Introductory Quantum Mechanics and Spectroscopy

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Lecture – 4

Part III

Expectation Values and Postulates in Quantum Mechanics

Welcome back to the lecture. We continue from what was there in the last lecture on the Heisenberg’s uncertainty principle and I introduced a simple quantity called the average value or the expectation value.

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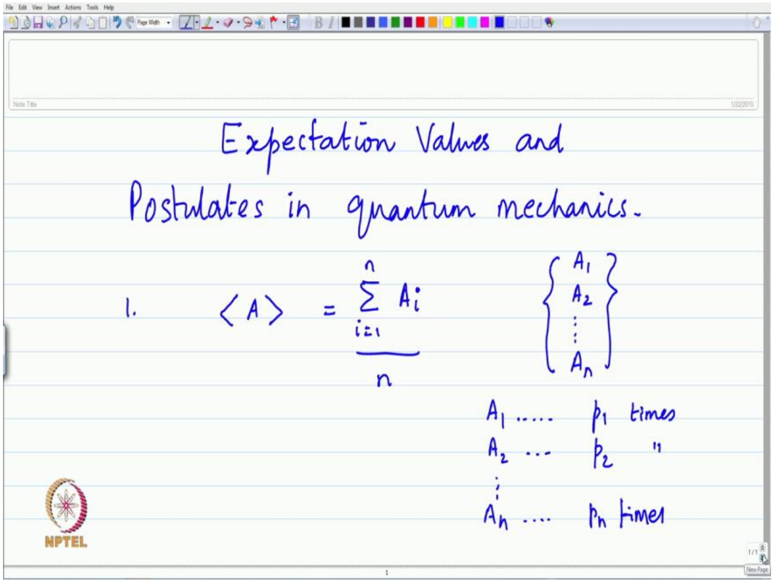

Expectation Values and Postulates in quantum mechanics.

1. $\langle A \rangle = \dfrac{\sum_{i=1}^{n} A_i}{n}$ $\quad \begin{Bmatrix} A_1 \\ A_2 \\ \vdots \\ A_n \end{Bmatrix}$

A_1 ..... p_1 times
A_2 ... p_2 "
$\vdots$
A_n .... p_n times

So, in this part of the lecture we will consider the formal definition for expectation values in quantum mechanics and if time permits I shall talk more about the postulatory bases, that is, bases with which mathematically we can start, that these are the starting points and then, quantum mechanics we can build, that is called the postulatory basis. And the postulatory basis in quantum mechanics will also be stated in very simple terms. The postulates are mathematical in nature, but we will see simple explanations hopefully.

First one is the expectation value, it is denoted by the average value bracket for any quantity. The average value is in general calculated according to the standard prescription, that if there are n measurements and these things happen with different outcomes for the measured quantity A with values A 1, A 2, A n for different measurements, then you know, that the average is nothing but the sum over i is equal to 1 to n A i divided by n .

Now, on the other hand, suppose you have A 1 occurring n 1 times in an experiment repeated many, many times, A 2 occurring n 2 times. Let me change n 1, n 2 to something else, which is standard p 1 times, p 2 times and likewise A n, and these are the only possible values. Let us see these are the only outcomes, that you have, occurs p n times.

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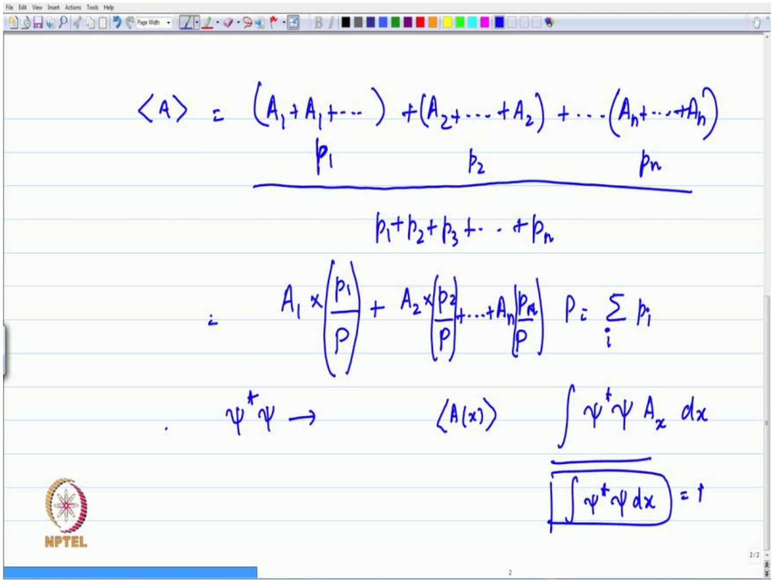

$$\langle A\rangle = \frac{\underset{p_1}{(A_1+A_1+\cdots)} + \underset{p_2}{(A_2+\cdots+A_2)} + \cdots \underset{p_n}{(A_n+\cdots+A_n)}}{p_1+p_2+p_3+\cdots+p_n}$$

$$= A_1\times\left(\frac{p_1}{P}\right) + A_2\times\left(\frac{p_2}{P}\right)+\cdots+A_n\left(\frac{p_n}{P}\right) \qquad P = \sum_i p_i$$

$$\psi^*\psi \rightarrow \qquad \langle A(x)\rangle \qquad \frac{\int \psi^*\psi A_x\, dx}{\boxed{\int \psi^*\psi\, dx}} = 1$$

Then, the average is calculated by adding all the A 1. So, the average is calculated by adding all the A 1 p 1 times and adding A 2, which has happened p 2 times and likewise, adding all the A n’s, which have occurred p n times dividing by p 1, p 2, p 3 up to p n. This is also the standard way in which you can calculate the averages. If some values repeat many times, then you want to find out how many times that it has repeated, what is the probability, that, that value is repeated and so on.

Now, the same thing can now be written by writing A 1 into p 1 by P, where P is the sum of all of the experiments p i. And therefore, p 1 by P gives you the probability, that you got A 1 for the measurement of A and likewise, A 2 into p 2 by P, which is the probability that you have the outcome A 2 and so on. Therefore, you have A n p n by P. So, this is a probability within brackets, that a given value occurs and then, what is the average when you do this experiment many, many times. This is standard way of representing probabilities.

And in quantum mechanics, you remember, psi star psi represents the probability density for the system at a given coordinate or at a given momentum, the variable x. So, in particularly one-dimensional box you talk about the psi star psi dx as the probability that the system is in the space between x and x plus dx. And in two-dimension psi star psi dx dy talks about the probability, that the system is in the area dx dy, which is enclosed between x and x plus dx and y and y plus dy, that is what it is. And therefore, psi star psi is a sort of a probability.

And then, what you have is the measured value, whatever that you measure. You measure the energy or you measure the position, you measure the momentum, it does not matter. Some experimentally observable quantity for which there is an operator associated with that in quantum mechanics, the measured value gives you the value with that probability. And then, the average value is the sum of all of those things, the measured value times the probability that it happens, summed over all such possible measured values.

Therefore, technically if you are looking at A as a function of x, because please remember, this is a continuous function, therefore A is defined for each and every value of x. So, what you think is, it is like psi star psi, which is the probability times the value A x, that happens in the x dx provided psi star psi represents the probability density, which means this integral psi star psi d x should be equal to 1, should be equal to 1.

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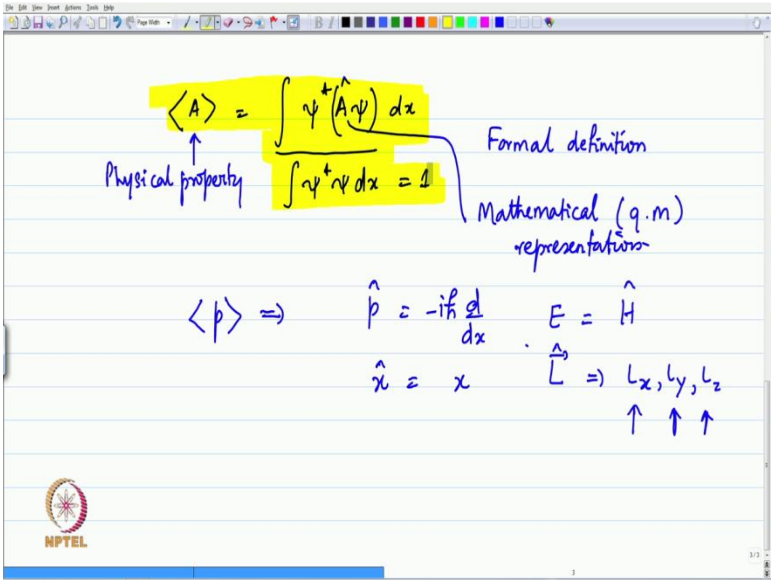

$$\langle A \rangle = \frac{\int \psi^* (\hat{A}\psi)\, dx}{\int \psi^* \psi\, dx = 1}$$

$$\langle p \rangle \Rightarrow \quad \hat{p} = -i\hbar \frac{d}{dx} \qquad E = \hat{H}$$

$$\hat{x} = x \qquad \hat{\vec{L}} \Rightarrow L_x, L_y, L_z$$

So, if you represent this, my probability density in quantum mechanics, the average value A is the probability times the value that happens with that probability summed over, but with one small technical difference namely, that the operator corresponding to A acting on psi giving you the measured value. And therefore, the measured value times the psi star psi is represented by this quantity divided by integral psi star psi dx, which of course, is set to 1 if we think of psi star psi as the probability.

So, this is the formal definition for the expectation value, and this A is the operator associated with the measured quantity, the physical property called A; this is the physical property. And this quantity is the mathematical representation or a quantum mechanical representation, quantum mechanical representation of that physical property.

You already know, because in the case of momentum, for example, the operator associated with p is minus i h bar d by dx or one-dimension. And then, what is the operator for the position? It is just dx itself. What is the operator for the energy? You have already seen, that it is the Hamiltonian operator. What is the operator associated with angular momentum, it is a vector and has three components in three dimensions or n components in n dimensions. So, if you write that in, say, three dimensions, you have three components, and each one of them is represented by a corresponding operator, which is slightly different from the, the notation, that we have here ((Refer Time: 09:10)) to all the derivatives.

So, the point is every measured quantity has a mathematical representation in quantum mechanics and the average value, that we expect by definition, the average mean, the average of an infinitely large number of measurements, the average value, that we expect to that system, that you see here, the average value is the psi star psi, psi star operator psi dx. This is a fundamentally important thing to remember. And again, when we introduce the postulates of quantum mechanics, this will be introduced as one of the postulates of quantum mechanics itself.

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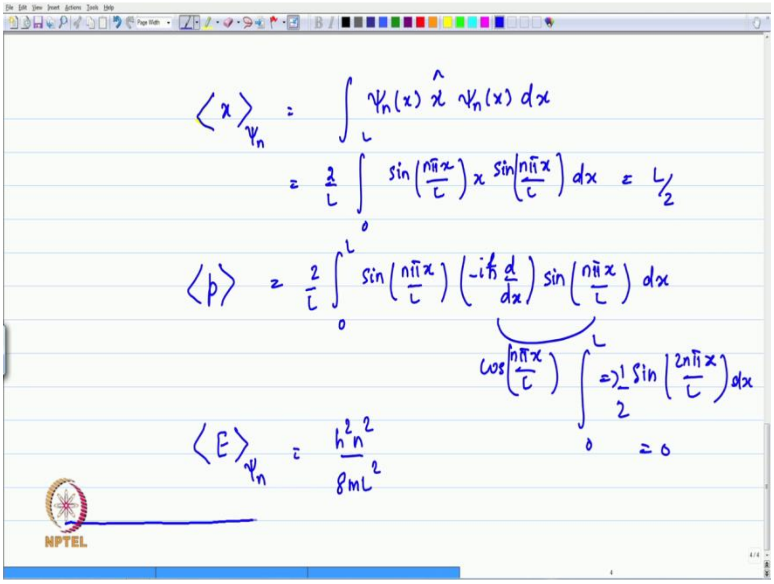

$$\langle x \rangle_{\psi_n} = \int_L \psi_n(x)\, \hat{x}\, \psi_n(x)\, dx$$

$$= \frac{2}{L} \int_0 \sin\left(\frac{n\pi x}{L}\right) x \sin\left(\frac{n\pi x}{L}\right) dx = L/2$$

$$\langle p \rangle = \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \underbrace{\left(-i\hbar \frac{d}{dx}\right) \sin\left(\frac{n\pi x}{L}\right)}_{\cos\left(\frac{n\pi x}{L}\right)} dx$$

$$\int_0^L \Rightarrow \frac{1}{2} \sin\left(\frac{2n\pi x}{L}\right) dx = 0$$

$$\langle E \rangle_{\psi_n} = \frac{h^2 n^2}{8mL^2}$$

Therefore, in the last lecture when I said, that the average value of the position, logically it turns out to be somewhere right in the middle of the box for a box of length L. You can calculate for one dimension.

The average value x to be psi n of x if the state of the system is psi n, then the average value in that state is psi n of x, the position operator x and psi n of x dx, and psi n being normalized to root 2 by L. Whatever you have, that is root 2 by L times sine n pi x by L, you have for the integral 0 to L sine n pi x by L x sine n pi x by L dx. So, this gives you, when you do the integral this gives you the answer L by 2. So, very simple integral it is. x sine square x and sine square x is, of course, you can write is as 1 minus cos 2 x by 2 and then you, you do the simple integral on x and x cos x. It is very easy to do.

Likewise, the average value for the momentum for the particle was also argued out to be 0 based on the fact, that the momentum is a vector and therefore, it has a positive or a definite negative direction at any point in space. If you do that the average value of the momentum will turn out to be 0 for the particle in one-dimensional box and that is also easy to verify by writing this down as 2 by L sine n pi x by L.

Now, you remember to put the operator in the middle i h bar d by dx sine n pi x by L times dx. Now, the derivative of the sine will give you a cosine n pi x by L, you can see mathematically, and the sin cosine will give you a sine 2 n pi x by L times 1 by 2, but that integral between 0 to L is a full sine wave and therefore, that goes to 0, d x.

So, it is easy to verify simple relations like p, expectation values for position, expectation values for momentum and these are the two things that you can think about. And if you have the kinetic energy, you already know, that the particle in the box is only kinetic energy inside the box. Therefore, the total energy is the same as that of kinetic energy. And you can see, that the average value E for the particle in the state psi n is h square n square by 8 m L square, that also comes out. So, these are simple prescriptions for doing calculations for the average values based on quantum mechanics.

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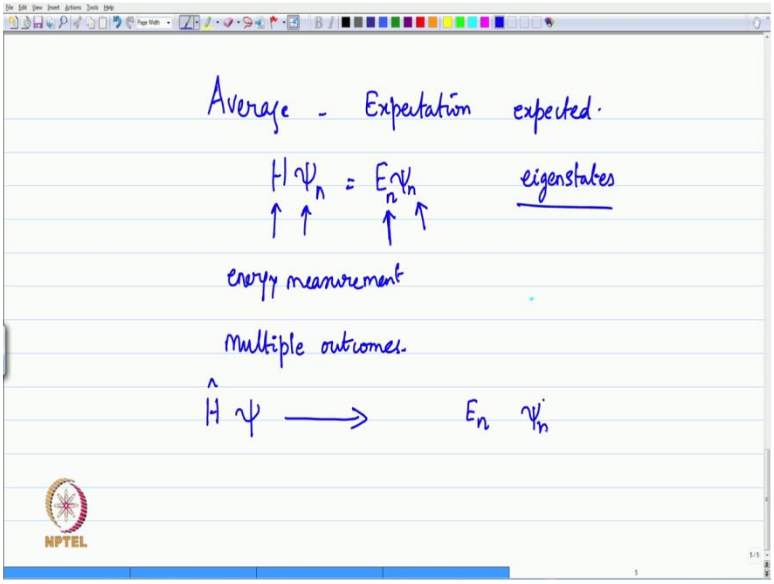

Average - Expectation expected.

$H\psi_n = E_n\psi_n$ eigenstates

$\uparrow \ \uparrow \quad \uparrow \ \uparrow$

energy measurement

multiple outcomes.

$\hat{H}\psi \longrightarrow E_n \quad \psi_n$

Now, please remember these are average values. Expectation values, that is, these are what are expected when you do many, many measurements. But if I do a singled experiment what value will I get? Is there a prescription in quantum mechanics? That is what this equation tells you. If the state of the system is in this function, is in this state psi n for the particle in the one-dimensional box, it does not matter how many times I make measurements on that state for the energy, for the energy; it does not matter. All the times I will get only one answer, namely, E n psi n of x.

It is like the simple analogy. You have a dye with six faces and you print only one dot on all the six faces. Therefore, the dye has only one state, namely, with an outcome of a single dot. No matter how many times you throw the dye, you get only one dot is the answer because that is how you prepared the state of the system. Such states are called Eigen states in quantum mechanics. In the case of a dye you have six possible things that you have for a single dye: 1 dot, 2 dot, 3 dot, 4 dot, 5 dot, and 6 dots. Therefore, you have six possible outcomes.

In the case of a particle in the box, if I make a measurement and I do not know what the state of the system is, what result can I expect for a single measurement? I have already told you what result we can expect for a very large number of measurements and then what is the average, that is what we did before. What is it for a single measurement? If you ask that question, the answer is one of the Eigen values of the system. In case of the dye, which is a normal dye or a regular dye, which has six different faces with 1, 2, 3, 4, 5, 6 dots, there are six possible outcomes, multiple outcomes.

Therefore, in a singled experiment of throwing the dye, we get a dot or 2 dot or 3 dot, all with identical probabilities, 1 by 6, if the dye is a perfect cube, because the dye is not prepared in any other way. Likewise in quantum mechanics, if the probabilities for all outcomes are uniform, then in a single measurement one of these energies will be the outcome. For the particle in a box if you measure the energy, only one of the E n's is possible, which of the E n statistics. Einstein was very unhappy. He said God does not play dice, and Niels Bohr told him, do not tell god what to do?

But there is an inherent statistical character built in the measurement outcomes according to what is called the Copenhagen school or the Niels Bohr school of quantum mechanics, which is still practiced by most of us. A single measurement will give you one of the Eigen values, and will result in the state of the system being one of that Eigen state, the Eigen state corresponding to that Eigen value.

Therefore, if we make a measurement for a particle in the one-dimensional box in an arbitrary state, that we do not know what it is, the result, that we will get out is only one result. And that result, the measurement will give you an Eigen value E n and the state of the system will become psi n. This is fundamental in quantum mechanics. And if the state is already an Eigen state, then no matter how many times you make copies of that state, and how many times you make the measurements you will always get the Eigen value.

That is why, I mean, I wrote the average value for E in the last slide or a few minutes ago, I go back to the screen, I have written that already here ((Refer Slide Time: 10:09)). If the state of the system is psi n, the measurement of energy every time will give you the same value h square m square by 8 m L square. And since it is a same value in all measurements, the average is also the same as the single measurement.

If you know the state of the system very precisely, that is what it is? If you do not know the state of the system to be an Eigen state, but an arbitrary psi, this is the result for an arbitrary psi. ((Refer Slide Time: 07:06)). Now, let me write down the tab psi here, that if the system is in the state psi, a measurement of a quantity physically will give you psi star A psi dx integrated over the domains completely available to the system. And for particle in a one dimensional box, it is between 0 to L, that is, the whole space available to the system. Therefore, you take the average by adding all the probabilities.

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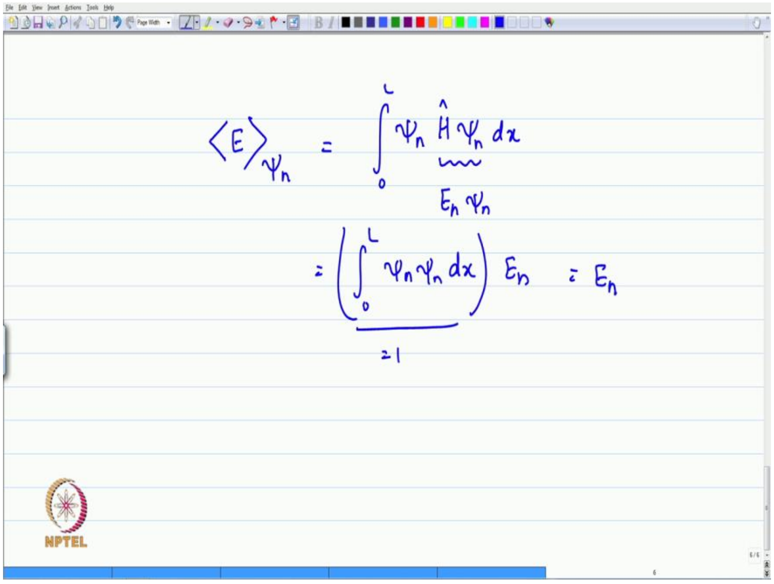

$$\langle E \rangle_{\psi_n} = \int_0^L \psi_n \underbrace{\hat{H}\psi_n}_{E_n \psi_n} dx$$

$$= \underbrace{\left(\int_0^L \psi_n \psi_n \, dx\right)}_{=1} E_n = E_n$$

It is very easy to see, that the same one is what you get because if you write E of psi n, which is an Eigen state of the Hamiltonian operator. Then, you see, that this relation is psi n H psi n dx. And you know, between 0 to L, you know, that H psi n is E n psi n and you know, that psi n is normalized. Therefore, the answer is 0 to L psi n psi n dx and with E n and this is equal to 1. And therefore, the average value is the same as the Eigen value for E n. Let me stop here and we will continue these discussions over the next few weeks on various aspects.

But it is important for us to remember, that the expectation value is a fundamentally important quantity and the fact that, that involves the wave faction and its complex conjugate is a very meaningful reason, very important reason, why? One is always interested in solving the Schrödinger equation to get that wave function first. That the wave function has an interpretation due to probability is one thing, but the wave function is extremely important in the actual calculations for the expectation values and the measurements.

And therefore you have a function, which you cannot physically explain or visualize, but it is very important and very useful for calculating average values, calculating other quantities called matrix elements, calculating the average values through various processes and so on. Therefore, the wave function has come to stay with all of us. We will continue this in the next lecture.

Thank you.