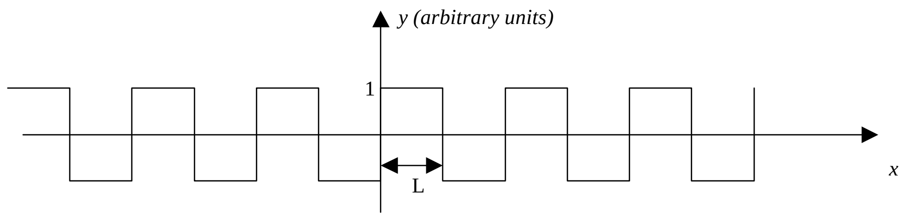
Fourier Analysis and the Uncertainty Principle

I. Fourier Series for a Periodic Function

A. Finding appropriate functions

1. Consider the square wave shown to the right.

   Sketch a single sine or cosine curve that best approximates the square wave.



   Write a mathematical representation of the function you have sketched. Explain how you came up with your answer.

B. Exploring the spreadsheet

1. Open up the spreadsheet ***Periodic Square Wave*** on the desktop. The sheet lets you add trigonometric functions of the form *Asin(kx)* and *Bcos(kx)*. In the spreadsheet, $k = {}^{np}\!/_{L}$.

   Note that the value of *k* is fixed for a given *n*, but the values of *n* and *A* can be varied.

   Find the value of *k* and the value of *n* for the function you obtained in part A.

   In the first function of the spreadsheet, enter the parameters of the function in part A.

2. Consider the blue line in the second graph (if it is not visible, scroll the screen down).

   Describe what the blue line represents in the second graph. Explain how you know. *(Hint: it is given the name "difference.")*

   The number to the right of the second graph gives the value of Δ^2, the area of the difference curve squared. What information does Δ^2 give you about your choice for the function describing the square wave? You may want to try different parameters for the function to see how Δ^2 changes.

Find the best possible value for *n* and *A* in your first function. Explain how you used Δ^2 to arrive at your answer.

C. *Adding more terms to get a better fit*

1. Consider the second graph on the spreadsheet. What curve could you add to the black curve in order to get the square wave?

   How could you best approximate the curve you describe with a sine or cosine curve? Explain.

   Determine values of *n* and *A* of your second function. Explain how you arrived at your answer.

2. Use the spreadsheet to add a third trigonometric function to better approximate the square wave. Explain how you optimized the values of *A* and *n* of the third function using the difference curve and Δ^2.

D. *Generalizing the Fourier Series*

1. What values of *n* would you expect for additional terms that describe the square wave on page 1? Describe the general pattern for the wave number, *k*.

   Suppose the pattern of successive approximations continues. Write the equation for an infinite series that describes the periodic square wave shown on page 1. (For now leave the coefficients undetermined.)

2. The general Fourier series describing an arbitrary function is given as

$$f(x) = {}^{a_o}\!/_{2} + \sum_{1}^{\infty}\{\ a_n \cos\left({}^{npx}\!/_{L}\right) + b_n \sin\left({}^{npx}\!/_{L}\right)\ \}$$

Compare the equation with the series you came up with in the previous question. State the similarities and differences.

The values of a_n and b_n can be obtained from the orthogonality conditions for trigonometric functions. We get $a_n = {}^{1}\!/_{L} \int_{-L}^{L} f(k)\cos\left({}^{npk}\!/_{L}\right) dk$ and $b_n = {}^{1}\!/_{L} \int_{-L}^{L} f(k)\sin\left({}^{npk}\!/_{L}\right) dk$.

II. Localizing an electron using a Fourier Series

A. Understanding Localization

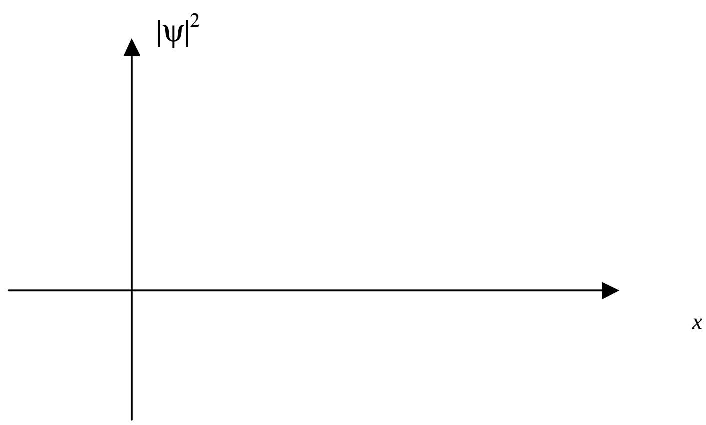
1. Consider an electron in a plane wave state with energy, *E*, and momentum, *p*.

Find the angular frequency, *w*, in terms of *E*, and the wave number, *k*, in terms of *p*.

Write out the wave function for the electron in terms of *w* and *k*.

In the space to the right, sketch the probability density for this electron.

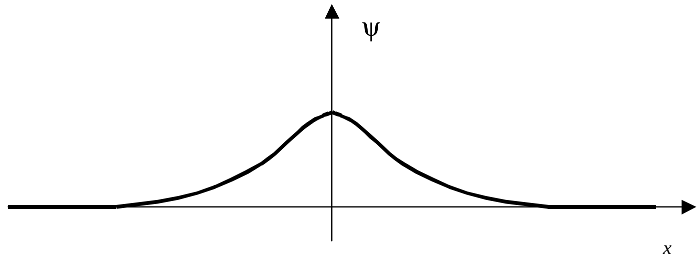
Based on the probability density, what can you say about the position of an electron with energy, *E*, and momentum, *p*?



Would you say the electron with energy, *E*, and momentum, *p*, is localized in space? What conditions have to be satisfied for localization? Explain.

2. Consider an electron described by the wave function shown at right.

   In this case would you say the electron is localized? Explain in terms of its probability density.



B. Exploring the spreadsheet

1. Open the spreadsheet ***Gaussian wave packet*** on the computer desktop. The sheet will add only cosine functions in the Fourier series shown on page 3. Again, the value of k is fixed but the values of n and A are not. Note that $k = {}^{2n\pi}\!/_{L}$ rather than $n\pi/L$, as before. In this spreadsheet, L = 6 units.

   Explain why sine functions are not included in this spreadsheet.

   Enter the parameters for only the constant term. Explain how you arrived at your answer.

   By adding more cosine functions on the spreadsheet, attempt to localize the electron in the given region (using integer values of n). Before adding each successive function, describe the shape of the difference curve when Δ^2 is optimized.

   Were you able to localize the electron? Predict what you would see outside the region shown. Explain.

In the graph window, double click on the "3" that indicates the scale of the x axis. Choose the *Scale* tab. Change both the *Minimum* and *Maximum* values from –3 to –6.

   What do you observe? Resolve any discrepancies with your prediction.

   How many terms would you need so that the electron is truly localized? Explain.