

PROFESSOR: Expectation values of operators. So this is, in a sense, one of our first steps that we're going to take towards the interpretation of quantum mechanics. We've had already that the wave function tells you about probabilities. But that's not quite enough to have the full interpretation of what we're doing. So let's think of operators and expectation values that we can motivate.

So for example, if you have a random variable q , that can take values-- so this could be a coin that can take values heads and tails. It could be a pair of dice that takes many values-- can take values in the set q_1 up to q_n with probabilities p_1 up to p_n , then in statistics, or 8044, you would say that this variable, this random variable has an expectation value. And the expectation value-- denoted by this angular symbols over here, left and right-- it's given by the sum over i , i equal 1 to n , of the possible values the random variable can take times the probabilities. It's a definition that makes sense. And it's thought to be, this expectation value is, the expected value, or average value, that you would obtain if you did the experiment of tossing the random variable many times. For each value of the random variable, you multiply by the probability. And that's the number you expect to get.

So in a quantum system, we follow this analogy very closely. So what do we have in a quantum system? In the quantum system you have that ψ^* of x and t . The x is the probability that the particle is in x , x plus dx . So that's the probability that the particle is going to be found between x and x plus dx . The position of this particle is like a random variable. You never know where you are going to find it. But he has different probabilities to find it.

So we could now define in complete analogy to here, the expectation value of the position operator, or the expectation value of the position, expectation value of \hat{x} , or the position, and say, well, I'm going to do exactly what I have here. I will sum the products of the position times the probability for the position. So I have to do it as an integral. And in this integral, I have to multiply the position times the probability for the position.

So the probability that the disc takes a value of x , basically all that is in the interval dx about x is this quantity. And that's the position that you get when you estimate this probability. So you must sum the values of the random variable times its probability. And that is taken in quantum mechanics to be a definition. We can define the expectation value of x by this quantity.

And what does it mean experimentally? It means that in quantum mechanics, if you have a

system represented by a wave function, you should build many copies of the system, 100 copies of the system. In all of these copies, you measure the position. And you make a table of the values that you measure the position. And you measure them at the same time in the 100 copies. There's an experimentalist on each one, and it measures the position of x . You construct the table, take the average, and that's what this quantity should be telling you.

So this quantity, as you can see, may depend on time. But it does give you the interpretation of expected value coinciding with a system, now the quantum mechanical system, for which the position is not anymore a quantity that is well defined and it's always the same. It's a random variable, and each measurement can give you a different value of the position. Quantum mechanically, this is the expected value. And the interpretation is, again if you measure many times, that is the value, the average value, you will observe.

But now we can do the same thing to understand expectation values. We can do it with the momentum. And this is a little more non-trivial. So we have also, just like we said here, that $\psi^* \psi dx$ is the probability that the particle is in there, you also have that $\phi^* \phi dp$ is the probability to find the particle with momentum in the range p to $p + dp$.

So how do we define the expected value of the momentum? The expected value of the momentum would be given by, again, the sum of the random variable, which is the momentum, times the probability that you get that value. So this is it. It's very analogous to this expression. But it's now with momentum.

Well, this is a pretty nice thing. But we can learn more about it by pushing the analogy more. And you could say, look, this is perfect. But it's all done in momentum space. What would happen if you would try to do this in position space? That is, you know how ψ is related to ψ of x . So write everything in terms of x . I would like to see this formula in terms of x . It would be a very good thing to have. So let's try to do that.

So we have to do a little bit of work here with integrals. So it's not so bad. $\int p \psi^* \psi dx$. And for this one, you have to write it as an integral over some position. So let me call it over position x' . This you will write this an integral over some position x . And then we're going to try to rewrite the whole thing in terms of coordinate space.

So what do we have here? We have $\int p dp$. And the first ψ^* would be the integral over dx' . We said there is the square root $2\pi\hbar$ that we can't forget. ψ , it would have an $e^{ipx'/\hbar}$, and a ψ^* of x' . So I did conjugate this ψ^*

of p . I may have it here. Yes, it's here. I conjugated it and did the integral over x' . And now we have another one, $\int \psi(x') e^{-ipx'/\hbar}$, and you have $\psi(x)$. Now there's a lot of integrals there, and let's try to get them simplified.

So we're going to try to do first the p integral. So let's try to clean up everything in such a way that we have only p done first. So we'll have a $1/2\pi\hbar$ from the two square roots. And I'll have the two integrals $\int dx' \psi(x') \star x \psi(x)$. So again, as we said, these integrals we just wrote them out. They cannot be done. So our only hope is to simplify first the p integral.

So here we would have integral of dp times p times $e^{ipx'/\hbar}$. And $e^{-ipx/\hbar}$. Now we need a little bit of-- probably if you were doing this, it would not be obvious what to do, unless you have some intuition of what the momentum operator used to be. The momentum operator used to be dv_x , basically.

Now this integral would be a delta function if the p was not here. But here is the p . So what I should try to do is get rid of that p in order to understand what we have. So here we'll do integral dp . And look, output here minus \hbar over idv_x . And leave everything here to the right, $e^{ipx'/\hbar} p e^{-ipx/\hbar}$. I claim this is the same. Because this operator, \hbar over $iddx$, well, it doesn't act on x' . But it acts here. And when it does, it will produce just the factor of p that you have. Because the minus i and the minus i will cancel. The \hbar will cancel. And the ddh will just bring down a p . So this is the way to have this work out quite nicely.

Now this thing is inside the integral. But it could as well be outside the integral. It has nothing to do with dp . So I'll rewrite this again. I'll write it as $\int dx' \psi(x') \star \int dx \psi(x)$. And I'll put this here, \hbar over $iddx$, in front of the integral. The $1/2\pi\hbar$ here. $\int dp e^{ipx'/\hbar} p e^{-ipx/\hbar}$. So I simply did a couple of things. I moved that $1/2\pi\hbar$ to the right. And then I said this derivative could be outside the integral. Because it's an integral over p . It doesn't interfere with x derivative, so I took it out.

Now the final two steps, we're almost there. The first step is to say, with this it's a ddx . And yes, this is a function of x and x' . But I don't want to take that derivative. Because I'm going to complicate things. In fact, this is already looking like a delta function. There's a dp . And the \hbar bars that actually would cancel. So this is a perfectly nice delta function. You can change variables. Do p equal u times \hbar and see that actually the \hbar doesn't matter. And

this is just $\delta(x' - x)$. And in here, you could act on the delta function. But you could say, no, let me do integration by parts and act on this one.

When you do integration by parts, you have to worry about the term at the boundary. But if your wave functions vanish sufficiently fast at infinity, there's no problem. So let's assume we're in that case. We will integrate by parts and then do the delta function. So what do we have here? I have $\int dx' \psi^*(x') \int dx \dots$. And now I have, because of the sign of integration by parts, $\int dx' \psi^*(x') \delta(x' - x)$. And then we have the delta function of $x' - x$. It's probably better still to write the integral like this, $\int dx' \psi^*(x') \delta(x' - x)$. And we're almost done, so that's good. We're almost done. We can do the integral over x' . And it will evaluate that wave function at x .

So at the end of the day, what have we found? We found that $\langle p \rangle$, the expectation value of p , equal $\int dx \psi^*(x) (-i\hbar \frac{d}{dx}) \psi(x)$. So we have $\int dx \psi^*(x) (-i\hbar \frac{d}{dx}) \psi(x)$. I'll write it two times, $\int dx \psi^*(x) (-i\hbar \frac{d}{dx}) \psi(x)$ and $\int dx \psi(x) (-i\hbar \frac{d}{dx}) \psi^*(x)$. I'm not sure I carried that times. I didn't put the time anywhere. So maybe I shouldn't put it here yet. This is what we did. And might as well write it in the standard order, where the complex conjugate function appears first.

This is what we found. So this is actually very neat. Let me put the time back everywhere you could put time. Because this is a time dependent thing. So $\langle p \rangle$, expectation value is $\int dx \psi^*(x, t) (-i\hbar \frac{d}{dx}) \psi(x, t)$. And now we have, if you wish, \hat{p} of ψ of x , where \hat{p} is what we used to call the momentum operator.

So look what has happened. We started with this expression for the expectation value of the momentum justified by the probabilistic interpretation of ψ . And we were led to this expression, which is very similar to this one. You see, you have the ψ^* , the ψ , and the x there. But here, the momentum appeared at this position, acting on the wave function ψ , not on ψ^* . And that's the way, in quantum mechanics, people define expectation values of operators in general.

So in general, for an operator q , we'll define the expectation value of q to be $\int dx \psi^*(x, t) q \psi(x, t)$. So you will always do this of putting the operator to act on the second part of the wave function, on the second appearance of the wave function. Not on the ψ^* , but on the ψ .

We can do other examples of this and our final theorem. This is, of course, time dependent. So let me do one example and our final time dependence analysis of this quantity. So for example, if you would think of the kinetic operator example. Kinetic operator \hat{T} is p^2 over $2m$ is a kinetic operator. How would you compute its expectation value? Expectation value of the kinetic operator is what?

Well, I could do the position space calculation, in which I think of the kinetic operator as an operator that acts in position space where the momentum is \hbar over i d/dx . So then I would have $\int dx \psi^*(x, t) \hat{T} \psi(x, t)$. And then I would have $-\hbar^2$ over $2m$ d^2/dx^2 of ψ of x and t . So here I did exactly what I was supposed to do given this formula.

But you could do another thing if you wished. You could say, look, I can work in momentum space. This is a momentum operator p . Just like I defined the expectation value of p , I could have the expectation value of p^2 . So the other possibility is that you have \hat{T} is equal to $\int dp p^2 \phi(p)$ over $2m$ times $\phi(p)$. This is the operator. And this is the probability.

Or you could write it more elegantly perhaps. $\int dp \phi^*(p, t) p^2 \phi(p, t)$ over $2m$ $\phi(p)$. These are just integrals of numbers. All these are numbers already. So in momentum space, it's easier to find the expectation value of the kinetic operator. In coordinate space, you have to do this. You might even say, look, this thing looks positive. Because it's p^2 of the number squared. In the center here, it looks negative. But that's an illusion. The second derivative can be partially integrated. One of the two derivatives can be integrated to act on this one. So if you do partial integration by parts, you would have $\int dx \hbar^2$ over $2m$. And then you would have $d\psi/dx$ squared by integration by parts. And that's clearly positive as well. So it's similar to this.