Interpretation of various parts of the 1DTISWE

(This is for 1D: Later, I’ll generalize the results for 3D)

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=-E\psi$$

Let’s consider potential free regions of space. Then:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$$

The result of the **operation** of $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2}$ upon the wave function is to produce an energy.

Let me show this for the case of the infinite square well. We had the wave functions:

$$\varphi=\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{n\pi x}{L}\right);n=1,2,\ldots$$

Application of that operator on the wave function gives:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}=-\frac{\hbar^2}{2m}\left[-\frac{n^2\pi^2}{L^2}\right]\varphi=n^2\frac{\hbar^2\pi^2}{2mL^2}\varphi=n^2E_1\varphi$$

It is for this reason that we call $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2}$ the energy operator.

I’ll invent a new symbol to represent an operator. The kinetic energy operator is thus given by:

$$\tilde{K}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

and it’s operation upon the wave function is to produce the kinetic energy.

The total energy operator is quite similar to this:

$$\tilde{E}=\tilde{K}+\tilde{V}$$

where the potential energy in the simplest of situations is a multiplication.

Now, we also know that the operator actually involves momentum:

Remember: $KE=\frac{P^2}{2m}$

It is useful to consider a method of writing the energy operator in terms of the momentum.

You can experiment with various forms … but I’d recommend trying this form:

$$-i\hbar\frac{\partial}{\partial x}\equiv\tilde{P}$$

Let me show you that this gives the kinetic energy operator:

$$\frac{\tilde{P}^2}{2m}=\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)$$

Now, you’re not at all used to seeing such a thing without a function that it operates on. Here is the secret to playing with operator mathematics: put a function in to get the manipulations right, and then take it out to show the results.

Try it on this function: Ξ

$$\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\Xi=\frac{i^2\hbar^2}{2m}\frac{\partial}{\partial x}\left[\frac{\partial\Xi}{\partial x}\right]=-\frac{\hbar^2}{2m}\frac{\partial^2\Xi}{\partial x^2}\Rightarrow\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

This is one subtle bit of mathematics, actually! When working with operators, you can see that this is true: (you’ve just seen that this is true)

$$\left(\frac{\partial}{\partial x}\right)^2=\frac{\partial^2}{\partial x^2}$$

We thus say that the momentum operator in 1D QM is thus given by:

$$\tilde{P} = -i\hbar\frac{\partial}{\partial x}$$

There is one more operator in QM that is of immediate need. This is the position operator, x. Without proof, I'll simply state that the position operator is simply multiplication by x. (These are not all the operators that you can define)

Operator	Symbol	Operation
Kinetic Energy	$\tilde{K}$	$\tilde{K} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$
Potential Energy	$\tilde{V}$	V (sometimes more)
Total Energy	$\tilde{E}$	$\tilde{E} = \tilde{K} + \tilde{V}$
Momentum	$\tilde{P}$	$\tilde{P} = -i\hbar\frac{\partial}{\partial x}$
Position	$\tilde{X}$	x

You might imagine that we could get a time operator. I'll get that as needed. Right now, we don't need it.

Now, each of these operators must produce a real result from operation on a wave function. This is extremely important to remember. These quantities are called "observables" and they must therefore be real.

This has some other important implications that we will not go into at the present time.

Let me show you now how to obtain the value of an observable.

Expectation Values

We have a very special short-hand notation to represent the expectation of an observable. The operation is relatively straight forward to do. Let me show you an example.

Calculate the expectation value of x a general square well eigenstate.

The mathematical operation required here is this:

$$\langle A \rangle = \int_{\substack{\text{all}\\\text{space}}} \varphi^*(x)\tilde{A}\varphi(x)\,dx$$

That is how it is done for a general operator A. The expectation value is basically the probabilistic average value. We're just using operators here to calculate it.

Ok, let me show you how to calculate the expectation value of x:

$$\langle x \rangle = \int_{x=0}^{x=L} \varphi^* x \varphi\,dx \equiv \langle \varphi | x | \varphi \rangle$$

Notice that short-hand symbol that I've introduced. This is called the "bra – ket" notation and is quite prevalent throughout QM.

For the square well, we have the eigenfunctions:

$$\varphi = \sqrt{\tfrac{2}{L}}\sin\left(\tfrac{n\pi x}{L}\right); n = 1, 2, \ldots$$

Thus, to calculate the expectation value, we do this:

$$\left\langle x \right\rangle = \tfrac{2}{L}\int\limits_{x=0}^{x=L} x \sin^2\left(\tfrac{n\pi x}{L}\right) dx$$

Then you enter x*Sin[b*x]*Sin[b*x] into the integrator.

The result is:

$$\left\langle x \right\rangle = \tfrac{2}{L}\left[\frac{x^2}{4} - \frac{\cos(2bx)}{8b^2} - \frac{x\sin(2bx)}{4b}\right]_{x=0}^{x=L}$$

I've used the obvious replacement for b, let me now put it back like it was:

$$\left\langle x \right\rangle = \tfrac{2}{L}\left[\frac{x^2}{4} - \frac{\cos\left(2\frac{n\pi}{L}x\right)}{8\left(\frac{n\pi}{L}\right)^2} - \frac{x\sin\left(2\frac{n\pi}{L}x\right)}{4\frac{n\pi}{L}}\right]_{x=0}^{x=L}$$

Now I'll evaluate the limits:

$$\left\langle x \right\rangle = \tfrac{2}{L}\left[\frac{x^2}{4} - \frac{\cos\left(2\frac{n\pi}{L}x\right)}{8\left(\frac{n\pi}{L}\right)^2} - \frac{x\sin\left(2\frac{n\pi}{L}x\right)}{4\frac{n\pi}{L}}\right]_{x=0}^{x=L}$$

$$= \tfrac{2}{L}\left\{\frac{L^2}{4} - \frac{\cos(2n\pi)}{8\left(\frac{n\pi}{L}\right)^2} - \frac{x\sin(2n\pi)}{4\frac{n\pi}{L}} - \frac{1}{8\left(\frac{n\pi}{L}\right)^2}\right\}$$

$$= \tfrac{2}{L}\left\{\frac{L^2}{4} - \frac{1}{8\left(\frac{n\pi}{L}\right)^2} - \frac{1}{8\left(\frac{n\pi}{L}\right)^2}\right\} = \frac{L}{2}$$

Now that you've seen the answer, you have to admit that you're not too surprised that this is the answer.

There's another important quantity to obtain … namely the value of $\left\langle x^2 \right\rangle$

This is gotten in exactly the same way, only different. Watch:

$$\left\langle x^2 \right\rangle = \int\limits_{\substack{\text{all}\\ \text{space}}} \varphi^* x^2 \varphi dx = \left\langle \varphi \middle| x^2 \middle| \varphi \right\rangle$$

In our case, then we have:

$$\left\langle x^2 \right\rangle = \tfrac{2}{L}\int\limits_{x=0}^{x=L} x^2 \sin^2\left(\tfrac{n\pi x}{L}\right) dx$$

This is easy to do via the integrator also:

I entered: x*x*Sin[b*x]*Sin[b*x]

and obtained:

$$\left\langle x^2 \right\rangle = \tfrac{2}{L}\left[\frac{x^3}{6} - \frac{x\cos(2bx)}{4b^2} - \frac{\left(-1+2b^2x^2\right)\sin(2bx)}{8b^3}\right]_{x=0}^{x=L}$$

Now I'm going to make the reverse placement for b:

$$\left\langle x^2 \right\rangle = \tfrac{2}{L}\left[\frac{x^3}{6} - \frac{x\cos\left(2\frac{n\pi}{L}x\right)}{4\left(\frac{n\pi}{L}\right)^2} - \frac{\left(-1+2\left(\frac{n\pi}{L}\right)^2x^2\right)\sin\left(2\left(\frac{n\pi}{L}\right)x\right)}{8\left(\frac{n\pi}{L}\right)^3}\right]_{x=0}^{x=L}$$

$$\left\langle x^2 \right\rangle = \frac{2}{L}\left[\frac{x^3}{6} - \frac{x\cos\left(2\frac{n\pi}{L}x\right)}{4\left(\frac{n\pi}{L}\right)^2} - \frac{\left(-1+2\left(\frac{n\pi}{L}\right)^2 x^2\right)\sin\left(2\left(\frac{n\pi}{L}\right)x\right)}{8\left(\frac{n\pi}{L}\right)^3} \right]\Bigg|_{x=0}^{x=L}$$

$$= \frac{2}{L}\left[\frac{L^3}{6} - \frac{L\cos(2n\pi)}{4\left(\frac{n\pi}{L}\right)^2} - \frac{\left(-1+2\left(\frac{n\pi}{L}\right)^2 L^2\right)\sin(2n\pi)}{8\left(\frac{n\pi}{L}\right)^3} \right] - [0-0-0]$$

$$= \frac{2}{L}\left[\frac{L^3}{6} - \frac{L^3}{4n^2\pi^2} \right] = L^2\left[\frac{1}{3} - \frac{1}{2n^2\pi^2} \right]$$

This result is less intuitive. Don’t let that bother you.
Now we define the uncertainty in an observable as:

$$\Delta x = \sqrt{\left\langle x^2 \right\rangle - \left\langle x \right\rangle^2}$$

Let me show you the uncertainty in x:

$$\Delta x = \sqrt{L^2\left[\frac{1}{3} - \frac{1}{2n^2\pi^2} \right] - \frac{L^2}{4}} = L\sqrt{\frac{1}{3} - \frac{1}{2n^2\pi^2} - \frac{1}{4}} = L\sqrt{\frac{8n^2\pi^2 - 12 - 6n^2\pi^2}{24n^2\pi^2}} = \frac{L}{\sqrt{24}n\pi}\sqrt{2n^2\pi^2 - 12}$$

Now let’s calculate ΔP
Firstly, the expectation value of P is zero because of two reasons:
(1) it is equally likely for the particle to go right as left and
(2) the momentum operator would not produce a real observable here which is absolutely required.

Then to calculate P^2, we have a very easy time:

$$\left\langle P^2 \right\rangle = \left\langle 2mE \right\rangle = 2m\left\langle E \right\rangle = 2m\left(n^2 E_1\right) = 2mn^2 \frac{\pi^2\hbar^2}{2mL^2} = n^2 \frac{\pi^2\hbar^2}{L^2}$$

The uncertainty in the momentum is then given by:

$$\Delta P = \sqrt{\left\langle P^2 \right\rangle - \left\langle P \right\rangle^2} = n\frac{\hbar\pi}{L}$$

Now let’s calculate the value of

$$(\Delta P)(\Delta X) = \left[n\frac{\hbar\pi}{L}\right]\left[\frac{L}{\sqrt{24}n\pi}\sqrt{2n^2\pi^2 - 12}\right] = \frac{\hbar}{\sqrt{24}}\sqrt{2n^2\pi^2 - 12}$$

This uncertainty is smallest for the n=1 state. In this state, we have:

$$(\Delta P)(\Delta X) = \frac{\hbar}{\sqrt{24}}\sqrt{2\pi^2 - 12} = 0.5679\hbar$$

Now, Heisenburg’s uncertainty principle says that the uncertainty is given by:

$$(\Delta P)(\Delta X) \geq \frac{\hbar}{2} = .5\hbar$$

So our result is thus in very nice agreement with Heisenburg’s uncertainty principle!

Of course, this is applied to a very simple problem. You might wonder what the meaning of the uncertainty principle is. It has a very clear meaning: you can not simultaneously measure momentum and position to any level of precision you want to. The exact value of the uncertainty principle comes from application to the tightest wave packet possible, namely the Gaussian wave packet. In this case, we’d get exactly the correct result.

This very principle has extremely important implications for all of physics as we know it. Indeed, if we make a measurement of position, we have as a consequence completely destroyed any hope we might have had of knowing anything about the momentum of the particle, and vice versa. Other relations similar to this involve E,t, and L,θ.

Now if you're ready let me show you a really remarkable property of our operators!

If you're going to measure P and X, you do this with one of the operators we've used above. Let me show you what happens:

$$\tilde{P}\tilde{X} = -i\hbar\left(\tfrac{\partial}{\partial x}\right)x$$

now do you remember what I told you about the way to work with these things? Put a function there to do the calculations and then take it out at the end. Thus:

$$\tilde{P}\tilde{X}\Xi = -i\hbar\left(\tfrac{\partial}{\partial x}\right)x\Xi = -i\hbar\tfrac{\partial(x\Xi)}{\partial x} = -i\hbar\left[\Xi + x\tfrac{\partial\Xi}{\partial x}\right]$$

$$\Rightarrow \tilde{P}\tilde{X} = -i\hbar\left[1 + x\tfrac{\partial}{\partial x}\right]$$

It is easier to calculate this the other way around:

$$\tilde{X}\tilde{P} = -i\hbar x\tfrac{\partial}{\partial x}$$

I'm going to now define something called the commutator:

$$\left[\tilde{X},\tilde{P}\right] \equiv \tilde{X}\tilde{P} - \tilde{P}\tilde{X}$$

This is a valid definition for any two operators, actually. In the case at hand, we have:

$$\left[\tilde{X},\tilde{P}\right] \equiv \tilde{X}\tilde{P} - \tilde{P}\tilde{X} = -i\hbar x\tfrac{\partial}{\partial x} + i\hbar + i\hbar x\tfrac{\partial}{\partial x} = i\hbar$$

This is a very simple result that has very deep consequences ...
Anytime the commutator of two observables is not zero, you can not simultaneously measure the two quantities to any arbitrary degree of certainty!

Not all observables behave like this. Here are some examples of commuting observables:

$$\left[x, x^m\right], [K,P]$$

You notice interestingly enough that the following is true:

$$[X,K] = x\left(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x^2}\right) - \left(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x^2}\right)x$$

$$= x\left(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2\Xi}{\partial x^2}\right) - \left(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x^2}\right)x\Xi = x\left(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2\Xi}{\partial x^2}\right) + \tfrac{\hbar^2}{2m}\tfrac{\partial}{\partial x}\left(\Xi + x\tfrac{\partial\Xi}{\partial x}\right)$$

$$= x\left(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2\Xi}{\partial x^2}\right) + \tfrac{\hbar^2}{2m}\left(\tfrac{\partial\Xi}{\partial x} + \tfrac{\partial\Xi}{\partial x} + x\tfrac{\partial^2\Xi}{\partial x^2}\right) = \tfrac{\hbar^2}{m}\tfrac{\partial}{\partial x}$$

Unsurprisingly, you can't simultaneously measure energy and position. This seems reasonable since you can't simultaneously measure momentum and position. Notice, however, that you can simultaneously measure momentum and energy.