Quantum Mechanics
Day 8

Today
I. Last Time
II. Refresher on Linearity
III. Fourier's Trick
IV. Hilbert Spaces

I. Last Time

- We introduced the idea that a function could be decomposed as a sum over basis *functions*

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n}{L}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi n}{L}x\right).$$

- Following Dirac we introduced a 'vector notation for functions'

  $|g\rangle = g(x)$ thought of as a vector

  $\langle f| =$ the transpose conjugate of $f(x)$ thought of as a 'dual' vector $= f^*(x)$.

- We defined an 'inner product' of functions

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)dx.$$

- Finally, we studied the 'Fourier basis' for functions and showed

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| \cos\left(\frac{2\pi n}{L}x\right)\right\rangle = \frac{L}{2}\delta_{mn}.$$

II. Refresher on Linearity

Recall that we call an operator M, any operator of any sort, *linear* if it distributes over sums and if constants pull through it. For example, if M is a matrix acting on a linear combination of vectors, we have

$$M(\alpha\vec{v} + \beta\vec{w}) = \alpha M\vec{v} + \beta M\vec{w}.$$

To check if a given operator is linear, you check if it satisfies this equality and your are good to go.

III. Fourier's Trick

The entire logic that we have pursued in this discussion is pushing us towards a single idea. We will, perhaps a bit idiosyncratically, call this idea Fourier's trick. The idea of Fourier's trick is to see if we can mimic the vector dot product method for extracting components in the context of functions. So, we first imagine, as we did above, that we can write

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n}{L}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi n}{L}x\right).$$

We want to find the coefficients a_0, a_n, and b_n that will make this a true equality. To that end we try computing

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| f(x) \right\rangle.$$

Because integration is a linear operation, we can distribute the inner product over sums and pull constants out front

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| f(x) \right\rangle = \left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n}{L}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi n}{L}x\right) \right\rangle$$
$$= \frac{1}{2}a_0 \left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| 1 \right\rangle + \sum_{n=1}^{\infty} a_n \left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| \cos\left(\frac{2\pi n}{L}x\right) \right\rangle + \sum_{n=1}^{\infty} b_n \left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| \sin\left(\frac{2\pi n}{L}x\right) \right\rangle.$$

I leave it to you to check that:

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| 1 \right\rangle = \delta_{m0} L$$

and

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| \sin\left(\frac{2\pi n}{L}x\right) \right\rangle = 0, \qquad \text{for all } m \text{ and } n.$$

If we take these two equalities for granted and assume we are interested in $m \neq 0$ for the moment , then we've shown that

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| f(x) \right\rangle = \sum_{n=1}^{\infty} a_n \left\langle \cos\left(\frac{2\pi m}{L}x\right) \middle| \cos\left(\frac{2\pi n}{L}x\right) \right\rangle$$
$$= \sum_{n=0}^{\infty} a_n \frac{L}{2} \delta_{mn}.$$

Now—and here is the magic of the Kronecker delta—if we sum over one of the indices of a Kronecker delta we *always* only pull out one element of the sum. Why? Well, it's because whenever $n \neq m$ the δ_{mn} is zero, and hence we're adding up (a whole bunch) of zeros, which is zero. But, when $n = m$ then $\delta_{mm} = 1$ and that single term is the value of the whole sum. In our present case we have

$$\sum_{n=1}^{\infty} a_n \frac{L}{2} \delta_{mn} = a_m \frac{L}{2}.$$

We love to see Kronecker deltas in a sum, it means we are going to have to do no work, only a little thinking, to evaluate the entire sum.

An example might help. Suppose we are considering the specific case $m = 3$, then

$$\left\langle \cos\left(\frac{2\pi \cdot 3}{L}x\right) \middle| f(x) \right\rangle = \sum_{n=1}^{\infty} a_n \frac{L}{2} \delta_{3n},$$

and all the terms of this sum vanish, except when $n = 3$, where we get

$$\begin{aligned}\left\langle \cos\left(\frac{2\pi \cdot 3}{L}x\right) \,\middle|\, f(x) \right\rangle &= \sum_{n=1}^{\infty} a_n \frac{L}{2}\delta_{3n}, \\ &= 0 + 0 + a_3\frac{L}{2}\delta_{33} + 0 + 0 + \cdots \\ &= a_3\frac{L}{2}.\end{aligned}$$

Leveraging an orthonormal basis in this way is what we call Fourier's trick.

Putting all these insights together, we see that we now have a way to extract the function's coefficients

$$\begin{aligned}a_3 &= \frac{2}{L}\left\langle \cos\left(\frac{2\pi \cdot 3}{L}x\right) \,\middle|\, f(x) \right\rangle \\ &= \frac{2}{L}\int_0^L \cos\left(\frac{2\pi \cdot 3}{L}x\right) f(x)\, dx.\end{aligned}$$

If we know what function $f(x)$ is, we can now compute the right-hand side and find a_3. Or, much more generally,

$$\begin{aligned}a_n &= \frac{2}{L}\left\langle \cos\left(\frac{2\pi n}{L}x\right) \,\middle|\, f(x) \right\rangle \\ &= \frac{2}{L}\int_0^L \cos\left(\frac{2\pi n}{L}x\right) f(x)\, dx, \qquad \text{for } n = 0, 1, 2, 3, \ldots.\end{aligned}$$

Hopefully you will practice all of the techniques outlined above to show that

$$\begin{aligned}b_n &= \frac{2}{L}\left\langle \sin\left(\frac{2\pi n}{L}x\right) \,\middle|\, f(x) \right\rangle \\ &= \frac{2}{L}\int_0^L \sin\left(\frac{2\pi n}{L}x\right) f(x)\, dx, \qquad \text{for } n = 1, 2, 3, \ldots.\end{aligned}$$

We have successfully defined an inner product. Indeed we have already seen ways in which it is useful for defining orthonormal bases of functions, e.g.

$$\left\langle \cos\left(\frac{2\pi m}{L}x\right) \,\middle|\, \cos\left(\frac{2\pi n}{L}x\right) \right\rangle = \frac{L}{2}\delta_{mn},$$

and for extracting Fourier coefficients, as in the two formulas above. It is also immensely useful conceptually and helps us to define the function spaces we are going to be working on.

IV. Hilbert Spaces

The set of all sufficiently well-behaved complex-valued functions on the real line {f(x)} is a vector space. You can check this by confirming that, e.g.,

$$z[f(x) + g(x)] = zf(x) + zg(x),$$

where $z \in \mathbb{C}$ and so on for all the other vector space axioms.

A key point, however, is that we are not interested in all sufficiently well-behaved functions. We want these functions to represent wave functions, $\Psi(x,t)$, and hence to be normalizable

$$\int_a^b |\Psi(x,t)|^2 dx = 1.$$

A *Hilbert space* is a vector space of functions equipped with an inner product whose members are functions that are *square integrable*, that is, they have finite values for their norms

$$\int_{-\infty}^{\infty} |f(x)|^2 dx < \infty.$$

Most often in the coming days we will work with Hilbert spaces defined on either the whole real line or on a segment of it and these Hilbert spaces are often written as $L^2(\mathbb{R})$ and $L^2([a,b])$ respectively. In shorthand notation

$$\mathscr{H} = L^2([a,b]) = \{\text{space of all functions } f(x) \text{ s.t. } \int_a^b |f(x)|^2 dx < \infty\},$$

and similarly for $L^2(\mathbb{R})$. The superscript 2 in these definitions is intended to make you think of the '2-norm' that we started out the course with!

There is one more important facet to Hilbert spaces. A set of functions $\{f_n(x)\}_{n=0}^{\infty}$ (or Hilbert space $\mathscr{H}$) is *complete* if any function $f(x) \in \mathscr{H}$ can be written in the form

$$f(x) = \sum_{n=0}^{\infty} c_n f_n(x).$$

In general the constants c_n are complex and Fourier's trick,

$$c_n = \langle f_n | f \rangle,$$

works if the set $\{f_n\}$ is orthonormal. When we say that some set of functions forms an Hilbert space $\mathscr{H}$ we are also saying that those functions are complete. When you can prove this, it is sometimes called Dirichlet's Theorem, see e.g. Boas, but we will mostly be leaving such proofs to mathematicians and just assume this property.

Let's briefly explore an example with complex c_n. Euler's famous identity

$$e^{i\theta} = \cos\theta + i \sin\theta$$

allows us to write the Fourier series we found above in a much more compact form. Write

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i\frac{2\pi n}{L}x}$$

and expand the exponential using Euler's identity, then

$$\begin{aligned} f(x) &= \sum_{n=-\infty}^{\infty} c_n \left[\cos\left(\frac{2\pi n}{L}x\right) + i\sin\left(\frac{2\pi n}{L}x\right)\right] \\ &= \sum_{n=1}^{\infty} c_{-n} \left[\cos\left(\frac{2\pi n}{L}x\right) - i\sin\left(\frac{2\pi n}{L}x\right)\right] + \sum_{n=0}^{\infty} c_n \left[\cos\left(\frac{2\pi n}{L}x\right) + i\sin\left(\frac{2\pi n}{L}x\right)\right] \\ &= c_0 + \sum_{n=1}^{\infty} (c_{-n} + c_n)\cos\left(\frac{2\pi n}{L}x\right) + \sum_{n=1}^{\infty} i(c_n - c_{-n})\sin\left(\frac{2\pi n}{L}x\right). \end{aligned}$$

Apparently this is equivalent to the standard Fourier series with coefficients

$$\begin{aligned} a_0 &= 2c_0, \\ a_n &= (c_{-n} + c_n) \\ b_n &= i(c_n - c_{-n}). \end{aligned}$$

You should check, using the appropriate Fourier's trick, that the a_n and b_n that arise from these definitions are always real. It's very cool how it all fits together so cleanly!