Lecture 3 - Fourier transforms

What's important:
- discrete Fourier transforms
- continuous Fourier transforms

Text: Gasiorowicz, App. A

The two probability distributions $P(x)$ and $P(p)$ for position and momentum introduced in Lec. 2 are not independent but linked through the Uncertainty Principle. The math which underlies the relationships is the same as that of Fourier series. We introduce discrete Fourier series in this lecture, then generalize to continuous variables. Although it looks like a mathematical diversion at this point, it establishes a helpful framework for introducing the Schrödinger equation.

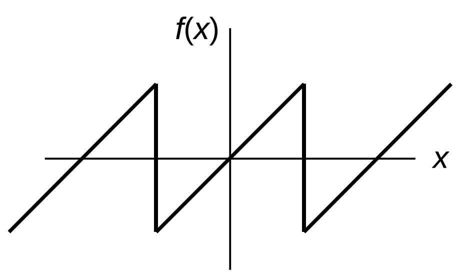
Fourier transforms - discrete

In second year calculus, series expansions are introduced as a way of representing complicated functions. For example, the sine function has the series expansion

$$\sin x = x - x^3/3! + x^5/5!... \qquad (1)$$

This expression can be useful in evaluating sine, or some of its integrals, in the region of small x. In using a polynomial expansion such as (1), one obviously must be concerned about the convergence of the series for the range of x of interest.

The de Broglie wavelength of particles provides a hint that the functions of interest in quantum mechanics are periodic. The series expansions of periodic functions can be conveniently based on other periodic functions, such as the sine and cosine functions of trigonometry. Suppose we have the simple sawtooth function $f(x) = x$, periodic over $-1 \le x \le 1$:



What functions would be useful in representing this particular $f(x)$?
1. $\sin(\pi x)$ is an obvious choice, as $\sin(0) = 0$, and it is appropriately periodic.
2. $\cos x$ is not a good choice, as $\cos(0) = 1$.
3. a constant a_o is also not useful, again because we require $f(0) = 0$.

So, we are tempted to write

$$f(x) = \Sigma_{n=1}\, a_n \sin(n\pi x) \qquad (2)$$

If $f(x)$ were of the form $f(x) = a_o + x$, then the summation in Eq. (2) would start at $n = 0$, rather than $n = 1$. The coefficients a_n are infinite in number, in principle; in practice, one only evaluates as many of them as are needed for the problem. How do we evaluate them? By multiplying both sides of the equation by $\sin(m\pi x)$, and then integrating over the allowed range of x, each coefficient in turn can be extracted, because the sine functions are orthogonal for $m \neq n$. That is:

$$\int_{-1}^{1} f(x) \sin(m\pi x)\, dx = \int_{-1}^{1} \sin(m\pi x) \Sigma_{n=1} a_n \sin(n\pi x)\, dx$$
$$= \Sigma_{n=1} a_n \int_{-1}^{1} \sin(m\pi x) \sin(n\pi x)\, dx. \qquad (3)$$

Working with the RHS:

$$\sin(m\pi x) \sin(n\pi x) = 1/2 \cos([m-n]\pi x) - 1/2 \cos([m+n]\pi x)$$
from trig identity $\sin a \sin b = [\cos(a-b) - \cos(a+b)]$ (4)

$$\text{RHS} = \int_{-1}^{1} \sin(m\pi x) \sin(n\pi x)\, dx$$
$$= 1/2 \int_{-1}^{1} \cos((m-n)\pi x)\, dx - 1/2 \int_{-1}^{1} \cos((m+n)\pi x)\, dx$$
$$= [1 / 2\pi(m-n)] \sin\theta|_{-(m-n)\pi}^{+(m-n)\pi} - [1 / 2\pi(m+n)] \sin\theta|_{-(m+n)\pi}^{+(m+n)\pi}$$

If $m \neq n$, then both terms give zero.
if $m=n$, first term gives 2/2, but the second still vanishes.
Thus,

$$\int_{-1}^{1} \sin(m\pi x) \sin(n\pi x)\, dx = \delta_{mn}. \qquad (5)$$

To solve for a_n we use

$$\text{LHS} = \int_{-1}^{1} x \sin(m\pi x)\, dx$$
$$= (m\pi)^{-2} \int_{-m\pi}^{m\pi} \cos z\, dz \quad - \quad (m\pi)^{-2}\, z \cos z\, |_{-m\pi}^{m\pi}$$
from $(z \cos z)' = \cos z - z \sin z$
$$= (m\pi)^{-2} \sin z\, |_{-m\pi}^{m\pi} \quad - \quad 2 \cos(m\pi) / m\pi$$
$$= \quad 0 \quad - \quad 2 (-1)^m / m\pi$$
$$= (2/m\pi)\bullet(-1)^{m+1} \qquad (6)$$

Combining (5) and (6) with (3) for the case $f(x) = x$

$$(2/m\pi)\bullet(-1)^{m+1} = \Sigma_{n=1} a_n \delta_{mn}$$

or

$$a_n = 2 (-1)^{n+1} / n\pi \qquad \text{for } f(x) = x. \qquad (7)$$

For a general function, we expect both sin and cos functions to be present in the series expansion, and can write:

$$f(x) = \Sigma_{n=1} a_n \sin(n\pi x) + \Sigma_{n=1} b_n \cos(n\pi x) \qquad (8)$$

aside from a constant to take care of $f(0)$. Now, this expression can be made more compact by allowing the expansion coefficients to be complex, and invoking

$$\exp(i\theta) = \sin\theta + i \cos\theta,$$

where the pure imaginary $i = \sqrt{-1}$. Thus, the general expression for the Fourier series is

$$f(x) = \Sigma_{n=-\infty}^{+\infty} a_n \exp(in\pi x / L). \qquad (9)$$

A couple of things to note in this expression:

1. The series involves positive and negative n, which may be needed to make the series pure real *etc*.
2. In general, x may carry dimensions which must be removed from the argument of the exponential. Thus, the physical period of the function must be incorporated, which is $2L$ in this definition. Other definitions are OK as well, but they may have different normalizations.

Now, it's trivial to invert Eq. (9) from

$$\frac{1}{2L}\int_{-L}^{L} e^{in\pi x/L} e^{-im\pi x/L} dx = \delta_{mn} \qquad (10)$$

yielding

$$a_n = \frac{1}{2L}\int_{-L}^{L} f(x) e^{-in\pi x/L} dx \qquad (11)$$

Fourier transforms - continuous

In the previous section, n takes on discrete values because of the periodicity of the system. Let's define a wavevector k from n which recognizes the periodic length through

$$k \equiv \pi n / L, \qquad (12)$$

where k has units of inverse length. Now, we can make the spacing between successive values of k smaller by increasing the repeat distance L. In other words, the more we wish to examine a "isolated" object, the larger we must make L, which we will do in a moment for an isolated wave packet. As the separation between successive k's decreases, the sum in Eq. (9) looks ever more like an integral. To make sure we have the correct density of states when taking the sum to an integral, we follow the same procedure as Appendix A of Gasiorowicz. First, multiply Eq. (9) by Δn, which equals one, as well as L/π and its inverse:

$$f(x) = \frac{L}{\pi}\sum_n a_n e^{in\pi x/L} \frac{\pi \Delta n}{L} \qquad (13)$$

From Eq. (7),

$$\Delta k \equiv (\pi/L)\,\Delta n \qquad (14)$$

so (13) is

$$f(x) = \sum_n \left(\frac{L}{\pi} a_n \right) e^{ikx} \Delta k \, . \qquad (15)$$

Lastly, we define a k-dependent function $A(k)$ as the continuous analog of the discrete coefficients a_n through

$$A(k) / (2\pi)^{1/2} \equiv L a_n / \pi \qquad (16)$$

which converts Eq. (15) to

$$f(x) = \Sigma_{n=-\infty}^{+\infty} A(k) \exp(ikx) \, \Delta k / (2\pi)^{1/2}.$$

The $(2\pi)^{1/2}$ in Eq. (16) is just a normalization constant, which can be chosen arbitrarily. Now that we have Δk appearing explicitly in the summation, we can just go over to the continuum limit with

$$f(x) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} A(k) \exp(ikx) \, dk. \qquad (17)$$

This is now a Fourier integral, instead of a Fourier series. To recover an expression for $A(k)$, we invert as usual by multiplying each side by $\exp(-iqx)$ and integrating:

$$\int_{-\infty}^{+\infty} f(x) \exp(-iqx) \, dx = (2\pi)^{-1/2} \int_{x=-\infty}^{+\infty} \int_{k=-\infty}^{+\infty} A(k) \exp(ikx) \exp(-iqx) \, dx \, dk.$$

The integral *over x* of the two exponentials gives a delta-function, with the normalization (see Appendix A of Gasiorowicz)

$$\int_{x=-\infty}^{+\infty} \exp(ikx) \exp(-iqx) \, dx = 2\pi \, \delta(k-q) \qquad (18)$$

Placing this into the integral *over k* in the previous line yields

$$\int_{-\infty}^{+\infty} f(x) \exp(-iqx) \, dx = 2\pi \bullet (2\pi)^{-1/2} \int_{k=-\infty}^{+\infty} A(k) \, \delta(k-q) \, dk$$

or

$$\int_{-\infty}^{+\infty} f(x) \exp(-iqx) \, dx = (2\pi)^{1/2} A(q)$$

$$A(k) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} f(x) \exp(-ikx) \, dx. \qquad (19)$$