CHM 532
Notes on Fourier Series, Fourier Transforms and the Dirac Delta Function

These notes provide additional details about some of the new concepts from mathematics given in lecture. Some of this mathematics is analogous to properties of ordinary vectors in three-dimensional space, and we review a few properties of vectors first.

1 Vectors

A *vector* is a mathematical object that has both magnitude and direction. Variables that have only a magnitude are called *scalars*. An example of a vector is the coordinate vector $\vec{r}$ that is defined as the vector that connects the origin of some coordinate system to a point in space. The magnitude of the coordinate vector is the distance between the origin of coordinates and the point in space, and the direction of the vector points to the specific point. A vector of zero length, denoted $\vec{0}$, points in no distinct direction.

We now introduce the definition of *linear independence* of two vectors:

Definition: Two distinct non-zero vectors $\vec{u}$ and $\vec{v}$ are said to be linearly independent if given two scalar coefficients a and b,

$$a\vec{u} + b\vec{v} = \vec{0}$$

only if $a = b = 0$. Two vectors that are not linearly independent are said to be linearly dependent.

Although the definition of linear dependence may appear a bit abstract, two linearly dependent vectors are parallel, and independent vectors are not parallel.

An important set of linearly independent vectors are the Cartesian unit vectors, $\hat{\imath}, \hat{\jmath}$ and $\hat{k}$. The Cartesian unit vector $\hat{\imath}$ is the coordinate vector of unit magnitude that begins at the origin of coordinates and lies on the x-axis. Similarly, $\hat{\jmath}$ is the unit vector on the y-axis and $\hat{k}$ is the unit vector along the z-axis. The three Cartesian unit vectors form a complete set of vectors in the sense of the following definition:

Definition: A set of vectors $\{\vec{u}_i\} i = 1, 2$ or 3 is said to be complete if given any vector $\vec{v}$ we can write

$$\vec{v} = \sum_{i=1}^{3} c_i \vec{u}_i$$

where the set $\{c_i\}$ are a set of scalar coefficients.

Because the Cartesian unit vectors are complete, we can write any vector $\vec{v}$ in the form

$$\vec{v} = v_x \hat{\imath} + v_y \hat{\jmath} + v_z \hat{k}. \tag{1}$$

The coefficients v_x, v_y and v_z are called the components of $\vec{v}$ along the x, y and z-axes respectively.

There are two methods of multiplying two vectors. Of the two methods, one (called the cross product) can be defined only for three-dimensional vectors. The other, defined now, is generalizable in a manner to be made clear in subsequent sections:

Definition: Let $\vec{u}$ and $\vec{v}$ be two vectors that can be written in terms of their Cartesian components

$$\vec{u} = u_x \hat{\imath} + u_y \hat{\jmath} + u_z \hat{k}$$

and

$$\vec{v} = v_x \hat{\imath} + v_y \hat{\jmath} + v_z \hat{k}.$$

Then the dot product (or inner product or scalar product) of $\vec{u}$ and $\vec{v}$ is defined to be

$$\vec{u} \cdot \vec{v} = u_x v_x + u_y v_y + u_z v_z.$$

Notice that the dot product of two vectors is a scalar. It is possible to show that for two vectors $\vec{u}$ and $\vec{v}$,

$$\vec{u} \cdot \vec{v} = uv \ \cos\theta \tag{2}$$

where u and v are the lengths of vectors $\vec{u}$ and $\vec{v}$ respectively, and θ is the angle between $\vec{u}$ and $\vec{v}$. The expression for the dot product in terms of angles helps us understand the next definition

Definition: Two vectors $\vec{u}$ and $\vec{v}$ are said to be orthogonal if

$$\vec{u} \cdot \vec{v} = 0.$$

The two vectors are said to be orthonormal if

$$\begin{cases} \vec{u} \cdot \vec{v} = 0 & \vec{u} \neq \vec{v} \\ \vec{u} \cdot \vec{v} = 1 & \vec{u} = \vec{v} \end{cases}$$

From the expansion of the dot product in terms of the angle between the two vectors, it is clear that two vectors are orthogonal if they are perpendicular.

Using the dot product, there is a simple method for determining the components of any vector. For example, consider

$$\vec{v} = v_x\hat{i} + v_y\hat{j} + v_z\hat{k}. \tag{3}$$

We now take the dot product of the left and right hand sides of Eq.(3) with the unit vector $\hat{i}$

$$\hat{i} \cdot \vec{v} = v_x\hat{i} \cdot \hat{i} + v_y\hat{i} \cdot \hat{j} + v_z\hat{i} \cdot \hat{k}. \tag{4}$$

Because the Cartesian unit vectors are orthonormal

$$\hat{i} \cdot \hat{j} = \hat{i} \cdot \hat{k} = 0 \qquad \hat{i} \cdot \hat{i} = 1 \tag{5}$$

and

$$v_x = \hat{i} \cdot \vec{v}. \tag{6}$$

In a similar way

$$v_y = \hat{j} \cdot \vec{v} \tag{7}$$

and

$$v_z = \hat{k} \cdot \vec{v}. \tag{8}$$

2 Complete Sets of Functions

The properties of vectors outlined in the previous section are not limited to three-dimensional space. We can imagine vectors in N dimensions described by N orthonormal unit vectors. We can also imagine the case where N becomes infinite. An application of such an infinite dimensional *vector space* is found with sets of functions having special properties. We begin by considering functions on some domain D. We make the following two definitions:

Definition: A set of functions $\{u_n(x)\}$ is said to be linearly independent if

$$\sum_n c_n u_n(x) = 0$$

for all x only if $c_n = 0$ for all n. If the set of functions are not linearly independent, the set is said to be linearly dependent.

Any member of a linearly dependent set of functions can be expressed as a linear sum of the remaining members of the set. Linearly independent sets are said to be complete in the sense of this next definition:

Definition: A set of functions $\{u_n(x)\}$ defined on a domain D is said to be complete if given any function $f(x)$ defined on D we can write

$$f(x) = \sum_n c_n u_n(x)$$

where c_n is a scalar coefficient.

We emphasize that all functions considered here can be complex, and as a consequence the coefficients c_n can be complex numbers. It is important to see the analogy between the definition of a complete set of functions and a complete set of vectors. In each case, a general member of the space can be expressed as a simple linear combination of the members of the complete set. The members of the complete set are often called a *basis* for the space.

For functions, we have the analog of the dot product as well. We define the notation

$$\langle u|v\rangle = \int_D u^*(x)v(x)dx \tag{9}$$

where we use the standard notation $u^*(x)$ for the complex conjugate of the function $u(x)$. We see that $\langle u|v\rangle$ is a kind of product between two functions the result of which is a number. In analogy with the dot product of two vectors, we refer to $\langle u|v\rangle$ as a scalar product. Additional analogies between the properties of vectors and sets of functions are found in the following definitions:

Definition: Two functions $u(x)$ and $v(x)$ defined on a domain D are said to be orthogonal if

$$\langle u|v\rangle = \int_D u^*(x)v(x)dx = 0.$$

Definition: The Kronecker delta is defined by

$$\delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j. \end{cases}$$

Definition: A set of functions $\{u_n(x)\}$ defined on a domain D is said to be orthonormal if

$$\langle u_n|u_m\rangle = \int_D u_n^*(x)u_m(x)\ dx = \delta_{nm}.$$

An important class of functions defined on a domain D are those that are both complete and orthonormal. Suppose $\{u_n(x)\}$ is such a complete orthonormal set and $f(x)$ is any function defined on the domain D. We can expand $f(x)$ in terms of our complete set, and a simple procedure can provide the expansion coefficients. We begin with the expression

$$f(x) = \sum_n c_n u_n(x). \tag{10}$$

In the case of a complete orthonormal set of vectors, the coefficients associated with each vector are determined by taking the dot product of each vector with the sum [See Eq.(4) and Eqs.(6)-(8)]. We perform the same procedure to obtain the coefficients c_n in Eq.(10). We multiply each side of Eq.(10) by the complex conjugate of a particular member of the complete set and the integrate over the domain D. The procedure, as given in the next equations, uses the scalar product of the complete orthonormal set instead of the dot product. We have

$$\int_D u_m^*(x) f(x)\ dx = \int_D u_m^*(x) \sum_n c_n u_n(x)\ dx \tag{11}$$

$$= \sum_n c_n \int_D u_m^*(x) u_n(x)\ dx \tag{12}$$

$$= \sum_n c_n \delta_{mn} = c_m. \tag{13}$$

In summary, we can expand any function $f(x)$ in a complete orthonormal set as given in Eq.(10) with the expansion coefficients given by

$$c_n = \int_D u_n^*(x) f(x)\ dx. \tag{14}$$

It is easiest to understand this procedure with the important example of the Fourier series.

3 The Fourier Series

Fourier has proved that the set of functions $\{\sin nx, \cos nx\}$ for $n = 0, 1, 2, \cdots$ is complete and orthogonal for any piecewise continuous function $f(x)$ defined on the domain $-\pi \leq x \leq \pi$. For any piecewise continuous function $f(x)$, we can write

$$f(x) = \frac{B_0}{2} + \sum_{n=1}^{\infty} [A_n \sin nx + B_n \cos nx] \tag{15}$$

where we have separated the $n = 0$ term to make the formulas for B_n uniform for any n. Equation (15) is usually called a Fourier series. To obtain the expansion coefficients, the following integrals are of use

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \sin nx\ \sin mx\ dx = \delta_{mn} \tag{16}$$

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \cos nx\ \cos mx\ dx = \delta_{mn} \tag{17}$$

and

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \sin nx\ \cos mx\ dx = 0. \tag{18}$$

The set of functions $\{\sin nx, \cos nx\}$ are orthogonal but not orthonormal on the domain $-\pi \leq x \leq \pi$. To find the coefficients of the Fourier series, we multiply each side of Eq. (15)

by a member of the complete set, multiply by $1/\pi$, and integrate on the interval $-\pi \leq x \leq \pi$. For example, to find the coefficient A_m

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \sin mx \; f(x) \; dx = \frac{1}{\pi}\int_{-\pi}^{\pi} \sin mx \left[\frac{B_0}{2} + \sum_{n=1}^{\infty}\{A_n \sin nx + B_n \cos nx\}\right] \; dx \tag{19}$$

$$= \frac{1}{\pi}\int_{-\pi}^{\pi} \sin mx \frac{B_0}{2} dx + \frac{1}{\pi}\sum_{n=1}^{\infty} A_n \int_{-\pi}^{\pi} \sin mx \sin nx \; dx + \frac{1}{\pi}\sum_{n=1}^{\infty} B_n \int_{-\pi}^{\pi} \sin mx \cos nx \; dx \tag{20}$$

$$= \sum_{n=1}^{\infty} A_n \delta_{mn} = A_m. \tag{21}$$

To find the coefficient B_m for $m \neq 0$

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \cos mx \; f(x) \; dx = \frac{1}{\pi}\int_{-\pi}^{\pi} \cos mx \left[\frac{B_0}{2} + \sum_{n=1}^{\infty}\{A_n \sin nx + B_n \cos nx\}\right] \; dx \tag{22}$$

$$= \frac{1}{\pi}\int_{-\pi}^{\pi} \cos mx \frac{B_0}{2} dx + \frac{1}{\pi}\sum_{n=1}^{\infty} A_n \int_{-\pi}^{\pi} \cos mx \sin nx \; dx + \frac{1}{\pi}\sum_{n=1}^{\infty} B_n \int_{-\pi}^{\pi} \cos mx \cos nx \; dx \tag{23}$$

$$= \sum_{n=1}^{\infty} B_n \delta_{mn} = B_m. \tag{24}$$

Finally, to find B_0, we multiply both sides of Eq. (15) by $1/\pi$ and integrate over the same integration domain

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \; f(x) \; dx = \frac{1}{\pi}\int_{-\pi}^{\pi} \left[\frac{B_0}{2} + \sum_{n=1}^{\infty}\{A_n \sin nx + B_n \cos nx\}\right] \; dx \tag{25}$$

$$= B_0. \tag{26}$$

The general expressions for the Fourier expansion coefficients are then given by

$$A_n = \frac{1}{\pi}\int_{-\pi}^{\pi} \sin nx f(x) \; dx \tag{27}$$

and

$$B_n = \frac{1}{\pi}\int_{-\pi}^{\pi} \cos nx f(x) \; dx \tag{28}$$

for all n.

In applications, it is generally best to determine the coefficients A_n and B_n first for $n \neq 0$ and then find the expression for B_0 separately. As an example, consider the function

$$f(x) = \begin{cases} 1 & -\pi/2 \leq x \leq \pi/2 \\ 0 & \text{otherwise.} \end{cases} \tag{29}$$

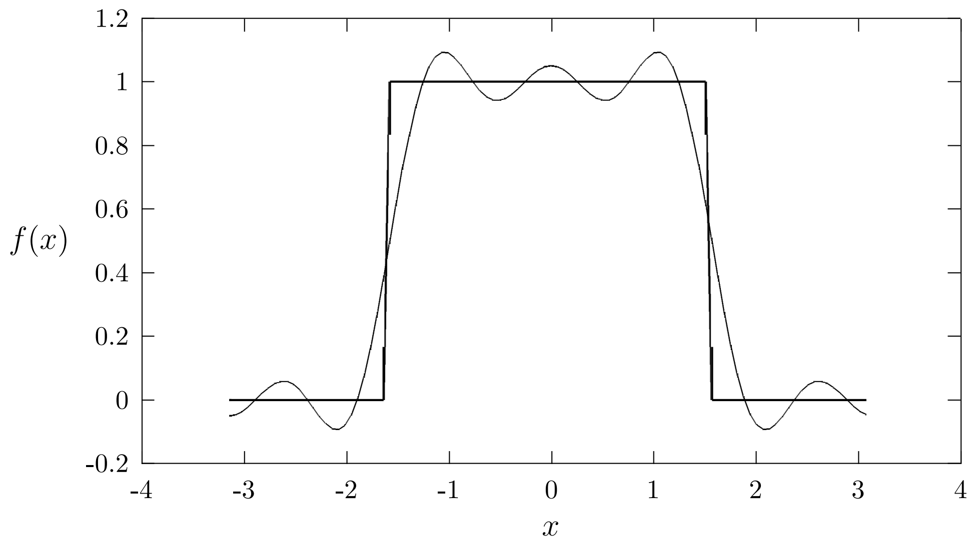
The function $f(x)$ is often called a *square wave*. Using the expressions for the Fourier coefficients, it is easy to show that

$$A_n = 0 \qquad B_0 = 1 \qquad B_n = \frac{2}{n\pi} \sin \frac{n\pi}{2} \tag{30}$$

so that the Fourier series for $f(x)$ is given by

$$f(x) = \frac{1}{2} + \frac{2}{\pi} \left[\cos x - \frac{\cos(3x)}{3} + \frac{\cos(5x)}{5} - \ldots \right] \tag{31}$$

The square wave and the Fourier series representation of the square wave using a maximum Fourier index of 5 are shown in the figure.



The Fourier series for the square wave gives the discrete sum of sinusoidal waves into which the square wave is decomposed. Each sinusoidal wave contribution [e.g. the $\cos x, \cos 3x, \ldots$] is included with a weight, the largest weights having the greatest contribution to the overall wave form. We can think of the Fourier series as a sum of sinusoidal waves with decreasing discrete wave lengths. The Fourier coefficients provide information about the importance of the different possible wave lengths to the overall wave form.

The wavelengths possible in a Fourier series are discrete. There are times when it is important to decompose a function into sinusoidal waves having continuous rather than discrete wavelengths. The extension that makes such a decomposition possible is called the Fourier transform. Before introducing the Fourier transform, we need a continuous analog of the Kronecker delta. The continuous analog is the subject of the next section.

4 The Dirac Delta Function

The Dirac delta function, invented by P.A.M. Dirac for his important formulations of quantum mechanics, is a continuous analog of the Kronecker delta. To appreciate the connection between the Kronecker delta and the delta function, it is important to recognize that subscripts are a kind of function. Recall that a function is a mapping between a set of numbers called the domain to another set of numbers called the range. When we use a subscript, we are defining a function whose domain is the set of integers. For example, suppose $a_j = j^2$ for $j = 0, 1, 2, \ldots$ Then for each integer j, a_j is a number (the square of j), and it is clear that the subscript operation just defines a function. In this sense, the Kronecker delta δ_{ij} is a function of two integer variables i and j. If $i = j$, the Kronecker delta returns 1, and the Kronecker delta returns 0 if $i \neq j$.

We next consider the effect of the Kronecker delta on a discrete sum. Consider

$$\sum_{i=0}^{\infty} a_i \delta_{ij} = a_j. \tag{32}$$

The result of the summation is a_j, because for any value of $i \neq j$, the Kronecker delta is 0. The Kronecker delta picks a single member from such an infinite sum.

To provide the continuous analogue of the Kronecker delta, we make the following definition:

Definition: The Dirac delta function (or just the delta function) $\delta(x - y)$ is defined by

$$\delta(x - y) = \begin{cases} 0 & x \neq y \\ \infty & x = y \end{cases}$$

such that for any function $f(x)$

$$\int_{-\infty}^{\infty} f(x) \delta(x - y)\; dx = f(y)$$

The Kronecker delta extracts a single element from an infinite sum, and the delta function extracts the value of a function at a single point from an integral. The Kronecker delta is zero everywhere except where $i = j$ when the Kronecker delta is 1. The delta function is zero everywhere except at the point $x = y$ where it is infinite in a way that allows the delta function to extract the value of a function at a single point.

It is important to emphasize that as defined, the delta function is not a function in the usual sense. The delta function does not satisfy the properties reserved for functions. When Dirac introduced the delta function in the 1930's, he introduced new mathematics that had no rigorous foundation. It was Dirac's insight that such a mathematical object had to exist. The rigorous mathematics connected with the delta function was developed in the 1950's with the theory of distributions. From our point of view, we can follow Dirac and avoid questions of mathematical rigor. We need to learn the rules for using the delta function, always keeping in mind that some standard mathematical practices may not work.

We now try some examples of applying the delta function in integration. Consider the integral

$$\int_{-\infty}^{\infty} x^3 \delta(x - 2)\; dx.$$

The integrand is zero everywhere except at the point $x = 2$. Then the integral must be 8. Next consider

$$\int_{-\infty}^{\infty} x^3 \delta(x+2)\ dx.$$

In this case, the integrand is zero everywhere except at the point $x = -2$. Then the integral is -8. Next consider

$$\int_{0}^{\infty} x^3 \delta(x+2)\ dx.$$

In this case, the integrand is zero everywhere except at $x = -2$, a point that is outside the range of integration. Consequently, the integral is 0.

An important property of the delta function can be understood from the integral

$$\int_{-\infty}^{\infty} \delta(x)\ \ dx.$$

We can rewrite this integral

$$\int_{-\infty}^{\infty} \delta(x)\ \ dx = \int_{-\infty}^{\infty} \delta(x-0) f(x)\ dx \tag{33}$$

where we take $f(x) = 1$ for all x. Because the integral is zero except at the point $x = 0$, the result is $f(0) = 1$. The implication is that although the value of the integrand is infinite at $x = 0$, the integral is finite and equal to 1; i.e. the delta function is an infinite spike at a single point with unit area. This description of the delta function can allow the representation of the delta function by various pre-limiting forms. For example, a Gaussian is a pre-limit form of a delta function as its width (standard deviation) becomes small

$$\delta(x) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}. \tag{34}$$

An important homework problem in CHM 532 is the proof that if $\{\phi_n(x)\}$ is a complete and orthonormal set of functions, it follows that

$$\sum_{n=0}^{\infty} \phi_n^*(a)\phi_n(x) = \delta(x-a). \tag{35}$$

Because the delta function is not really a function in the usual sense, it is of interest to see how Eq.(35) evolves numerically. As discussed in class, the set of function $\{(2/L)^{1/2} \sin n\pi x/L\}$ for $n = 1, 2, \ldots$ is complete and orthonormal on the domain $0 \le x \le L$ for all functions that vanish at $x = 0$ and $x = L$. We evaluate the sum

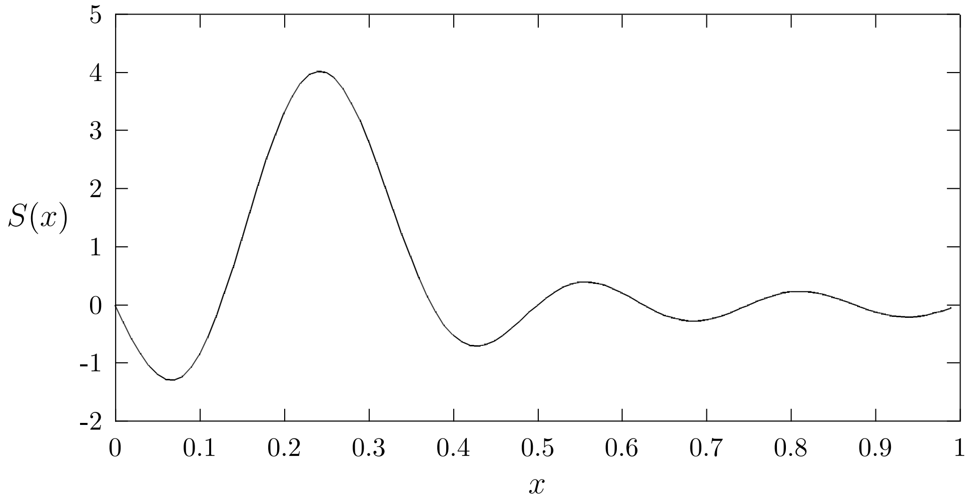
$$S(x) = \sum_{n=1}^{N} \sin n\pi x\ \sin \frac{n\pi}{4} \tag{36}$$

for different values of N. From Eq. (35) we know that

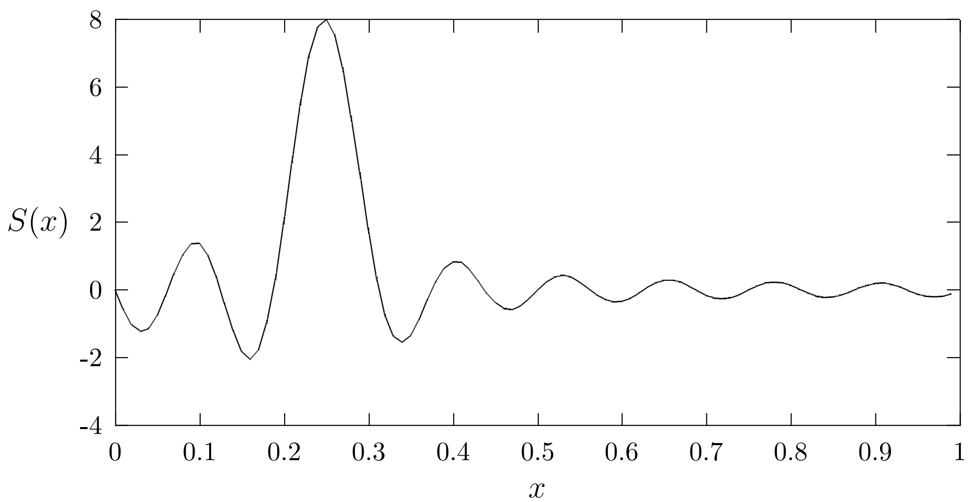
$$\lim_{N\to\infty} S(x) = \frac{1}{2}\delta(x - 0.25). \tag{37}$$

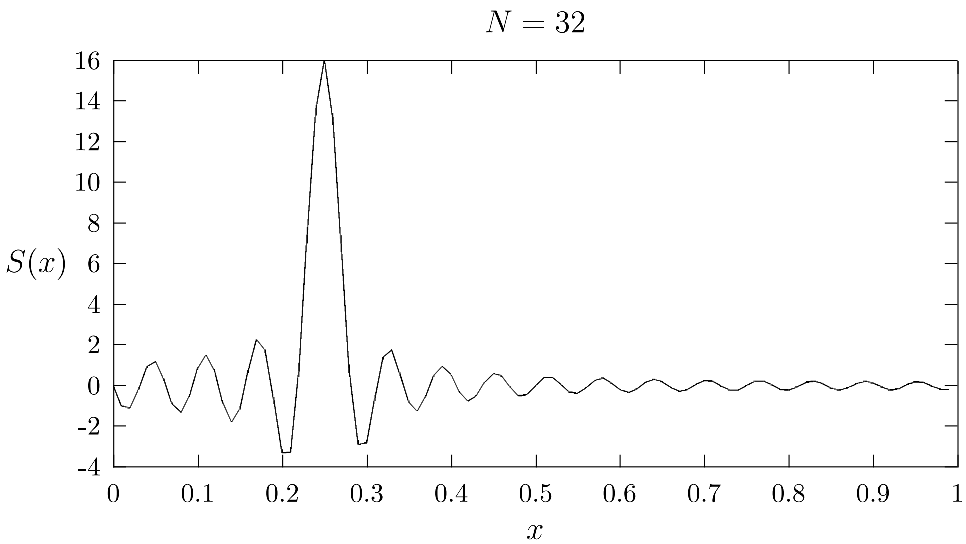
Graphs of $S(x)$ for $N = 8, 16, 32$ and 64 are plotted below:

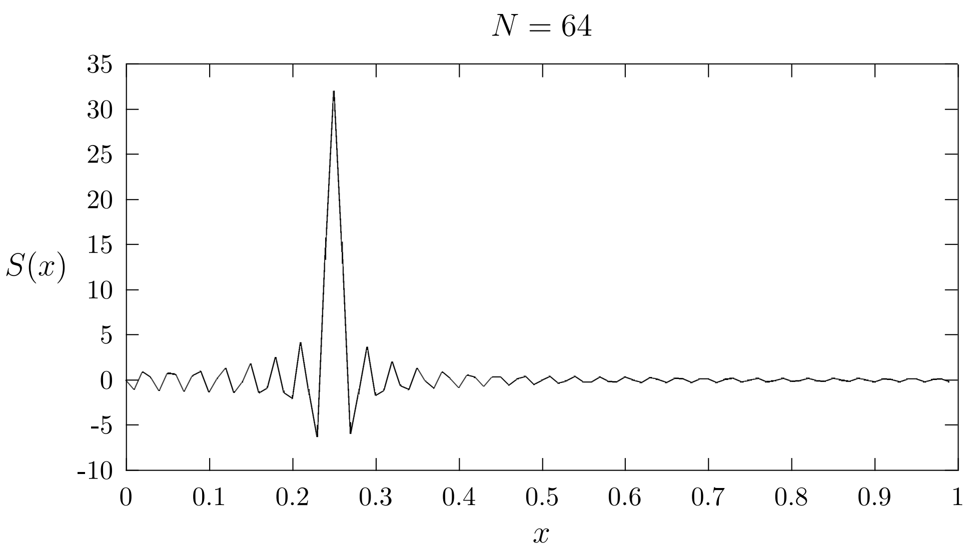
$N = 8$



$N = 16$







We see $S(x)$ constructively grows about the point $x = 0.25$ while the contributions to $S(x)$ outside this region approach zero. We can also observe that the magnitude of $S(x)$ about the point $x = 0.25$ increases with increasing N.

5 The Fourier Transform

We have seen how the Fourier series allows the decomposition of a function on a finite domain into a series of sinusoidal functions at discrete wavelengths. The Fourier transform allows the same kind of decomposition for functions defined on an infinite interval in terms of a continuous set of wavelengths. The basic notion of the Fourier transform is based on the completeness of the set of functions

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{38}$$

For $-\infty < k < \infty$. The exponential evaluated at an imaginary argument is given in terms of Euler's formula

$$e^{ix} = \cos x + i \sin x. \tag{39}$$

The parameter k is often called the *wave vector*, and k is simply related to the wavelength of the sinusoidal functions given in Eq.(38). From the properties of the trigonometric functions, it is easy to show that

$$\exp(ikx) = \exp\left(ik\left[x + \frac{2\pi}{k}\right]\right) \tag{40}$$

so that the wavelength is expressed in terms of the wave vector by

$$\lambda = \frac{2\pi}{k}. \tag{41}$$

For continuous complete set of functions, Eq.(35) is represented by an integral rather than a sum

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(k-k')x} dx = \delta(k - k'). \tag{42}$$

Equation (42) is often called the *integral representation of the delta function*. It is important not to attempt to evaluate Eq.(42) like an ordinary integral; i.e. we cannot evaluate the simple integral of the exponential in the usual way and then attempt to evaluate the result at the end points of $\pm\infty$. The integral in Eq.(42) so evaluated does not exist. We must just recognize that integrals of the form given in Eq.(42) are delta functions. Remember, delta functions are not really functions, and we learn to work with them using certain rules like that given in Eq.(42).

The Fourier transform of a function are the coefficients of a linear combination of the complete set $\{1/\sqrt{2\pi}\exp(ikx)\}$. Because the complete set is continuous, we use an integral rather than a sum. We then write for any $f(x)$ for which the Fourier transform exists

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k) e^{ikx}\, dk \tag{43}$$

where $g(k)$ is said to be the Fourier transform of $f(x)$. The Fourier transform $g(k)$ is to the Fourier transform what the coefficients A_n and B_n are to a Fourier series [See Eq. (15)]; i.e. the expansion coefficients. To determine the Fourier transform coefficients $g(k)$, we follow the same procedure we have used for complete sets of functions. We multiply each side of Eq. (43) by the complex conjugate of a different member of the complete set, and we then integrate over the domain of x. We then obtain

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ik'x} f(x)\, dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\; e^{-ik'x}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)\; e^{ikx}\, dk \tag{44}$$

$$= \int_{-\infty}^{\infty} dk\ g(k) \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{i(k-k')x} \tag{45}$$

$$= \int_{-\infty}^{\infty} dk\ g(k)\ \delta(k-k') \tag{46}$$

$$= g(k'). \tag{47}$$

We see that $f(x)$ is the Fourier transform of its own Fourier transform. The formulas are symmetric.

To illustrate Fourier transforms, we calculate the Fourier transform of the function given in Eq.(29) for which we have already determined the Fourier series

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx}\ dx \tag{48}$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\pi/2}^{\pi/2} e^{-ikx}\ dx \tag{49}$$

$$= -\frac{1}{\sqrt{2\pi}} \frac{1}{ik} e^{-ikx} |_{-\pi/2}^{\pi/2} \tag{50}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{ik} \left[e^{ik\pi/2} - e^{-ik\pi/2} \right] \tag{51}$$

$$= \frac{2}{k\sqrt{2\pi}} \sin\left(\frac{k\pi}{2}\right). \tag{52}$$

We interpret $g(k)$ to mean the relative weights of the continuous set of sinusoidal functions each having wavelength $2\pi/k$ that combine to give $f(x)$; i.e. we can write

$$f(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin(k\pi/2)}{k} e^{ikx} dk. \tag{53}$$