Chemistry I - CY1001
Introductory Quantum Mechanics and Spectroscopy
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Lecture – 06
Lecture 4: Part II - Uncertainty principle

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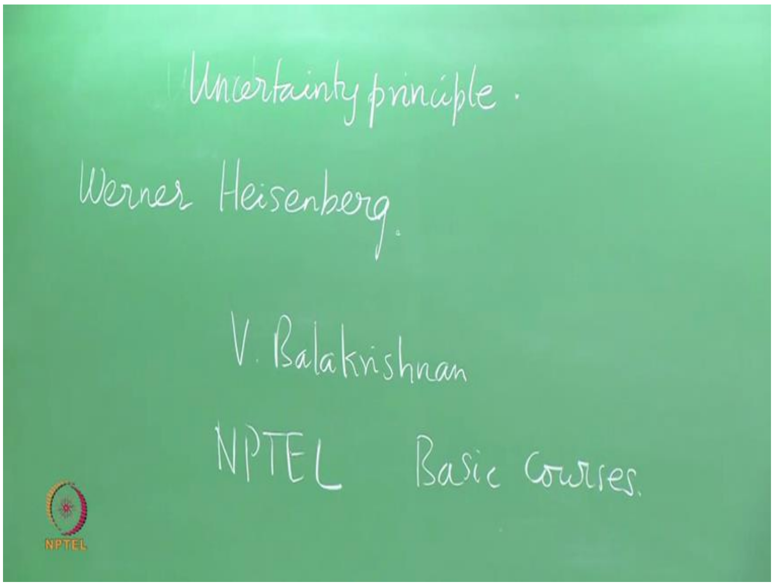

So, we shall continue the particle inner two d box, but for the moment let us consider a little bit on this famous principle called the Uncertainty principle which was first put forward by Werner Heisenberg. Now there is a very beautiful lecture on the Heisenberg uncertainty principle by professor V Balakrishnan and it is there in the NPTEL website under basic courses or in physics, uses on (Refer Time: 01:04) mechanics.

The very first lecture is on the Heisenberg uncertainty principle, I would like to recommend that to everyone of you to go through that lecture, but this is very very preliminary; it is not anything like what was there, but you would appreciate that lecture far more when you listen to professor Balakrishnan's account of how the Heisenberg uncertainty principle is to be understood.

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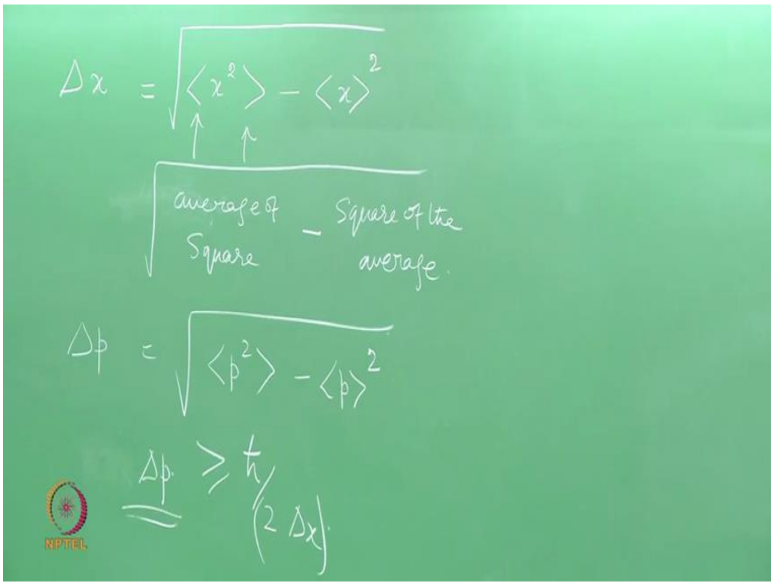

We will do a much simpler exercise since you are beginning this is meant for the introductory very first year students. The uncertainty delta x in any measurement quantity x is given by this simple statement that it is the difference between the average of the square of that variable minus the square of the average of that variable and this whole thing is under a square root. This is the angular brackets to (Refer Time: 02:27), the average value.

What is inside is - the one for which the average is taken. Therefore, the average is taken for the square of that value x, here the average is taken for the value x (Refer Time: 02:45) and then it is squared. The difference between the two the square root of this is called the uncertainty average of the square minus square of the average; this I do not know how to say it in English, it is a square root or you can write within bracket square root.

Likewise the uncertainty, this is for the precision variable and this is for the momentum variable. I have introduced this in a separate account I might tell you how this formula comes about and so on. But let us just introduce these things as defined in textbooks, the delta p is again the average of the square of the momentum minus the momentum square. Delta x delta p; the product of the two is greater than or equal to h bar by 2. This is the Heisenberg’s statement about the uncertainty between the x and p. What it means is that if for some preparation of the states, we are able to minimize this by making sure that this average and this squared average are very close to each other, therefore we are able to measure the position very very very accurately; if you do that what uncertainty principle tells you that is in the denominator therefore, the uncertainty in delta p is very large; it is not possible for us to control the uncertainties to both of them to absolute minimum except not to violate this particular relation.

Therefore, this is one of the statements that you might see in textbooks very often regarding the uncertainty in the position measurement and uncertainty in the momentum measurement. But it also means is that position and momentum cannot be simultaneously used as variables for describing the state of a particle as independent quantities for describing the state of the particle.

The state of the particle can either be very precisely stated using the position or very precisely stated using its momentum, but not more and therefore, this brings down the whole structure of classical mechanics where one would imagine in the solution of the Newton's equation, the precise statement for the position and the velocity of a particle at one instance of time and be able to solve. Therefore, if you can specify the velocity of these you can also specify the momentum of the particle therefore, position of momentum can be simultaneously used as descriptors for defining the state of a classical particle, but they cannot be used as descriptors for the state of a quantum particle and the relation between the two is given by this famous Heisenberg uncertainty principle and professor Balakrishnan's lecture tells you how to generalize the Heisenberg uncertainty states in using other classical formulations and eventually what is known as the commutator.

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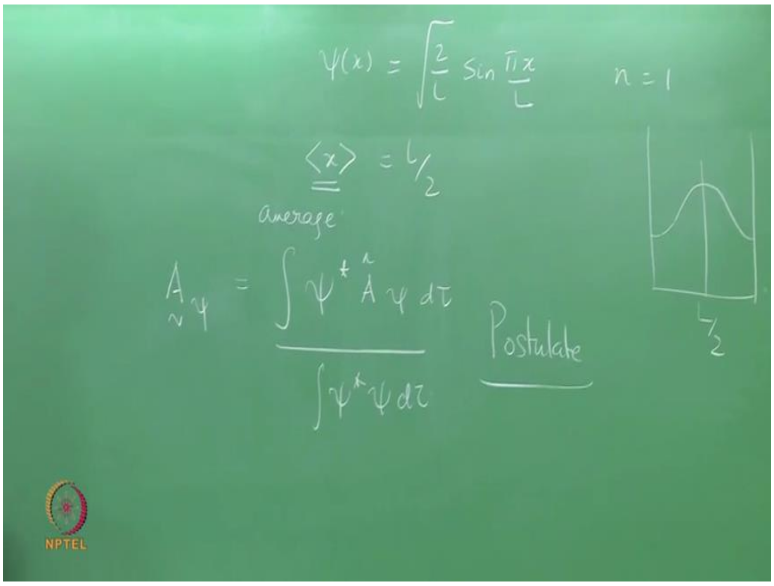

Now, let us use the wave function psi of x for the one dimensional box; root 2 by L sin pi x by L. We will take the L equal to 1 in case quantum number and if we try to calculate the average value x for the particle in this state whose wave function and the probability of the particular variance points is symmetrically the same or either side of L by 2. It should be immediately clear that the average value for the particle position given that these are the probabilities for the particles position being here or here or here or here; by looking at this being a symmetrical graph, you can immediately say x should be L by 2.

That is also the expectation value or the average value, this is true. The average value in quantum mechanics for any variable A in the state psi is given by psi star A on psi d tau which is the volume element or the area element or the length element similar to whether it is a one dimensional box or a two or a three dimensional divided by the interval psi star psi d tau; this is a postulate. I do not want to tell you how this can be arrived at using arguments, we will find such things in physics books but for the particular course that you have started taking, this is the postulatory introduction for the expectation value of any variable A whose corresponding representation as an operator is given by this A hat and A hat is between the wave function psi and the complex conjugate psi star if psi is a complex function, otherwise both of them are psi.

This prescription must be kept in mind, this is introduced as a postulatory form and let me calculate the x for the particle; it is very easy now.

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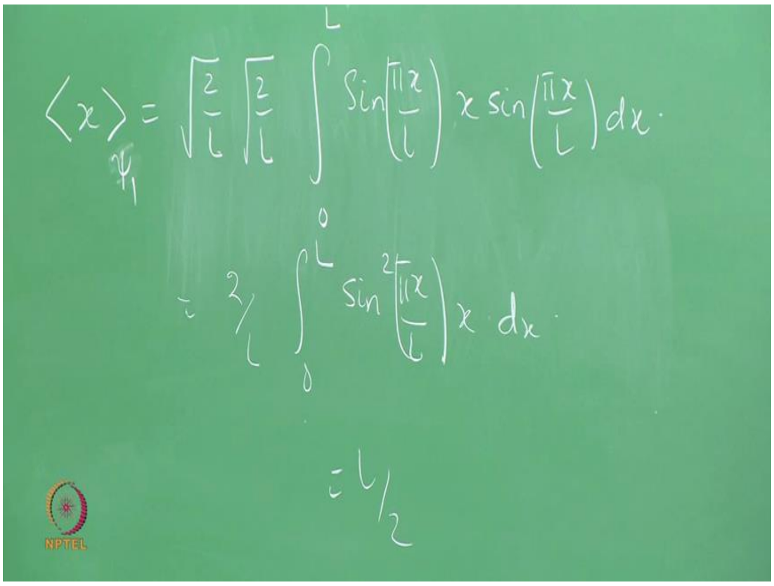

Now, for the average value x is given by the integral root 2 by L, root 2 by L because it is psi star psi and you have sin pi x by L; x sin pi x by L; d x between 0 and L, for the particle in the quantum state with the quantum number 1 which is what we call as psi 1 and x of course, does not change anything, I mean it simply multiplies to this. Therefore, this integral is 2 by L 0 to L; sin square pi x by L multiplied by x dx. Calculate this integral and show that the answer is L by 2.

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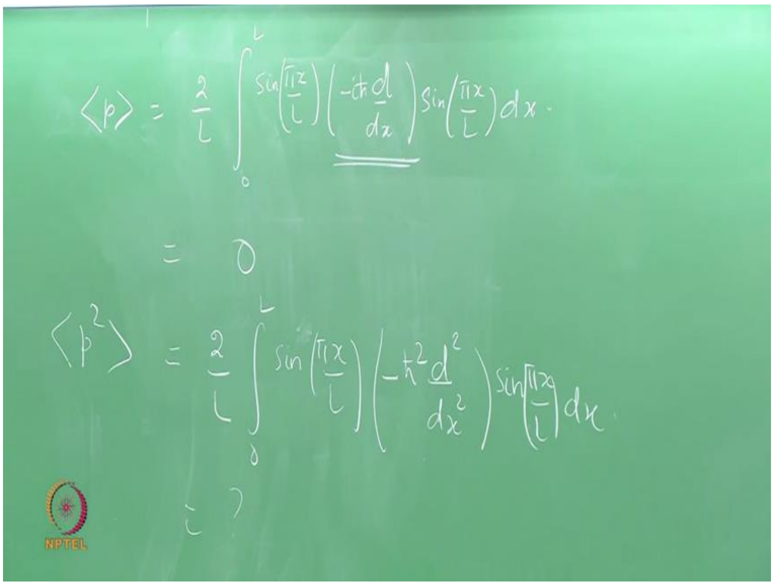

Let us carry out to the re exercise, what about the momentum? You have to be careful in ensuring that the momentum operator which is a derivative operator is placed as written here mainly 2 by L that comes from the two constants psi star psi, then we have sin pi x by L, between 0 to L and the momentum operator is minus i h bar d by dx; acting on sin pi x by L dx, see that the operator is sandwiched between the wave function and the complex conjugate of the wave function, but here the wave function is real, therefore you do not see the difference between the two. What is this? It is very easy to see that this will give you the derivative will give you a cos and a sin cos will give you a sin 2 pi x by L and that in this interval is actually 0.

What about the average value p square? The average value p square is given by 2 by L again sin pi x by L and now you remember, it is minus h bar square, d square by d x square for the operator p square; sin pi x by L dx and it is between 0 and L. I did not write the denominator because we have chosen the wave function by ensuring that the wave function is the integral of the square of the wave function is actually 1 in the entire region, therefore I did not write the denominator; that is 1.

This of course, you know is nothing but 2 m e; the total energy, this is p square on the wave function; you remember p square by 2 m on the wave function gave you the E. Therefore, this is 2 m E therefore you see that p square is immediately given by the energy that we know you can write that.

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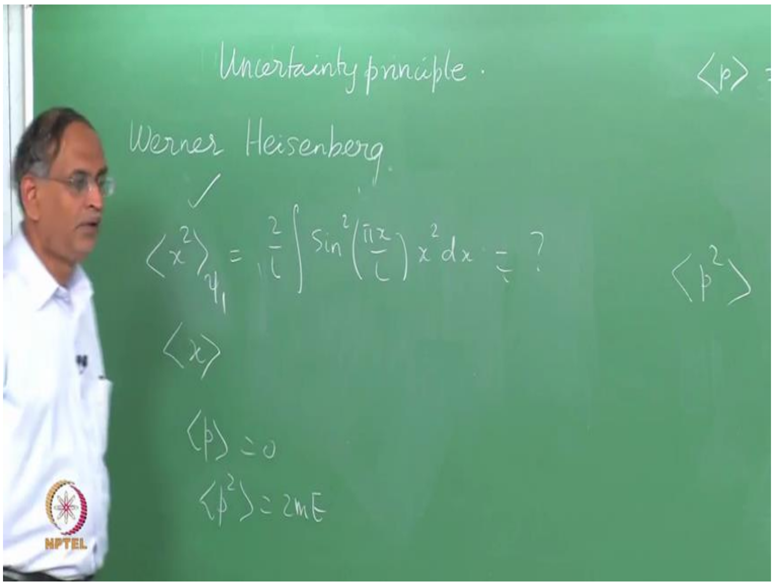

What about the d x square? If I have to do x square all I need to do the same thing; write x square on psi 1 and I have the integral that needs to be evaluated is integral 2 by L; sin square pi x by L into x square d x, therefore you know the value of x square, you know the value of x, you know the value of p as 0, we know the value of p square as nothing but 2 m E; this is the only integral that I have not calculated.

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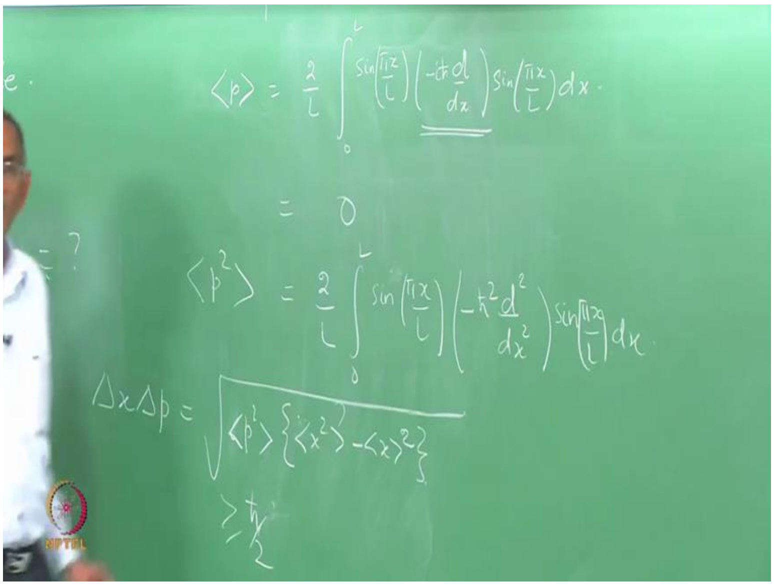

Once you have done that, you can calculate delta x delta p as nothing, but the square root of p square minus p of course, you know that is 0 times x square minus x whole square and you should be able to verify that this answer is greater than or equal to h bar by 2. So, this is the statement of the Heisenberg uncertainty principle for the particle in a one dimensional box. Now exactly the same statement can be extend, I mean it can be extended to particle in a two dimensional box except that now we have x and y as two independent coordinates p x and p y as two independent coordinates.

Therefore, you have a corresponding uncertainty relation in two dimensions with one exception mainly x and y are independent coordinates therefore, x and p y can be simultaneously measured or it can be ascribed as a property to the system; y and p x can be simultaneously specified for the particle, x and y can be specified p x and p y can be specified, but not x and p x and y and p y that is the only thing you have to remember.

The independence of the degrees of freedom ensures that the operators corresponding to those degrees of freedom commute with each other and if I have not spoken to you much about commutation that will be in the next lecture. But in this part I would simply want you to calculate the Heisenberg's uncertainty principle as given this is one simple way of doing it, you can find similar treatments for the uncertainty when you go to study the other systems like the harmonic oscillator the hydrogen atom and so on.

What is key to remember is the definition for real delta x I gave you and the definition for the delta p I gave you, those are fundamental. I have not told you where they come from; maybe in a separate lecture or in the class when we discuss these things through elaborations, I will tell you what the origin of the delta x and delta p, but these are definitions which you have to start with working and then feel more comfortable, go back and look at the whole process of the derivation.

We will continue this exercise to complete what is known as the introductory, but postulatary basis of quantum mechanics for this course. In the next part of this lecture which is the third part for the particle in a two dimensional box with that we will complete the two simple models particle in a one d and a two d box. We will meet again for the last portion of the particle in a two d box lecture the next time.

Thank you.