5.3: Operators and Observables

Quantum State Information

Something we discussed only obliquely in an earlier section is the idea of a quantum state and the information contained within it. There are some very strange features associated with the concept of a quantum state. High among those it the fact that it is *non-local*. We are used to the classical notion that the mass, charge, and other features of a particle are located *at the particle* – we can literally point to the point to the position in space where these quantities can be found. But now we have to accept the fact that even the location of the particle itself is not something that is well-defined. The wave function of a particle exists everywhere in space at the same time, and it isn't until it interacts with a measuring device that its location is defined. To emphasize this point: It isn't that the particle is somewhere but we just don't know where (like the result of a coin flip still concealed by someone's hand), it actually not located anywhere until it is observed.

All of this mysterious mumbo-jumbo might tempt us to throw up our hands in despair that we can't do any of the predictive science that we've become accustomed to in classical physics, but the quantum state of a particle *does* contain useful information about it. Indeed, the theory claims that the quantum state contains *all* of the accessible information about the particle. Much of it is probabilistic, but this is still useful. We have already discussed a bit about how to extract this information from the quantum state – we take averages using the probability density. We have slightly oversimplified this process, but we will correct that now.

Expectation Value Computation

The key to pulling information from the quantum state is calculating expectation values. Even when we want to compute uncertainties, to do this we need to be able to compute averages. So far, we have seen that the method for doing this is to multiply the quantities measured by their associated probability densities, and integrate over all the possible values. For example, if we wish to calculate the average position:

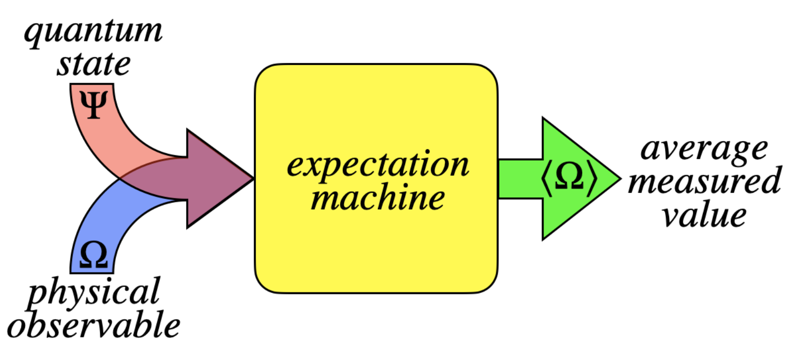
$$\langle x\rangle = \int\limits_{-\infty}^{+\infty} \mathcal{P}(x)\; x\;dx = \int\limits_{-\infty}^{+\infty} |\Psi|^2\; x\;dx = \int\limits_{-\infty}^{+\infty} \Psi^*\Psi\; x\;dx \tag{5.3.1}$$

If we instead which to calculate the average momentum, we can Fourier-transform the position wave function to get the momentum version, and use it in the integral along with a k and dk in place of x and dx (this will give an average wave number, which can then be multiplied by $\hbar$ to get an average momentum). Notice that in the momentum case we can't use the usual $\mathcal{P}(x)$, because the momentum values are not a function of x. Lucky that we have the Fourier transform! But what if there are other observable quantities for which we wish to compute an average (energy, angular momentum, etc.)?

Quantum mechanics provides an alternate means that is totally equivalent to the one above for position and momentum, without the need for a Fourier transform, and which works for other quantities. What is more, this process for computing averages embodies the idea that measurements affect the very quantum state they seek to measure. We'll start with a basic description for how this works...

We begin with two things: The quantum state we are working with, and the observable whose the expectation value we wish to compute. We throw these both into a machine, which in turn spits out the expectation value:

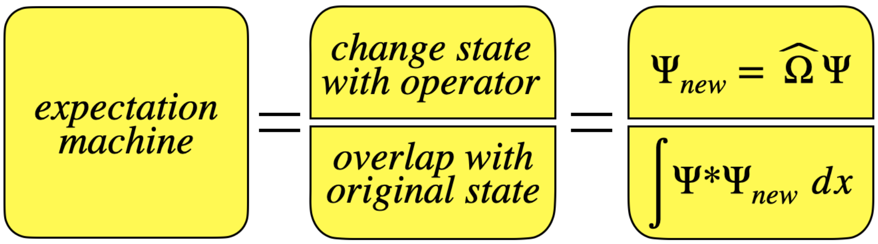
Figure 5.3.1 – Expectation Value Machine



Well, this is just fine, but of course we need to peek behind the curtain to see precisely how this expectation machine functions. It works in a few steps:

1. It invents an *operator* that belongs to the given observable. It is one of the postulates of quantum theory that every quantity that can be measured and is stored in a quantum state has an associated operator.
2. The operator "acts upon" the state, changing it into a new state. This is the part of the process where the observation of a physical property of a particle alters the state of the particle being observed.
3. The "overlap integral" of new state and the original state is computed. As we have said before, the integral of the product of two functions is like a dot product (e.g. odd functions are "orthogonal" to even functions, as their overlap integral is zero). So this overlap integral gives us a sense of how far the wave function has been altered from its original one.

Figure 5.3.2 – Machine Inner Workings



It's probably not immediately clear how this process gives us the average value we wish to compute, so let's look a bit closer.

The Position and Momentum Operators

Let's look first at the simple case of $\langle x\rangle$. In this case, the "new state" has a wave function for position that is simply the product of x and the previous wave function:

$$\Psi_{new} = x\,\Psi \quad \Rightarrow \quad \langle x\rangle = \int\limits_{-\infty}^{+\infty} \Psi^*\Psi_{new} dx = \int\limits_{-\infty}^{+\infty} \Psi^*\left(x\,\Psi\right)dx = \int\limits_{-\infty}^{+\infty} x\left|\Psi\right|^2 dx = \int\limits_{-\infty}^{+\infty} x\,\mathcal{P}\left(x\right)dx \tag{5.3.2}$$

If we now wish to do the same with momentum, it is not clear how the momentum operator creates a new quantum state from the old one, when we describe that quantum state in terms of position. We *do* know how it changes the quantum state when it is described in terms of momentum (or wave number) – it works the same way as x did:

$$\Phi_{new} = p\,\Phi \quad \Rightarrow \quad \langle p\rangle = \int\limits_{-\infty}^{+\infty} \Phi^*\Phi_{new} dk = \int\limits_{-\infty}^{+\infty} \Phi^*\left(p\,\Phi\right)dk = \int\limits_{-\infty}^{+\infty} p\left|\Phi\right|^2 dk = \int\limits_{-\infty}^{+\infty} p\,\mathcal{P}\left(k\right)dk \tag{5.3.3}$$

But now we are interested in how the momentum affects the quantum state *when the wave function is viewed in terms of position*. To do this, we turn to our "translation" device - the Fourier transform. Noting that $\Phi_{new} = p\Phi$, we can do an inverse Fourier transform to get both the original wave function Ψ and the newly-altered function Ψ_{new}:

$$\Psi = \int\limits_{-\infty}^{+\infty} \Phi\; e^{ikx} dk\;, \quad \Psi_{new} = \int\limits_{-\infty}^{+\infty} \Phi_{new}\; e^{ikx} dk = \int\limits_{-\infty}^{+\infty} p\;\Phi\; e^{ikx} dk = \int\limits_{-\infty}^{+\infty} \hbar k\;\Phi\; e^{ikx} dk \tag{5.3.4}$$

Now we seek some operation we can perform on Ψ that can give us Ψ_{new}. Without further ado, we declare that if we act on Ψ with the operation $-i\hbar\frac{d}{dx}$, that will do the trick. The wave function Φ is only a function of k (not x), so:

$$\Psi_{new} = -i\hbar\frac{d}{dx}\Psi = -i\hbar\frac{d}{dx}\int\limits_{-\infty}^{+\infty} \Phi\; e^{ikx} dk = -i\hbar\int\limits_{-\infty}^{+\infty} \Phi\;\frac{d}{dx} e^{ikx} dk = \int\limits_{-\infty}^{+\infty} \hbar k\;\Phi\; e^{ikx} dk \tag{5.3.5}$$

To summarize, the x-direction momentum operator for use on wave functions expressed in terms of position is (when we eventually go beyond 1-dimension, this will become a partial derivative):

$$\hat{p}_x = -i\hbar\frac{d}{dx} \tag{5.3.6}$$

The little "hat" above the p is a reminder to us that we are talking about an operator that changes a quantum state, and not just the value of momentum. What this operator actually is depends upon the type of wave function it is acting on. That is:

$$\hat{p}_x\,\psi(x) = -i\hbar\frac{d}{dx}\psi(x)\;, \quad \hat{p}_x\,\phi(k) = \hbar k\,\phi(k) \tag{5.3.7}$$

Similarly, the operator $\widehat{x}$ is just the function $f(x) = x$ when acting on a wave function expressed in terms of position, and will involve a derivative when acting on a wave function expressed in terms of wave number (it is left as an exercise o the reader to determine the operator $\widehat{x}$ that acts on $\phi(k)$).

Going back to the original discussion of computing expectation values, we see that we have:

$$\langle p\rangle = \int\limits_{-\infty}^{+\infty}\Psi^*\left(\hat{p}\;\Psi\right)dx = \int\limits_{-\infty}^{+\infty}\Psi^*\left(-i\hbar\frac{d}{dx}\Psi\right)dx \tag{5.3.8}$$

Building More Operators

We can build new operators for other physical observables from $\widehat{x}$ and $\hat{p}$. Most notable among these is the kinetic energy operator:

$$\widehat{KE} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{5.3.9}$$

This looks familiar! It is precisely what acts on the wave function in the Schrödinger equation, which we already said accounts for the particle's kinetic energy. Now we see the Schrödinger equation in a whole new light – as an equation that relates the effects of operators. The potential $V(x)$ is just a function of x, so it is an operator formed from $\widehat{x}$. Together, the operators $\widehat{KE}$ and $\widehat{V(x)}$ account for the total energy, and as a shorthand we sometimes use:

$$\widehat{H} \equiv \widehat{KE} + \widehat{V(x)} \tag{5.3.10}$$

This "total energy operator" is commonly referred to as the *Hamiltonian*. Note that Schrödinger's equation states that the Hamiltonian's actions in on the wave function expressed in terms of position are equivalent to another operator's actions. The other operator (sometimes called the "total energy operator") is what we see on the right hand side of the Schrödinger equation:

$$\widehat{E} \equiv i\hbar\frac{\partial}{\partial t} \tag{5.3.11}$$

Uncertainty Principle

We have already seen that measurements of position and momentum are "incompatible" in that the measurement of one affects the measurement of the other – the more we take care to precisely one of them, the less able we are to measure the other. This comes through very clearly with this idea that operators change quantum states into new states. We would expect that the alteration of the state by one of these two operators will have an effect on the measurement of the expectation for the other, and it does. Suppose, for example, that for whatever reason, we wish to know the expectation value of the product of the position and momentum, xp. We follow our "expectation machine" method, but since we now have two operators, we have to do them in sequence – first change the quantum state by one of the operators, and then by the other. If we use the momentum operator first, we get:

$$\Psi_{new} = \widehat{x}\;\left(\hat{p}\;\Psi\right) = x\;\left(-i\hbar\frac{d}{dx}\Psi\right) = -i\hbar x\;\frac{d\Psi}{dx} \tag{5.3.12}$$

But if we perform the operation in the other order, we get a different result:

$$\Psi_{new} = \hat{p}\;\left(\widehat{x}\;\Psi\right) = -i\hbar\frac{d}{dx}\left(x\Psi\right) = -i\hbar\left(\Psi + x\;\frac{d\Psi}{dx}\right) \tag{5.3.13}$$

This effect of two operators "tripping over each other" is directly related to an uncertainty principle between those two operators – changing the state by one of them affects the measurement of the other. When two operators do not acheive the same result when performed in either order, we say that that do not *commute* with each other. Note that any function of $\widehat{x}$ (like $\widehat{V}(x)$) will commute with any other function of $\widehat{x}$, and any function of $\hat{p}$ (like $\widehat{KE}$) will commute with any other function of $\hat{p}$. So measuring the momentum will not have an effect on measuring the kinetic energy.