform and Inverse Fourier Transform

The inverse Fourier transform can be operated on the momentum wave function to derive the position wave function:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p,t)e^{ipx/\hbar} \, dp$$

where $\Psi(x,t)$ is the position wave function and the $\phi(k)$ is the momentum wave function.

The Fourier transform can be used on the momentum wave function to derive the momentum wave function:

$$\phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,t)e^{-ipx/\hbar} \, dx$$

Plancherel's Theorem states that the inverse Fourier transform of a Fourier transform is the starting function. Therefore, if either the momentum or position wave function is known, then the other can be determined using the inverse Fourier transform and the Fourier transform, respectively. Then, by using Fourier transform and the inverse Fourier transform, respectively, the original wave function can be recovered. Through the use of these transformations, one can freely change from momentum space to position space, or vice versa.

Demonstration Application of the Fourier Analysis of the Wave Packet and the Uncertainty Relation

The demonstration application helps the user understand the concept of the Fourier transform and inverse Fourier transform. After the momentum wave function is defined, the application will produce the position wave function but also create a 3-dimensional model that combines the momentum and the individual sinusoidal waves that are superimposed to create the wave function through the relationship of the Fourier transform.

By defining a Gaussian momentum wave function (see Figure 1), one can use the demonstration application to find the position wave function (see Figure 2) that is enveloped by a Gaussian wave packet. This is performed by taking the defined momentum wave function and performing the inverse Fourier transformation.
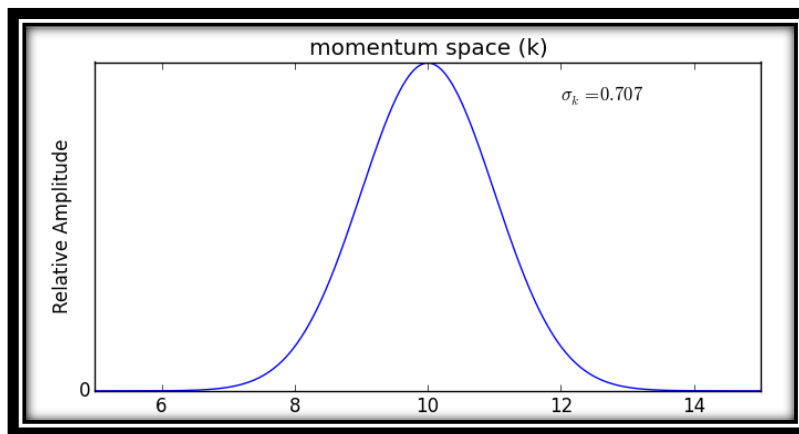

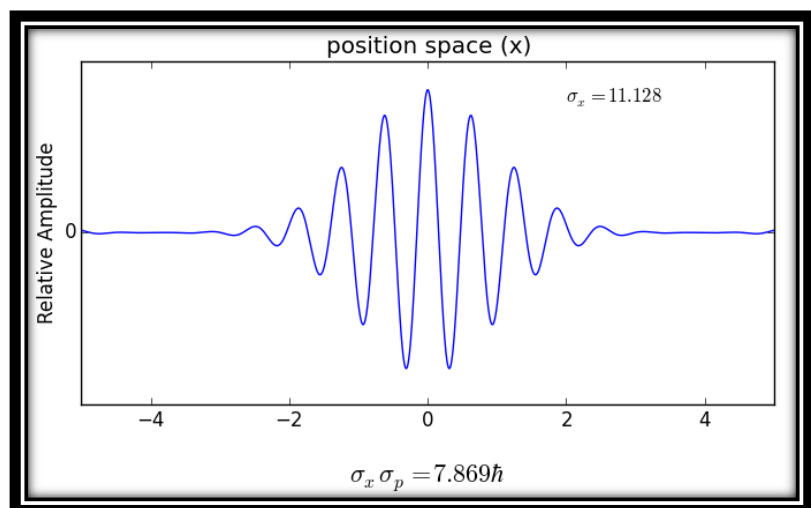*Figure 1: The defined momentum wave function*

Figure 2: Position wave packet resulting from the inverse Fourier transform of the defined momentum wave function. It can be seen that the wave function is "grouped" together to make the wave packet.

The uncertainty of the momentum wave function is defined by the user and the uncertainty of the position wave function will be calculated by the application. It is then shown that the product of the uncertainty of the momentum and position wave function is greater than or equal to $\hbar/2$ (i.e. Heisenberg uncertainty principle will be conserved).

In fact, for any Gaussian wave packet (i.e. any wave functions produced with this application), the Uncertainty Principle holds to equality: $\sigma_x \sigma_p = \hbar/2$. However, in the images above, the product of the uncertainties shown is much larger than $\hbar/2$; this occurs because of the use of a small finite number of component waves in the application simulation (this in turn allows for the reappearance of identical wave packets at regular intervals in x-space, not seen in the image). In order to increase the accuracy of the uncertainty product, larger numbers of component wave are used (see images below); in reality, the Fourier transformation uses an infinite number of infinitely-densely-spaced component waves, which can only be approximated in the simulation.

The application will produce a 3-D model that relate the momentum and position space through the Fourier transform. The model will show the relationship of the momentum wave function and the individual sinusoidal waves that forms the position wave function when superimposed (Figure 3, 4, 5).
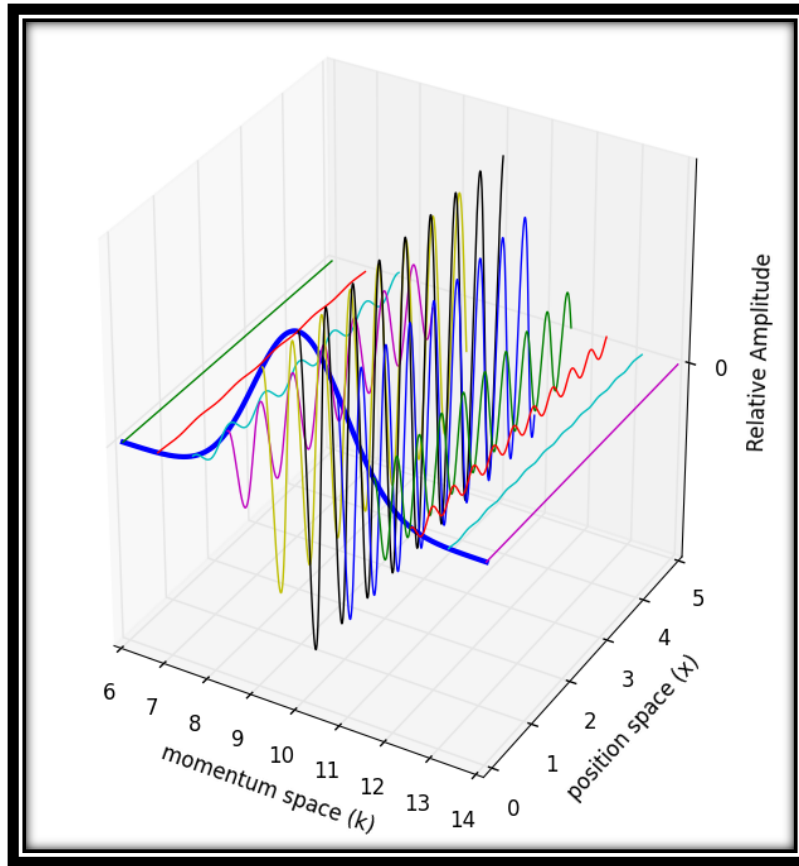
Figure 3: The 3-D model that relates the momentum space and position space through the Fourier transform
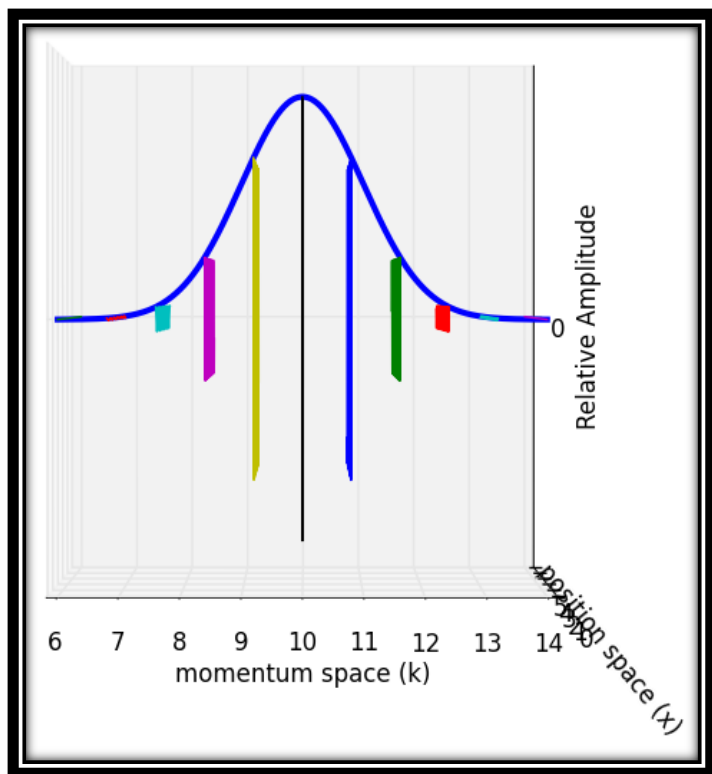
Figure 4: The momentum wave function is made up of the amplitudes of the individual waves that are superimposed to create the wave function
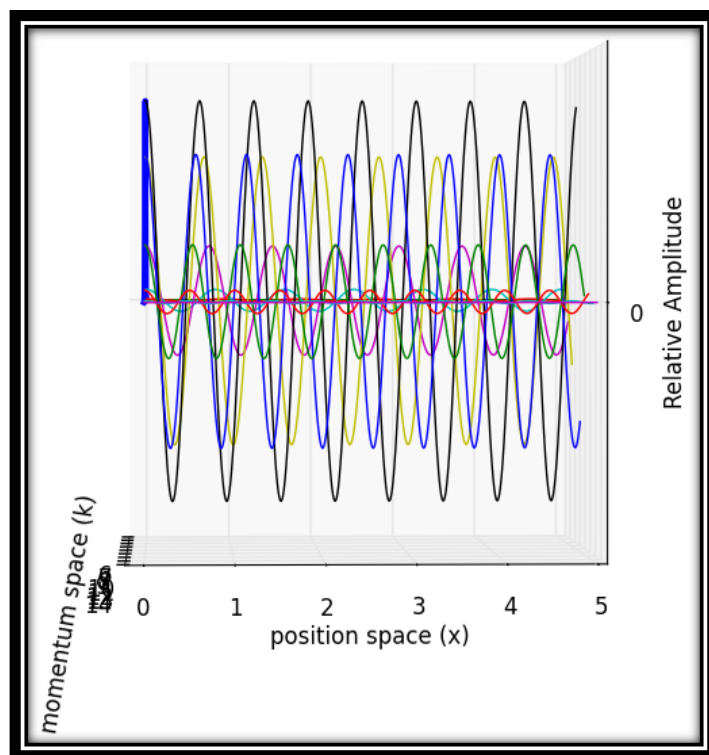

Figure 5: The individual waves that are superimposed to create the position wave function.

Examples of the Demonstration Application

Three examples will be shown with the application. Each example will minimize the uncertainties while still conserving the uncertainty principle.

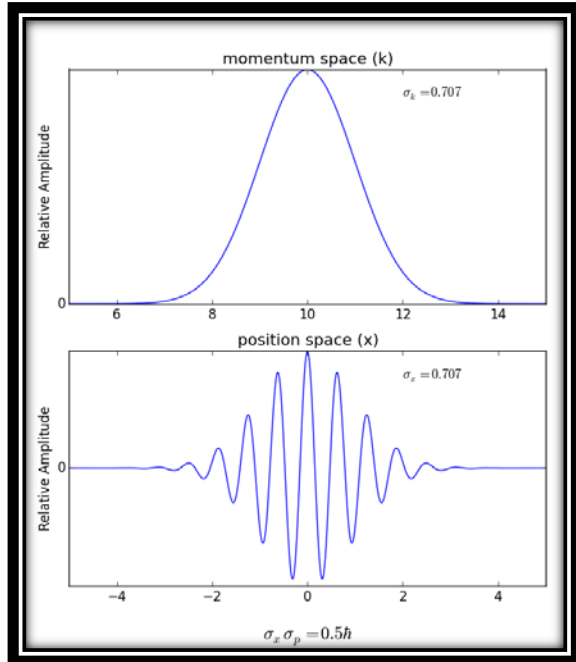1. Momentum uncertainty and position uncertainty are the same:

Figure 6: A Gaussian momentum wave function is defined and the application will perform the inverse Fourier
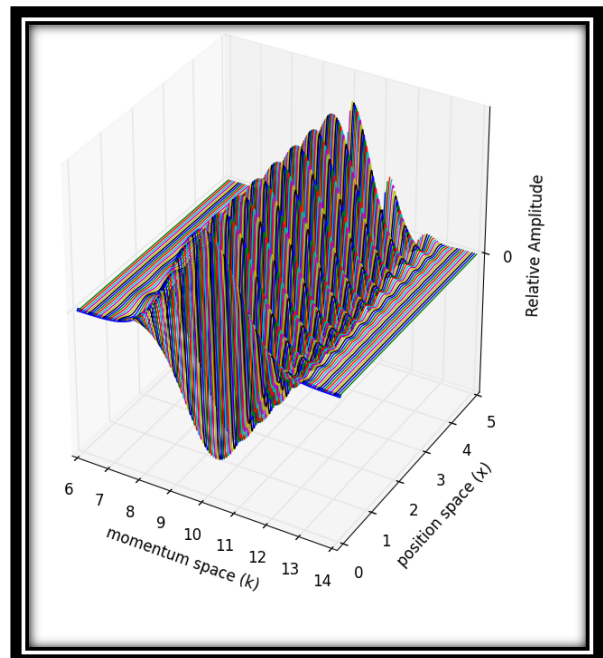

Figure 7: Many individual sinusoidal position waves were used in this 3-D model. The amount of waves can be changed in this application.

2. Momentum uncertainty is large and position uncertainty is small:

    By giving the momentum wave function a large uncertainty (i.e. make the wave spread out), the position wave packet is able to have a small uncertainty (i.e. localized).
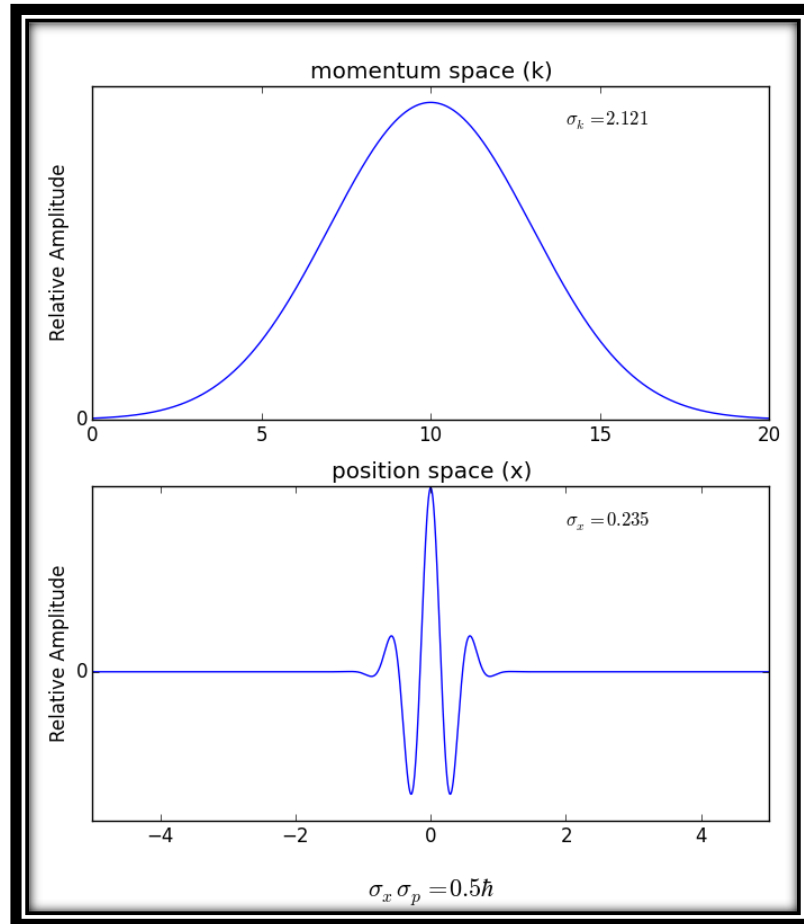

Figure 8: The momentum wave was given a large uncertainty which resulted in a position wave function with a small uncertainty. The Heisenberg uncertainty principle is still conserved.

3. Momentum uncertainty is small and position uncertainty is large:

   By giving the momentum wave function a small uncertainty (i.e. localized), the position wave packet must have a large uncertainty (i.e. spread out).
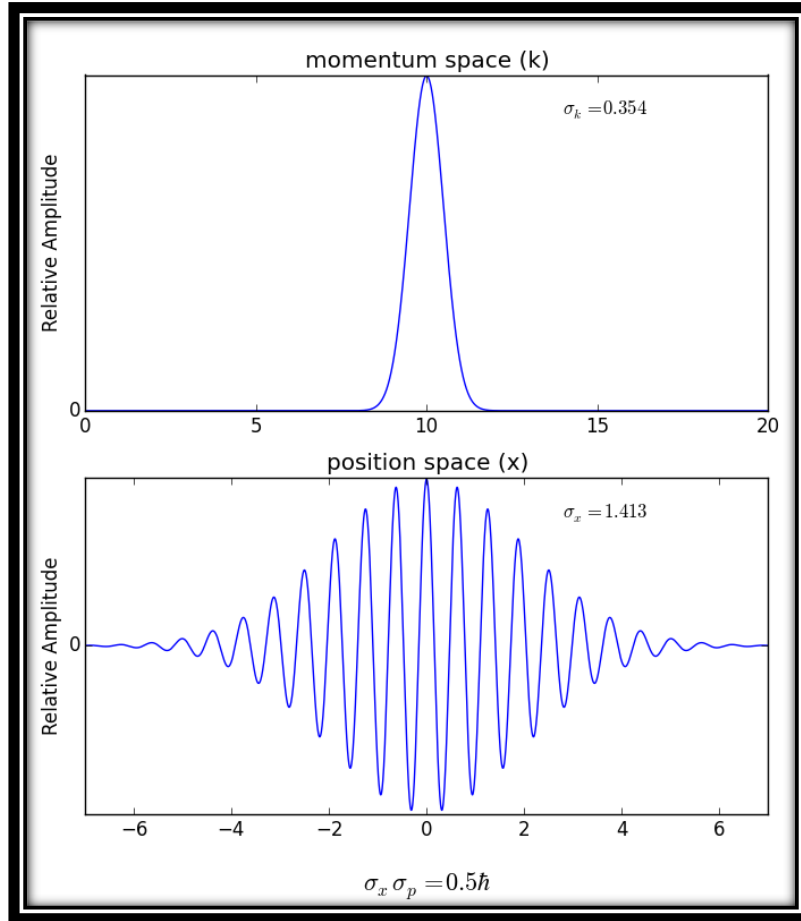

Figure 9:The momentum wave was given a small uncertainty (to simulate localization) which resulted in a position wave function with a large uncertainty. The Heisenberg uncertainty principle is still conserved.

How to use the application

When one starts the program, it will give the user an introduction, the current distribution, and a list of its functions (Figure 10).

```
Hello there! Welcome to
Fourier Transformations &
Understanding Uncertainty


Your current transformation is:

Gaussian k-distribution centered at 10 with sigma 1
showing 11 component waves, 5 < k < 15 & -5 < x < 5

To view your current transformation, just type "go".
To adjust the Gaussian center, type "cen=#" for center at
#.
To adjust the Gaussian sigma, type "sig=#" for a sigma of
#.
To adjust the number of wave components shown, type
"num=#".
To adjust k scale from a to b, type "klo=a" and "khi=b".
To adjust x scale from c to d, type "xlo=c" and "xhi=d".
To view probability distributions (|f|^2), type "sqd=1".
Separate multiple commands with a comma.
If you wanna quit, just say "bye".
>>>
```

Figure 10: The program's introductory instructions

The momentum wave function can be determined by the functions "`cen=#`" and "`sig=#`". To determine range of k values to be viewed, use the functions "`klo=#`", and "`khi=#`".

For the position wave function, the range of x values to be viewed is determined with the functions "`xlo=#`" and "`xhi=#`". To control the number of individual sinusoidal waves that are superimposed to form the wave function, use the function "`num=#`".

To view the wave functions and the 3-D model of the Fourier Transform, one just needs to type "go".

Note: One can view the actual probability distributions (instead of just the amplitudes) with the "`sqd=1`" command, as shown.
To exit the image window, just close the window. Then a new transformation can be defined. When the user wants to quick the program, use the "`bye`" command.

Example
A Gaussian momentum wave function with a peak centered at the k value 15, a k value range from 0 to 30, with 100 decomposed sinusoidal waves use the command shown on Figure 11.

```
>>> num=100, cen=15, klo=0, khi=30, go
```

Figure 11: The example command