Quantum Mechanics
Day 7

Today

I. Last Time

- We discussed Schrödinger's insight that the dimensionless classical action
$$\frac{1}{\hbar}S = \frac{1}{\hbar}\int_{t_i}^{t_f}(p\dot{x} - H)dt$$
could be viewed as a phase function for a wave theory of matter particles and how this leads to
$$p = \frac{h}{\lambda} \qquad \text{de Broglie's relation,}$$
and Einstein's relation
$$E = \hbar\omega = h\nu.$$

- This led into introducing a plane matter wave
$$\Psi_{\text{plane}}(x,t) = Re^{\frac{1}{\hbar}S},$$
where R is an amplitude and the exponent is again the classical action function.

- We were then able to see that conservation of energy could be expressed as an equation relating operators acting on these matter waves. This gave Schrödinger's equation
$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi.}$$

II. Functions as Vectors?!

I don't need to convince you of the utility of the idea of a vector—you've seen it. You also know the power of choosing a basis: once you've chosen a basis *any* vector an be decomposed as a linear combination of your basis vectors. For example, in the vector space $\mathbb{R}^2$ we might choose the basis $\{\hat{x}, \hat{y}\}$ and decompose

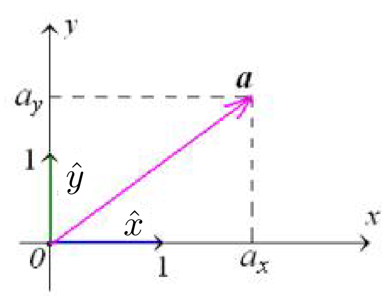

Figure 1: Decomposition of a vector **a** into its components in a basis.

$$\vec{a} = a_x\hat{x} + a_y\hat{y}.$$

We've already been using these ideas in our matrix computations, where we've been writing this same basis as

$$\hat{x} = \begin{pmatrix}1\\0\end{pmatrix} \qquad \text{and} \qquad \hat{y} = \begin{pmatrix}0\\1\end{pmatrix}.$$

In much of this course we are going to focus on wave functions $\Psi(x,t)$. Is there an analogous set of tools for *functions*? Can we decompose a function into pieces? Can we introduce sets of functions that act as a basis for all functions? If we could do this, what would it require? Certainly it won't be the same tool as in the 2D example above. What specifically will be different? Remarkably, we can implement these ideas with functions $f(x)$.

Suppose $f(x)$ is a periodic function with period L, then we can write

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

Here the *infinite* collection of functions

$$\cos\left(\frac{2\pi n}{L}x\right) \qquad n = 0, 1, 2, 3, \ldots,$$

and

$$\sin\left(\frac{2\pi n}{L}x\right) \qquad n = 1, 2, 3, \ldots,$$

are acting as a basis for the periodic function $f(x)$. Notice that we include $n = 0$ in the first set to allow for the possibility of a constant term in the expansion. (See if you can spot why the a_0 term is multiplied by $1/2$ as we proceed. Including $n = 0$ in the sine series does nothing, since $\sin(0) = 0$). Also note that once again we have a wave number $k_n = 2\pi n/L$ that makes the units in the arguments of our basis functions make sense. This way of writing $f(x)$ is called its Fourier series.

III. The Components of a Function

If I give you a function $f(x)$, how do you extract the constant 'component' coefficients a_n and b_n? Answering this question is a central goal for our entire course. If we can figure out a way to do this, we will be able to solve a whole host of practical problems in quantum theory.

Notice that even though we don't always think about it this way, that we do have an algorithm for doing this in the familiar vector case. Given the vector $\vec{a}$, I can extract its x-component by computing

$$a_x = \hat{x} \cdot \vec{a},$$

and similarly

$$a_y = \hat{y} \cdot \vec{a}.$$

Why does this work? Well, it's because $\{\hat{x}, \hat{y}\}$ is an 'orthonormal' basis. Let's break this jargon down. The 'ortho' part refers to the fact that the basis is orthogonal, that is, $\hat{x} \cdot \hat{y} = 0$. The 'normal' part refers to the fact that the basis is normalized, that is, for both $\hat{x}$ and $\hat{y}$ we have $\hat{x}\cdot\hat{x}=\hat{y}\cdot\hat{y}=1$. These properties of the basis allow us to expand

$$\hat{x}\cdot\vec{a}=\hat{x}\cdot(a_x\hat{x}+a_y\hat{y})=a_x(\hat{x}\cdot\hat{x})+a_y(\hat{x}\cdot\hat{y})=a_x.$$

If we want to generalize these ideas, the first thing we are going to need is an 'inner product', that is, a continuum generalization of the dot product used above. To signify that we are thinking of functions, say $f(x)$ and $g(x)$, as a special kind of vector we introduce a new notation, the Dirac 'bra-ket' notation (this name is supposed make you think of a *bracket*): we write $g(x)$ as a 'ket' that is as $g(x)\rightsquigarrow|g\rangle$. We also write the transpose-conjugate of $f(x)$ as $f^*(x)\rightsquigarrow\langle f|$. (Notice that the transpose does nothing to the function, as at any particular x it is just a number; I only mention it here because it will come up when we return to matrix mechanics.)

With this notation in place, we introduce the inner product

$$\langle f|g\rangle\equiv\int_a^b f^*(x)g(x)dx,$$

and, as usual, the juxtaposition of the two functions on the right just indicates multiplication. With this definition we can now ask if two *functions* are orthogonal; let's try $\cos\left(\frac{2\pi}{L}x\right)$ and $\cos\left(\frac{2\pi(2)}{L}x\right)$ over the full region of periodicity $[0,L]$,

$$\begin{aligned}\left\langle\cos\left(\frac{2\pi}{L}x\right)\Big|\cos\left(\frac{4\pi}{L}x\right)\right\rangle&=\int_0^L\cos\left(\frac{2\pi}{L}x\right)\cos\left(\frac{4\pi}{L}x\right)dx\\&=\frac{1}{2}\int_0^L\left[\cos\left(\frac{2\pi}{L}x+\frac{4\pi}{L}x\right)+\cos\left(\frac{2\pi}{L}x-\frac{4\pi}{L}x\right)\right]dx\\&=0,\end{aligned}$$

where the last equality follows from the fact that we are integrating cosine functions that go through an integer number of periods in the region $x\in[0,L]$, and the integral of a cosine over a full period is zero. Generalizing this example, you will find that for all $m\neq n$

$$\left\langle\cos\left(\frac{2\pi m}{L}x\right)\Big|\cos\left(\frac{2\pi n}{L}x\right)\right\rangle=0.$$

Apparently the cosine functions with wave numbers k_n determined by the integers n are all orthogonal! This is starting to look like a promising basis. What about the case where $m=n$? Let's try $m=n=1$, so that

$$\begin{aligned}\left\langle\cos\left(\frac{2\pi}{L}x\right)\Big|\cos\left(\frac{2\pi}{L}x\right)\right\rangle&=\int_0^L\cos\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}x\right)dx\\&=\frac{1}{2}\int_0^L\left[\cos\left(\frac{2\pi}{L}x+\frac{2\pi}{L}x\right)+\cos\left(\frac{2\pi}{L}x-\frac{2\pi}{L}x\right)\right]dx\\&=0+\frac{1}{2}\int_0^L 1dx=\frac{L}{2}.\end{aligned}$$

Again, it's a good exercise to check that this computation yields the same result for all $m = n$. Apparently, these functions aren't normalized. But, that's not a big deal, you've been practicing normalizing functions on the homework. All we need to do to get a normalized basis of functions is to change the set of functions we're working with

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

Now, notice that were you do the exercises I mention above you would arrive at an infinite collection of results, one for each value of m and n. It is very convenient to introduce a shorthand notation that summarizes all of these result. Define

$$\delta_{mn} \equiv \begin{cases} 0 & \text{if } m \neq n, \\ 1 & \text{if } m = n, \end{cases}$$

this symbol is known as the Kronecker delta and is a very efficient way to summarize orthonormality. For example, we have just argued

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

For most of the course we will prefer to work with this and other normalized bases. However, for just the remainder of today and next time we will continue working with the unnormalized basis

$$\cos\left(\frac{2\pi n}{L}x\right).$$

The only reason for this is that it is what people conventionally do in the context of Fourier series.