

Fourier's Theorem, Fourier Transforms, and the Uncertainty Principle

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1 The Vector Analogy

A vector in ordinary space is completely specified by its displacement in each spatial direction. Lets look at this familiar picture a bit formally, to prepare us to apply it in a less intuitive (but mathematically equivalent) setting. The first thing we will need to know how to do is to calculate the dot product between any two vectors:

$$\vec{v} \cdot \vec{w} = v_x w_x + v_y w_y + v_z w_z$$

You already know how to do this for ordinary vectors. In other settings, we use the more general term *inner product*. To describe any vector we need a set of *basis vectors*, in this case \hat{x} , \hat{y} , and \hat{z} . These basis vectors are orthogonal:

$$\hat{x} \cdot \hat{y} = \hat{y} \cdot \hat{z} = \hat{z} \cdot \hat{x} = 0$$

and normalized:

$$\hat{x} \cdot \hat{x} = \hat{y} \cdot \hat{y} = \hat{z} \cdot \hat{z} = 1.$$

When the basis vectors have both of these properties, we call them *orthonormal*.

For any possible vector \vec{v} , we can calculate its component in the direction of each basis vector by calculating the inner product:

$$v_x = \vec{v} \cdot \hat{x}$$

$$v_y = \vec{v} \cdot \hat{y}$$

$$v_z = \vec{v} \cdot \hat{z}$$

We say that the basis vectors \hat{x} , \hat{y} , and \hat{z} are *complete*, because specifying the values of v_x , v_y , and v_z completely describes the vector v . The set of basis vectors \hat{x} and \hat{z} are orthonormal, but they are not complete in three dimensional space, because there are vectors which we cannot write using only these two directions. For instance, there are no possible values for v_x and v_z which make

$$\vec{v}_1 = v_x \hat{x} + v_z \hat{z}$$

equal to the vector

$$\vec{v}_2 = 3\hat{x} + 2\hat{y} + 7\hat{z}.$$

2 The Fourier Series

Using the language of vectors, the Fourier Theorem states that the sines and cosines form a complete orthonormal basis for describing any periodic function.

To make sense of this, we need to define the inner product. If we restrict ourselves to real functions of x with period L , the inner product between any two functions $f(x)$ and $g(x)$ is defined to be the integral:

$$\langle f, g \rangle \equiv \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x)g(x) dx$$

The orthonormal basis vectors are the specific sine and cosine functions

$$s_n(x) \equiv \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi n}{L} x\right)$$

$$c_n(x) \equiv \sqrt{\frac{2}{L}} \cos\left(\frac{2\pi n}{L} x\right)$$

which are defined for $n = 1, 2, 3, \dots$. They are normalized because by our definition for the inner product we can see that:

$$\langle s_n, s_n \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin^2\left(\frac{2\pi n}{L} x\right) dx = 1$$

$$\langle c_n, c_n \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos^2\left(\frac{2\pi n}{L} x\right) dx = 1$$

The demonstration that they are orthogonal is left as an exercise:

$$\langle s_n, s_m \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{2\pi n}{L} x\right) \sin\left(\frac{2\pi m}{L} x\right) dx = 0 \quad (n \neq m) \quad (1)$$

$$\langle c_n, c_m \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos\left(\frac{2\pi n}{L} x\right) \cos\left(\frac{2\pi m}{L} x\right) dx = 0 \quad (n \neq m) \quad (2)$$

$$\langle s_n, c_m \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{2\pi n}{L} x\right) \cos\left(\frac{2\pi m}{L} x\right) dx = 0 \quad (3)$$

We can combine the normalization and orthogonality conditions using the Kronecker delta symbol:

$$\delta_{nm} = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{otherwise} \end{cases}$$

and write the above five equations as:

$$\langle s_n, s_m \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{2\pi n}{L} x\right) \sin\left(\frac{2\pi m}{L} x\right) dx = \delta_{nm}$$

$$\langle c_n, c_m \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos\left(\frac{2\pi n}{L} x\right) \cos\left(\frac{2\pi m}{L} x\right) dx = \delta_{nm}$$

$$\langle s_n, c_m \rangle = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{2\pi n}{L} x\right) \cos\left(\frac{2\pi m}{L} x\right) dx = 0 \quad (4)$$

Last of all, they are *complete* because any periodic function with period L can be written as a sum of these sines and cosines:

$$f(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} A_n \cos\left(\frac{2\pi n}{L} x\right) + \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} B_n \sin\left(\frac{2\pi n}{L} x\right) + C \quad (5)$$

The values A_n , B_n , and C are called *Fourier coefficients*. There are different conventions for handling the constant term C which are discussed in the exercises. Technically the n th term in the Fourier Series refers to the approximation for $f(x)$ from the first N terms in the infinite sum above, and we say that the Fourier Series converges to the function $f(x)$. The demonstration of completeness is optional reading, available in the Appendix. For a visual example of the Fourier Series, the first terms of the Fourier Series for a step function are shown in Fig. 1.

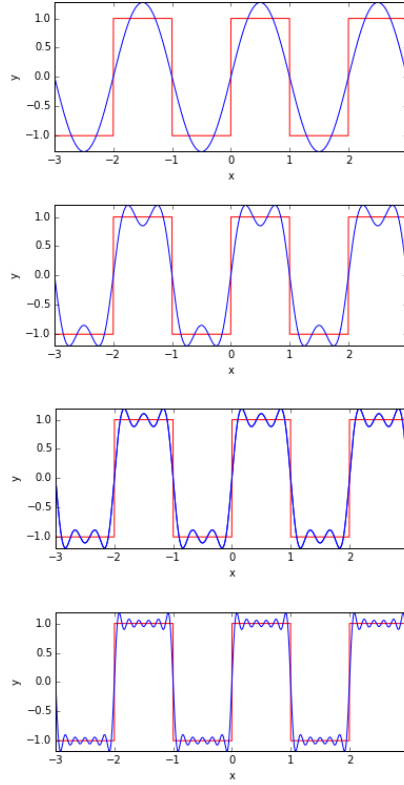


Figure 1: The Fourier Series for a step function including one term, three terms, five terms, and nineteen terms. The Fourier Theorem states that the series will converge, reproducing the original function, as the number of terms approaches infinity.

3 Determining the Fourier Coefficients

Just as in the vector analogy, we can determine the Fourier coefficients of a function f by computing the inner products:

$$\begin{aligned} A_n &= \langle c_n, f \rangle \\ B_n &= \langle s_n, f \rangle \end{aligned}$$

or, in terms of the inner product integrals:

$$\begin{aligned} A_n &= \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos\left(\frac{2\pi n}{L} x\right) dx \\ B_n &= \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \sin\left(\frac{2\pi n}{L} x\right) dx \end{aligned} \quad (6)$$

Just as in the vector analogy, the inner product determines the correct coefficients only because the basis functions are complete and orthonormal. We will illustrate this with a function that has all of the B_n equal to zero. Start with the completeness equation, but change the index from n to m in order to make the next step clearer.

$$f(x) = \sqrt{\frac{2}{L}} \sum_{m=0}^{\infty} A_m \cos\left(\frac{2\pi m}{L} x\right)$$

Now we apply the prescription in Equation 6 to both sides of this equation:

$$\begin{aligned} \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos\left(\frac{2\pi n}{L} x\right) dx &= \sqrt{\frac{2}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \left\{ \sqrt{\frac{2}{L}} \sum_{m=0}^{\infty} A_m \cos\left(\frac{2\pi m}{L} x\right) \right\} \cos\left(\frac{2\pi n}{L} x\right) dx \\ &= \sum_{m=0}^{\infty} A_m \left\{ \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos\left(\frac{2\pi m}{L} x\right) \cos\left(\frac{2\pi n}{L} x\right) dx \right\} \\ &= \sum_{m=0}^{\infty} A_m \delta_{nm} \\ &= A_n \end{aligned}$$

4 Compact Form of the Fourier Series

The Fourier Series developed above has the considerable advantage that it makes explicit the role of the sine and cosine functions as an orthonormal basis. But it is a bit unwieldy and seldom encountered in that form. Consider Equation 5 again:

$$f(x) = \sqrt{\frac{2}{L}} \sum_{n=0}^{\infty} A_n \cos\left(\frac{2\pi n}{L} x\right) + \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} B_n \sin\left(\frac{2\pi n}{L} x\right) + C$$

It is convenient to absorb the normalization factor $\sqrt{2/L}$ into the coefficients. The series is therefore most often written in the much more compact form:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \{a_n \cos(k_n x) + b_n \sin(k_n x)\} \quad (7)$$

where we have introduced the wave numbers:

$$k_n \equiv \frac{2\pi n}{L} \quad (8)$$

and the new Fourier Coefficients:

$$a_n \equiv \sqrt{\frac{2}{L}} A_n = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos(k_n x) dx \quad (9)$$

$$b_n \equiv \sqrt{\frac{2}{L}} B_n = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \sin(k_n x) dx \quad (10)$$

5 Fourier Series for Complex Functions

The Fourier Series can be expressed in terms of the complex exponential by noting that:

$$\begin{aligned}\cos(k_n x) &= \frac{\exp(ik_n x) + \exp(-ik_n x)}{2} \\ \sin(k_n x) &= \frac{\exp(ik_n x) - \exp(-ik_n x)}{2i}\end{aligned}$$

So that Equation 7 can be rewritten as:

$$\begin{aligned}f(x) &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \{a_n \cos(k_n x) + b_n \sin(k_n x)\} \\ &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left\{ a_n \frac{\exp(ik_n x) + \exp(-ik_n x)}{2} + b_n \frac{\exp(ik_n x) - \exp(-ik_n x)}{2i} \right\} \\ &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left\{ \frac{a_n - ib_n}{2} \exp(ik_n x) + \frac{a_n + ib_n}{2} \exp(-ik_n x) \right\} \\ &= c_0 + \sum_{n=1}^{\infty} \{c_n \exp(ik_n x) + c_n^* \exp(-ik_n x)\}\end{aligned}\tag{11}$$

Where in the last step we have introduced the complex Fourier coefficient:

$$c_n \equiv \frac{a_n - ib_n}{2}.\tag{12}$$

Notice in Equation 11 that c_0 is real because $b_0 = 0$ in Equation 12, and each summand in the sum is of the form $z + z^*$, hence $f(x)$ is real, as we assumed initially. Each summand in Equation 11 is of form $z + z^*$ because the coefficients of the complex exponentials are complex conjugates. If we replace our initial real function $f(x)$ with a complex valued function $\Psi(x)$ (such as a wave function in Quantum Mechanics!), the constraint that these coefficients are complex conjugates vanishes, and we can replace c_n^* with new independent¹ complex Fourier coefficients d_n . Furthermore, the constant c_0 which was real is now allowed to be complex.

$$\Psi(x) = c_0 + \sum_{n=1}^{\infty} \{c_n \exp(ik_n x) + d_n \exp(-ik_n x)\}$$

And finally, we note that we can simplify this equation even further by being quite clever, noting that $k_{(-n)} = -k_n$ and defining $c_{(-n)} \equiv d_n$:

$$\begin{aligned}\Psi(x) &= c_0 + \sum_{n=1}^{\infty} c_n \exp(ik_n x) + \sum_{n=1}^{\infty} d_n \exp(-ik_n x) \\ &= c_0 + \sum_{n=1}^{\infty} c_n \exp(ik_n x) + \sum_{n=-\infty}^{-1} c_n \exp(ik_n x) \\ \Psi(x) &= \sum_{n=-\infty}^{\infty} c_n \exp(ik_n x).\end{aligned}\tag{13}$$

¹If you prefer, you can construct the complex function from two real functions: $\Psi(x) = f(x) + ig(x)$. Either way, you have twice as many independent Fourier coefficients when the function is complex valued.

It's amusing to compare the size of Equation 5 with Equation 13, and note that the latter form is considerably more powerful. To determine the complex Fourier coefficients we calculate:

$$\begin{aligned}
c_n &\equiv \frac{a_n - ib_n}{2} \\
&= \frac{1}{2} \left\{ \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi(x) \cos(k_n x) dx - i \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi(x) \sin(k_n x) dx \right\} \\
&= \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi(x) \{ \cos(k_n x) - i \sin(k_n x) \} dx \\
c_n &= \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi(x) \exp(-ik_n x) dx
\end{aligned} \tag{14}$$

Now look closely at Equation 13 and Equation 14 and spot the negative sign in the exponential function of the latter. It seems something strange has happened. Instead of the sines and cosines, we would like to think of our new orthonormal basis as the complex exponential functions

$$e_n(x) \equiv \frac{1}{\sqrt{L}} \exp(ik_n x). \tag{15}$$

But to calculate the coefficient of $\exp(ik_n x)$, we integrate with respect to a *different* function $\exp(-ik_n x)$. Can our vector analogy survive this? It seems as though we are calculating the component along \hat{x} by taking the dot product with $-\hat{x}$.

It turns out that for complex valued functions, we need to modify our inner product to include complex conjugation of one of the functions:

$$\langle \Psi, \phi \rangle \equiv \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi^*(x) \phi(x) dx \tag{16}$$

With this simple tune up, the vector analogy for complex valued functions is saved! We still have orthonormal basis functions:

$$\begin{aligned}
\langle e_n, e_m \rangle &= \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \exp(-ik_n x) \exp(ik_m x) dx \\
&= \delta_{nm}
\end{aligned} \tag{17}$$

and we still calculate the coefficient of each $e_n(x)$ from the inner product:

$$c_n = \frac{1}{L} \langle e_n, \Psi \rangle = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi(x) \exp(-ik_n x) dx \tag{18}$$

6 The Fourier Transform

The Fourier Series is sufficient for periodic functions. Unfortunately, this is of rather limited use in physics. To realize the full potential of the Fourier Theorem, we need to extend the concept to apply to any function, with the only caveat that the function must approach zero as x approaches both negative and positive infinity.

The trick is to consider such a function as periodic with period L in the limit $L \rightarrow \infty$. Recall Equation 8:

$$k_n \equiv \frac{2\pi n}{L}.$$

When L is very large, we will obtain a non-zero value for k_n only for comparably large values of n . But since n is very large, the difference between k_n and k_{n+1} is infinitesimal. We have moved from the discrete case, where we only have certain wave numbers k_n for each integer $n = 0, 1, 2, \dots$, to the continuous case, where k can take any real value. Fortunately, our vector analogy survives intact.

Our inner product now extends between positive and negative infinity:

$$\langle \Psi, \phi \rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x) \phi(x) dx \quad (19)$$

Our basis functions, which are now defined for any value of k ,

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx) \quad (20)$$

are still orthonormal, but the condition looks a bit different in the continuum case:

$$\langle e_k, e_{k'} \rangle = \delta(k - k')$$

See the appendix for more details on the Dirac delta function $\delta(x)$, which is zero everywhere but at $x = 0$, where it is infinite. It is the continuous version of δ_{nm} .

Our basis functions are also still complete. In the discrete case we have a complex Fourier coefficient for every integer n . Now we have a complex Fourier coefficient for any real value of k . In place of Fourier coefficients, we have instead a function of k which we call the Fourier transform: $\tilde{\Psi}(k)$. Instead of a sum over discrete terms, we now have to integrate over all values of k :

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\Psi}(k) \exp(ikx) dk. \quad (21)$$

Just as in the discrete case, we determine the Fourier transform from the inner product:

$$\tilde{\Psi}(k) = \langle e_k, \Psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx) dx \quad (22)$$

Equation 22 is generally referred to as the *Fourier Transform*, while Equation 21 is referred to as the *Inverse Fourier Transform*.

7 The Fourier Transform in Quantum Mechanics

So far we have been considering the Fourier transform with respect to position x and wave-number k . A much more useful pair of variables for Quantum Mechanics turns out to be momentum p and position x . To relate p to k we need only apply the DeBroglie relation to the wavelength in the definition of the wavenumber:

$$k \equiv \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

We could therefore make the substitution $k \rightarrow p/\hbar$ (and $dk \rightarrow dp/\hbar$) in Equations 21 and 22. It turns out that a marginally more useful equation results if we make the normalization factors symmetric, by splitting the normalization factor of $1/\hbar$ across both equations with $1/\sqrt{\hbar}$ applied to each:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\Psi}(p) \exp(ipx/\hbar) dp \quad (23)$$

$$\tilde{\Psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar) dx \quad (24)$$

The major benefit of this symmetric form is that the normalization of $\Psi(x)$ and $\tilde{\Psi}(p)$ in this case turns out to be the same:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = \int_{-\infty}^{\infty} |\tilde{\Psi}(p)|^2 dp = 1$$

Because we can always calculate $\Psi(x)$ from $\tilde{\Psi}(p)$ either one completely describes the quantum mechanical state. We call $\tilde{\Psi}(p)$ the momentum wave function. Whereas $|\Psi(x)|^2$ gives us the probability density for the quanton to be at position x , $|\Psi(p)|^2$ gives us the probability density for the quanton to have momentum p .

8 The Uncertainty Principle

Imagine that a particle is near $x = 0$ with some uncertainty σ_x . One way we might describe such a state is that the probability distribution is a Gaussian (bell-curve) distribution:

$$|\Psi(x)|^2 = N_x^2 \exp\left(-\frac{x^2}{2\sigma_x^2}\right)$$

where N_x is a normalization factor chosen such that

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1.$$

One wave function that would lead to such a probability distribution is

$$\Psi(x) = N_x \exp\left(-\frac{x^2}{4\sigma_x^2}\right).$$

Let's look at the momentum wave function for this particle:

$$\tilde{\Psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar) dx \quad (25)$$

$$= \frac{N}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4\sigma_x^2} - \frac{ipx}{\hbar}\right) dx \quad (26)$$

The trick to solving this integral is called *completing the square*, we add and subtract the missing term needed to write this as $(x + a)^2 + b$:

$$\begin{aligned} X &= -\frac{x^2}{4\sigma_x^2} - \frac{ipx}{\hbar} \\ &= -\frac{1}{4\sigma_x^2}(x^2 - 4ipx\sigma_x^2/\hbar) \\ &= -\frac{1}{4\sigma_x^2}(x^2 - 4ipx\sigma_x^2/\hbar + 4i^2p^2\sigma_x^4/\hbar^2 - 4i^2p^2\sigma_x^2/\hbar^2) \\ &= -\frac{(x - 2ip\sigma_x^2/\hbar)^2}{4\sigma_x^2} - p^2\sigma_x^2/\hbar^2 \end{aligned}$$

The whole point of this is that because x runs from $-\infty$ to ∞ we can now make a change of variables $x - 2ip\sigma_x^2/\hbar \rightarrow x$ to clean things up dramatically:

$$X = -\frac{x^2}{4\sigma_x^2} - p^2\sigma_x^2/\hbar^2$$

Our integral now becomes:

$$\begin{aligned}
\tilde{\Psi}(p) &= \frac{N}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4\sigma_x^2} - p^2\sigma_x^2/\hbar^2\right) dx \\
&= \left\{ \frac{N}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4\sigma_x^2}\right) \right\} \exp(-p^2\sigma_x^2/\hbar^2) \\
&= N_p \exp(-p^2\sigma_x^2/\hbar^2)
\end{aligned} \tag{27}$$

Where in the last step we have noted that the term in brackets is just a constant and set $N_p = \{\dots\}$.

Fortunately the term in brackets does not depend on p at all... there's no need to calculate it, it will just give us a normalized momentum wave function. We might as well just set it to N_p : Recall that we started with a wave function which had a Gaussian (bell-shaped) probability distribution with uncertainty σ_x :

$$|\Psi(x)|^2 = N_x^2 \exp\left(-\frac{x^2}{2\sigma_x^2}\right).$$

We found that the momentum wave function also has a Gaussian probability distribution, if we call the uncertainty on the momentum σ_p , the probability distribution should have form the same form:

$$|\tilde{\Psi}(p)|^2 = N_p^2 \exp\left(-\frac{p^2}{2\sigma_p^2}\right)$$

Comparing this to Equation 27 we conclude:

$$\sigma_p = \frac{\hbar}{2\sigma_x}$$

or:

$$\sigma_x \sigma_p = \frac{\hbar}{2}$$

Since uncertainties can always be worse than the best case, we have more generally:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

This is the Heisenberg uncertainty principle of quantum mechanics. The more precisely the position is determined, the less precisely the momentum is determined, and vice versa. It is a direct consequence of the wave like nature of matter.

9 Frequency Space

One of the more confusing aspects of the Fourier Theorem is the bewildering variation in the applications. But this is merely an inevitable consequence of how fundamental and powerful a tool it is. As Fourier pairs we most often see the dimensionless quantities kx , px/\hbar , ωt , $2\pi ft$, and Et/\hbar , but any dimensionless quantity formed from two variables will work. Once the Fourier pair is chosen, one then has to decide how to normalize the Fourier Transform and Inverse Fourier Transform. But whatever unfamiliar ground you find yourself on, it is always true that:

$$\int_{-\infty}^{\infty} \exp(ikx) dx = 2\pi\delta(k).$$

That 2π has to go somewhere!

By far the most popular choice for the Fourier is frequency and time. In this case, the 2π remains in the exponent, and we have simply:

$$\tilde{V}(f) = \int_{-\infty}^{\infty} \exp(-i2\pi ft) V(t) dt \quad (28)$$

$$V(t) = \int_{-\infty}^{\infty} \exp(i2\pi ft) \tilde{V}(f) df \quad (29)$$

$$(30)$$

10 Energy Spectral Density

Consider:

$$\begin{aligned} \int_{-\infty}^{\infty} dt |V(t)|^2 &= \int_{-\infty}^{\infty} df V^*(t) V(t) \\ &= \int_{-\infty}^{\infty} df \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} df' \tilde{V}(f') \exp(-i2\pi f't) \right)^* \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} df'' \tilde{V}(f'') \exp(-i2\pi f''t) \right) \\ &= \int_{-\infty}^{\infty} df \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} df' \tilde{V}^*(f') \exp(i2\pi f't) \right) \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} df'' \tilde{V}(f'') \exp(-i2\pi f''t) \right) \\ &= \int_{-\infty}^{\infty} df \int_{-\infty}^{\infty} df' \tilde{V}^*(f') \tilde{V}(f'') \int_{-\infty}^{\infty} dt \exp(i2\pi(f'' - f')t) \\ &= \int_{-\infty}^{\infty} df \int_{-\infty}^{\infty} df' \tilde{V}^*(f') \tilde{V}(f') \delta(f'' - f') \\ &= \int_{-\infty}^{\infty} df |\tilde{V}(f)|^2 \end{aligned}$$

which is called Parseval's Theorem in all its guises, which always relates the integrated norm of a function to that of its Fourier coefficient. But take care that sometimes there are normalization factors, for instance: if we try to hide the factor of 2π by using variable $\omega = 2\pi f$ instead of f , we find:

$$\int_{-\infty}^{\infty} dt |V(t)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega |V(\omega)|^2$$

That 2π factor always appears somewhere!

In many cases, the power of a time varying signal goes as an amplitude squared, so for instance:

$$U = \frac{1}{2} CV^2$$

and so the total energy of the signal can be calculated as:

$$E \propto \int dt |V(t)|^2 \quad (31)$$

but Parseval's theorem implies

$$E \propto \int df |\tilde{V}(f)|^2$$

We can therefore associate the quantity $|\tilde{V}(f)|^2$, which we call the Energy Spectral Density, with the amount of energy contained in the signal at frequency f .

11 Autocorrelation

A widely useful quantity for signal processing is the autocorrelation function, which simply integrates a function multiplied by a delayed copy of itself:

$$R(\tau) = \int_{-\infty}^{\infty} du V(u) V(u + \tau) \quad (32)$$

Notice that $R(-\tau) = R(\tau)$ (by changing integration variables). Also notice that $R(\tau) \leq R(0)$, that is, R is monotonically decreasing. For most (non-periodic) physical signals, the autocorrelation vanishes quickly. This turns out to be very useful in cases (like Noise!) where the Fourier transform of the signal itself cannot be calculated. But first let's have a look at the Fourier Transform $S(f)$ of the autocorrelation function when the Fourier transforms of the signal V can be calculated:

$$\begin{aligned} S(f) &\equiv \int_{-\infty}^{+\infty} d\tau R(\tau) \exp(-i2\pi\tau) \\ &= \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} d\tau V(u) V(u - \tau) \exp(-i2\pi\tau) \\ &= \int_{-\infty}^{+\infty} du V(u) \exp(i2\pi\tau) \left\{ \int_{-\infty}^{+\infty} d\tau V(u - \tau) \exp(i2\pi(u - \tau)) \right\} \\ &= \int_{-\infty}^{+\infty} du V(u) \exp(i2\pi\tau) \left\{ \int_{-\infty}^{+\infty} d\tau' V(\tau') \exp(i2\pi(\tau')) \right\} \\ &= |\tilde{V}(f)|^2 \end{aligned}$$

So the Fourier Transform of the Autocorrelation function is the Energy spectral density. This fascinating outcome is quite useful, as we shall see, when we encounter signals $V(t)$ for which the Fourier transform does not exist. It also makes good sense if you think about it. The Fourier transform measures the amplitude of the periodic functions contained within a signal, and the autocorrelation function preserves the periodicity of the original function.

12 Power Spectral Density

The definitions above work well for a limited time duration pulses with finite total energy, and the integral in Equation 31 is calculable. However, for continuous signals, that are present for all time, the total energy is infinite and so the energy spectral density is undefined. Yet it certainly makes sense to ask what the frequency distribution of a continuous signal is. The answer is to normalize these distribution, essentially turning them into expectation values with respect to time. Even if this integral diverges:

$$\int_{-\infty}^{\infty} dt f(t) \rightarrow \infty$$

this limit, because of the normalization factor T , will often converge:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt f(t) \equiv \langle f(t) \rangle,$$

and represents the expectation value of f over all time. For $f(t) = V^2(t)$ the integral in Equation 31 yielded the total power, while the expectation value gives the average power:

$$P_{\text{avg}} \propto \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt |V(t)|^2 = \langle V^2(t) \rangle. \quad (33)$$

Signals with a finite energy are called "energy signals" and have a well-defined energy spectral density. Signals with a finite average power and therefore infinite energy are called "power signals". Of course, there are no actual power signals in the universe, but many signals last much longer than the time interval of interest, and are therefore effectively power signals.

When it exists, the Fourier transform $\tilde{V}(f)$ contains useful information about the frequency distribution of a power signal. However, there are many important cases, such as for random noise, that the Fourier transform of $V(t)$ does not exist. Recall that for energy signals, the Fourier transform of the autocorrelation gave the energy spectral density. In this case, the correlation function as defined in Equation 32 diverges, but if we normalize it:

$$\mathcal{R}(\tau) \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt V(t)V(t-\tau) = \langle V(t)V(t-\tau) \rangle \quad (34)$$

this function is usually well behaved, and part of a Fourier Transform pair:

$$\mathcal{S}(f) \equiv \int_{-\infty}^{\infty} d\tau \mathcal{R}(\tau) \exp(-i2\pi f\tau) \quad (35)$$

$$\mathcal{R}(\tau) = \int_{-\infty}^{\infty} df \mathcal{S}(f) \exp(i2\pi f\tau) \quad (36)$$

But how should we interpret $\mathcal{S}(f)$ which we hope contains useful information about the frequency distribution of our signal? We start by noting that Definition 34 implies that:

$$R(0) = \langle V^2(t) \rangle \equiv P_{\text{avg}}$$

but from Equation 36 we also have:

$$\begin{aligned} R(0) &= \int_{-\infty}^{\infty} df \mathcal{S}(f) \exp(i2\pi f0) \\ &= \int_{-\infty}^{\infty} df \mathcal{S}(f) \end{aligned}$$

or in other words:

$$P_{\text{avg}} \equiv \langle V^2(t) \rangle = \int_{-\infty}^{\infty} df \mathcal{S}(f)$$

That is to say $\mathcal{S}(f)$ is the average power contained at frequency f . To calculate $\mathcal{S}(f)$ we simply calculate the Fourier transform of the autocorrection function:

$$\mathcal{R}(\tau) \equiv \langle V(t)V(t-\tau) \rangle. \quad (37)$$

13 The Periodogram

Suppose $V(t)$ is continuous with some period T so that it is represented by a Fourier Series:

$$V(t) = \sum_{n=-\infty}^{\infty} c_n \exp(i2\pi f_n t)$$

where $f_n = n/T$. The Fourier coefficients are determined from:

$$c_n = \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} dt V(t) \exp(-i2\pi f_n t), \quad (38)$$

and in this context Parseval's theorem is:

$$\frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} |V(t)|^2 dt = \sum_n |c_n|^2$$

or equivalently:

$$P_{\text{avg}} \equiv \langle |V(t)|^2 \rangle = \sum_n |c_n|^2$$

which we can interpret to mean that $|c_n|^2$ represents the average power $P_{\text{avg}}^{(n)}$ at frequency f_n . Since the frequencies associated with each coefficient are discrete values separated by $\Delta f = f_{n+1} - f_n = 1/T$, the power spectral distribution for the discrete Fourier Series is

$$\mathcal{S}(f_n) = \frac{P_{\text{avg}}^{(n)}}{\Delta f} = T|c_n|^2.$$

Furthermore, since we often do not care about the *phase* information in the two-sided power spectral distribution, that is, we don't care to distinguish between power at f_n and power at $-f_n$, the one-sided power spectral distribution is:

$$\mathcal{S}_+(f_n) = \frac{P_{\text{avg}}^{(n)}}{\Delta f} = T(|c_n|^2 + |c_{-n}|^2) \quad (39)$$

In the exercises, you will show that for

$$f(t) = A \cos(2\pi f_n t)$$

the one-sided power spectral distribution is:

$$\mathcal{S}_+(f_n) = \frac{T}{2}|A|^2 \quad (40)$$

which is absolutely essential for calibrating a PSD using a function generator!

In many cases, we wish to estimate the PSD from a discrete data set. Instead of a continuous function of time $f(t)$ on the interval T we instead have N samples of f each separated by time $\tau = T/N$, which we record as x_i . We can replace $f(t)$ with its discrete version:

$$f(t) \rightarrow \sum_{m=0}^{N-1} x_m \delta(t - i\tau) \tau \quad (41)$$

so chosen because any integral over the discrete version

$$\int_{t_1}^{t_2} dt \sum_{m=0}^{N-1} x_m \delta(t - i\tau) \tau = \sum_{m=m_1}^{m_2} x_m \tau \rightarrow \int_{t_1}^{t_2} dt f(t)$$

approaches the integral over the continuous function in the limit $N \rightarrow \infty$. Note that m in the middle sum runs over the indices of the samples in the time interval t_1 to t_2 .

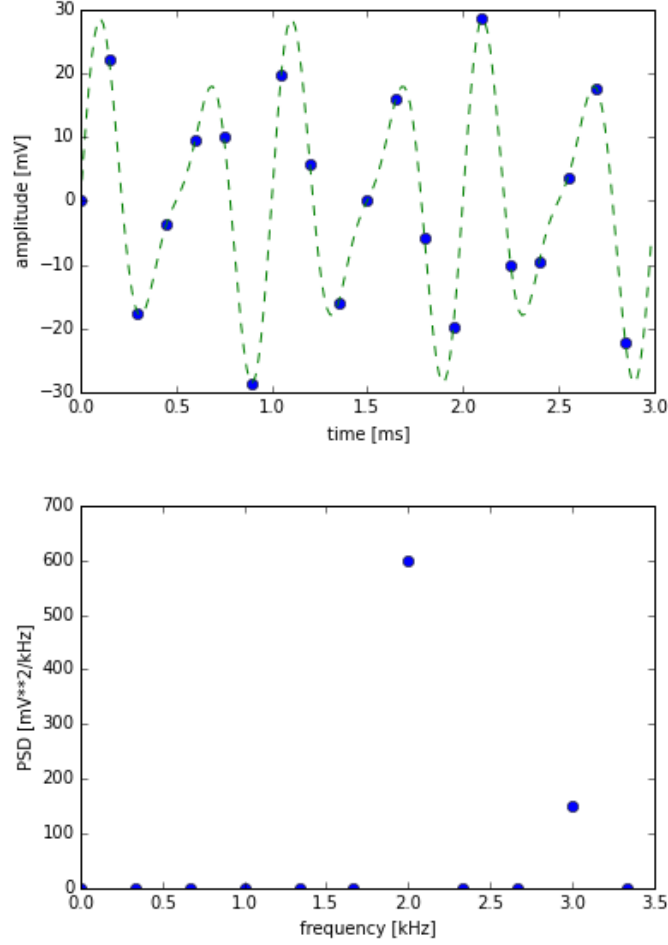


Figure 2: An example periodogram calculated from 20 samples over 3 ms from a signal composed of two sine waves with amplitudes 10 mV and 20 mV. There are two peaks in the periodogram with PSD values $\mathcal{S}_+(f_n) = 150$ and $600 \text{ mV}^2/\text{kHz}$ as expected from Equation 40.

Simply inserting the discrete version of $f(t)$ from Equation 41 into the formula for determining the coefficients of the Fourier series Equation 38:

$$\begin{aligned}
 c_n &= \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} dt V(t) \exp(-i2\pi f_n t) \\
 &= \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} dt \exp\left(\frac{-i2\pi n t}{T}\right) \sum_{m=0}^{N-1} x_m \delta(t - i\tau) \tau \\
 &= \frac{\tau}{T} \sum_{m=0}^{N-1} \exp\left(\frac{-i2\pi n m \tau}{T}\right) x_m \\
 &= \frac{1}{N} \sum_{m=0}^{N-1} \exp\left(\frac{-i2\pi n m}{N}\right) x_m
 \end{aligned} \tag{42}$$

This is an example of a discrete Fourier Transform (DFT). There are more computationally efficient methods to calculate the coefficients c_n , but they all reproduce this calculation.

The Nyquist-Shannon sampling theorem states that if the highest frequency component of a

signal is f_0 , and the signal is sampled at a rate $1/\tau \geq 2f_0$ then no information is lost. The Fourier coefficients determined from the DFT can be used to exactly reproduce the original signal at any time. This may seem surprising at first glance. But consider that we are already familiar with a continuous function being exactly represented by a discrete set of Fourier coefficients. If a signal has a maximum frequency component f_0 , we can think of its Fourier transform as a periodic function on the interval $(-f_0, f_0)$. Its inverse Fourier transform will then be discrete!

Given N samples x_i taken at sample rate $1/\tau$, we calculate the DFT as the coefficients in Equation 42, then we calculate the one-sided power spectrum distribution as in Equation 39. If we have satisfied the Nyquist-Shannon sampling theorem, only the coefficients corresponding to $1/2\tau$ will be non-zero, so we need only report $\mathcal{S}_+(f_n)$ at the $N/2$ values from $f = 1/T$ to $f = N/2T = 1/2\tau$. The plot of $\mathcal{S}_+(f_n)$ versus f_n for these $N/2$ values is known as periodogram, and is a staple of digital signal processing. An example periodogram resulting from a sine wave is shown in Fig. 2.

14 Exercises

Problem 1: Show that the sines and cosines are orthogonal functions as claimed in Equations 1–3. You can compute the integrals using the trigonometric identities:

$$\begin{aligned}\sin \alpha \sin \beta &= \frac{1}{2} \{ \cos(\alpha - \beta) - \cos(\alpha + \beta) \} \\ \cos \alpha \cos \beta &= \frac{1}{2} \{ \cos(\alpha - \beta) + \cos(\alpha + \beta) \} \\ \cos \alpha \sin \beta &= \frac{1}{2} \{ \sin(\alpha + \beta) - \sin(\alpha - \beta) \}\end{aligned}$$

Problem 2: There are different conventions for the constant term C in Equation 5. Since this is the only term that gives $f(x)$ a mean value, we must in every case have:

$$C = \frac{1}{L} \int_{-\frac{L}{2}}^{-\frac{L}{2}} dx f(x).$$

Show that we can extend Equation 4 so that

$$\langle c_n, c_m \rangle = \delta_{nm}$$

even for $n = m = 0$ for a suitable definition of the constant “function” c_0 . Further show that then if we define $A_0 = \langle c_0, f \rangle$ then we must have $C = A_0/\sqrt{L}$. A much more common approach is to extend Equations 9 and 10

$$\begin{aligned}a_n &= \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos(k_n x) dx \\ b_n &= \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \sin(k_n x) dx\end{aligned}$$

to include $n = 0$. Show that in this case $b_0 = 0$ always, and that we must have $C = a_0/2$, just as in Equation 7.

Problem 3: Consider the function $f(x) = x$ for the interval $[-1, 1]$. For its Fourier Series representation following the convention of Equation 7, calculate the coefficients a_0 , a_1 and b_1 . What about a_2 and a_3 ?

Problem 4: Verify Equation 17 in two different ways: (a) by explicitly calculating the integral, and (b) by using Euler's Equation and the orthogonality of the sines and cosines.

Problem 5: Using the compact form of the Fourier Series (Equation 13) show that the prescription for determining the coefficients (Equations 14) is valid. Use the same method as was used at the end of Section 3.

Problem 6: For the function $f(x) = \sin(2\pi f_n x)$ find all of the non-zero Fourier coefficients in the Fourier Series of Equation 13.

Problem 7: Suppose that instead of being in an Eigenstate of Energy, a particle in a box has equal probability to be anywhere in the box, so the wave function is:

$$\Psi(x) = \begin{cases} 1/d & \text{if } -d/2 < x < d/2 \\ 0 & \text{otherwise} \end{cases}$$

Compute the corresponding momentum wave function by taking the Fourier Transform.

Problem 8: Show that the auto-correlation function $\mathcal{R}(\tau) = \langle f(t)f^*(t - \tau) \rangle$ of $f(t) = \exp(i2\pi ft)$ is simply $f(\tau)$. Therefore, show that the PSD for $f(t)$ is a delta function at f .

Problem 8: Show that the auto-correlation function $\mathcal{R}(\tau) = \langle f(t)f^*(t - \tau) \rangle$ of $f(t) = \exp(i2\pi ft)$ is simply $f(\tau)$. Therefore, show that the PSD for $f(t)$ is a delta function at f .

Problem 9: Suppose that a signal $f(t) = A\delta(t)$. Calculate the autocorrelation function $R(\tau) = \int_{-\infty}^{+\infty} dt$ and then show that the Energy Spectral Density has the constant value A^2 .

15 Appendix

This is optional reading. A proper mathematical proof of these concepts requires about a one year course. Fortunately, physicist are generally satisfied with informal proofs of mathematical concepts, because for us the ultimate validation is experiment!

15.1 The Dirac Delta Function

These proofs make extensive use of the Dirac delta function, $\delta(x)$, which is zero everywhere but at $x = 0$, where it is infinite. Mathematically, the delta function only makes formal sense inside an integral, where it has the following defining properties:

$$\int_{-\infty}^{\infty} f(x') \delta(x - x') dx' = f(x) \quad (43)$$

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 \quad (44)$$

The delta function simply picks out from the integral the one value of the integrand which makes the argument of the delta function zero. This makes intuitive sense, because the delta function is zero everywhere else. The second equation shows the normalization of the delta function, which follows from the first if you take $f(x) = 1$.

15.2 The completeness of the sines and cosines

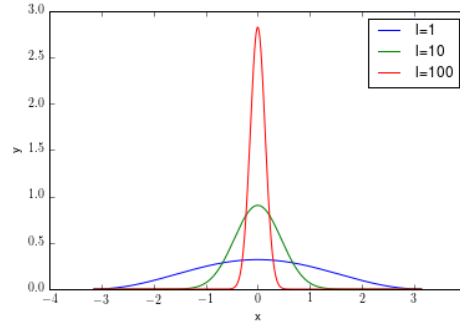


Figure 3: The function $h_\ell(x)$ for increasingly large values of ℓ .

To demonstrate the completeness of sines and cosines² we construct a peculiar but useful set of functions defined for $\ell = 1, 2, 3, \dots$:

$$h_\ell(x) = c_\ell \left(\frac{1 + \cos(x)}{2} \right)^\ell$$

We chose each factor c_ℓ such that:

$$\int_{-\pi}^{\pi} h_\ell(x) = 1$$

The shape of h_ℓ is shown in Fig. 3. As ℓ increases, h_ℓ becomes more and more narrow at $x = 0$, while the normalization is as in Equation 44. It looks more and more like the delta function:

$$\lim_{\ell \rightarrow \infty} h_\ell(x) = \delta(x)$$

It has one other important feature: $h_\ell(x)$ is simply a sum of cosines of nx with coefficients that don't depend on x . To see how this can be, note that we can always turn a product of cosines into a sum via the trigonometric identity:

$$\cos \alpha \cos \beta = \frac{1}{2} \{ \cos(\alpha - \beta) + \cos(\alpha + \beta) \}.$$

So, for instance, we can write:

$$\begin{aligned} h_2(x) &= \frac{c_2}{4} + \frac{c_2 \cos(x)}{2} + \frac{c_2 \cos^2(x)}{4} \\ &= \frac{c_2}{4} + \frac{c_2 \cos(x)}{2} + \frac{c_2 \cos(2x)}{8} \end{aligned}$$

²This proof taken from <http://web.mit.edu/jorloff/www/18.03-esg/notes/fourier-complete.pdf>

This property implies that the function $h_\ell(x - a)$ for some constant a is simply a sum of *both* sines and cosines of nx with coefficients that don't depend on x , as:

$$\cos(nx - na) = \cos(nx) \cos(na) + \sin(nx) \sin(na).$$

With this technology in hand we are ready to demonstrate the completeness of the sines and cosines. For simplicity, it suffices to consider only functions with period $L = 2\pi$ (i.e. $k_n = n$). The general case can then be inferred by transformation of coordinates. Consider a real function $f(x)$ which is periodic for $L = 2\pi$. For now just define the function $F(x)$ to be the infinite series:

$$F(x) \equiv a_0 + \sum_{n=1}^{\infty} \{a_n \cos(nx) + b_n \sin(nx)\}. \quad (45)$$

This is the compact form of the Fourier Series for this special case $L = 2\pi$, so $k_n = n$. We assume the coefficients are determined in the usual way:

$$\begin{aligned} a_n &= \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos(nx) dx \\ b_n &= \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \sin(nx) dx. \end{aligned}$$

We need to show that $F(x) = f(x)$, or

$$g(x) = F(x) - f(x) = 0$$

The proof hinges on the fact that $F(x)$ and $f(x)$ have the same Fourier coefficients, so that:

$$\begin{aligned} \int_{-\pi}^{\pi} g(x) \sin(nx) dx &= \int_{-\pi}^{\pi} F(x) \sin(nx) dx - \int_{-\pi}^{\pi} f(x) \sin(nx) dx \\ &= b_n - b_n \\ &= 0 \\ \int_{-\pi}^{\pi} g(x) \cos(nx) dx &= \int_{-\pi}^{\pi} F(x) \cos(nx) dx - \int_{-\pi}^{\pi} f(x) \cos(nx) dx \\ &= a_n - a_n \\ &= 0 \end{aligned}$$

This shows that the integral of $g(x)$ times any sine or cosine is zero. But our special function $h_\ell(x - a)$ function is just a sum of sines and cosines of nx for any value of a . This means that:

$$\int_{-\pi}^{\pi} h_\ell(x - a) g(x) dx = 0$$

If we take the limit as $\ell \rightarrow \infty$, we obtain:

$$\begin{aligned} \int_{-\pi}^{\pi} \delta(x - a) g(x) dx &= 0 \\ g(a) &= 0 \end{aligned}$$

Since this is true for any value of a , we have $g(x) = 0$ and so $F(x) = f(x)$.

15.3 The orthogonality and completeness of the complex exponential function

The first thing we need to show is that:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ikx) dk = \delta(x) \quad (46)$$

To see this we first calculate:

$$\begin{aligned} \frac{1}{2\pi} \int_{-a}^a \exp(ikx) dk &= \frac{1}{2\pi} \frac{\exp(iax) - \exp(-iax)}{ix} \\ &= \frac{1}{\pi} \frac{\sin(ax)}{x} \\ &= \frac{a}{\pi} \text{sinc}(ax) \end{aligned}$$

An integration shows that:

$$\int_{-\infty}^{\infty} \frac{a}{\pi} \text{sinc}(ax) dx = 1 \quad (47)$$

exactly as needed for Equation 44.

Fig. 4 shows that this function peaks at zero and becomes more and more narrow for progressively larger values of a . Since it has the correct normalization, we conclude that:

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ikx) dk &= \lim_{a \rightarrow \infty} \frac{1}{2\pi} \int_{-a}^a \exp(ikx) dk \\ &= \lim_{a \rightarrow \infty} \frac{a}{\pi} \text{sinc}(ax) \\ &= \delta(x) \end{aligned} \quad (48)$$

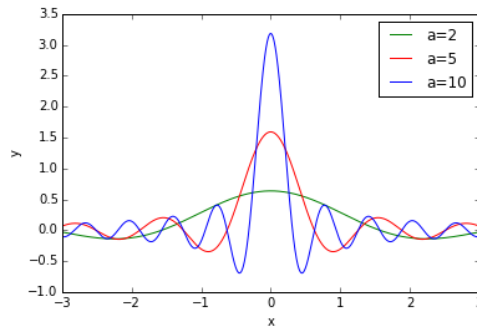


Figure 4: The function $a \text{sinc}(ax)/\pi$ for progressively larger values of a . As $a \rightarrow \infty$, this function approaches the delta function $\delta(x)$.

We are now fully equip to show that the complex exponential functions:

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx)$$

are orthonormal. Calculating the inner product

$$\begin{aligned}
\langle e_k, e_{k'} \rangle &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp(-ikx) \frac{1}{\sqrt{2\pi}} \exp(ik'x) dx \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\{i(k' - k)x\} dx \\
&= \delta(k - k')
\end{aligned}$$

where we have used Equation 48 but with the roles of x and k exchanged. To prove completeness, we can now show that:

$$\begin{aligned}
\Psi(x) &= \int_{-\infty}^{\infty} \Psi(x') \delta(x - x') dx' \\
&= \int_{-\infty}^{\infty} f(x') \left\{ \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp\{ik(x - x')\} dk \right\} dx' \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x') \exp(-ikx') dx' \right\} \exp(ikx) dk \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\Psi}(k) \exp(ikx) dk
\end{aligned}$$

where:

$$\tilde{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx) dx$$