Indian Institute of Technology Madras
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NPTEL
NATIONAL PROGRAMME ON TECHNOLOGY ENHANCED LEARNING

Chemistry I
Introduction to Quantum Chemistry
And Molecular Spectroscopy

Lecture – 12
Particle in a One-dimensional Box: Part II
Uncertainty Principle

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So we shall continue the particle in a 2D 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.

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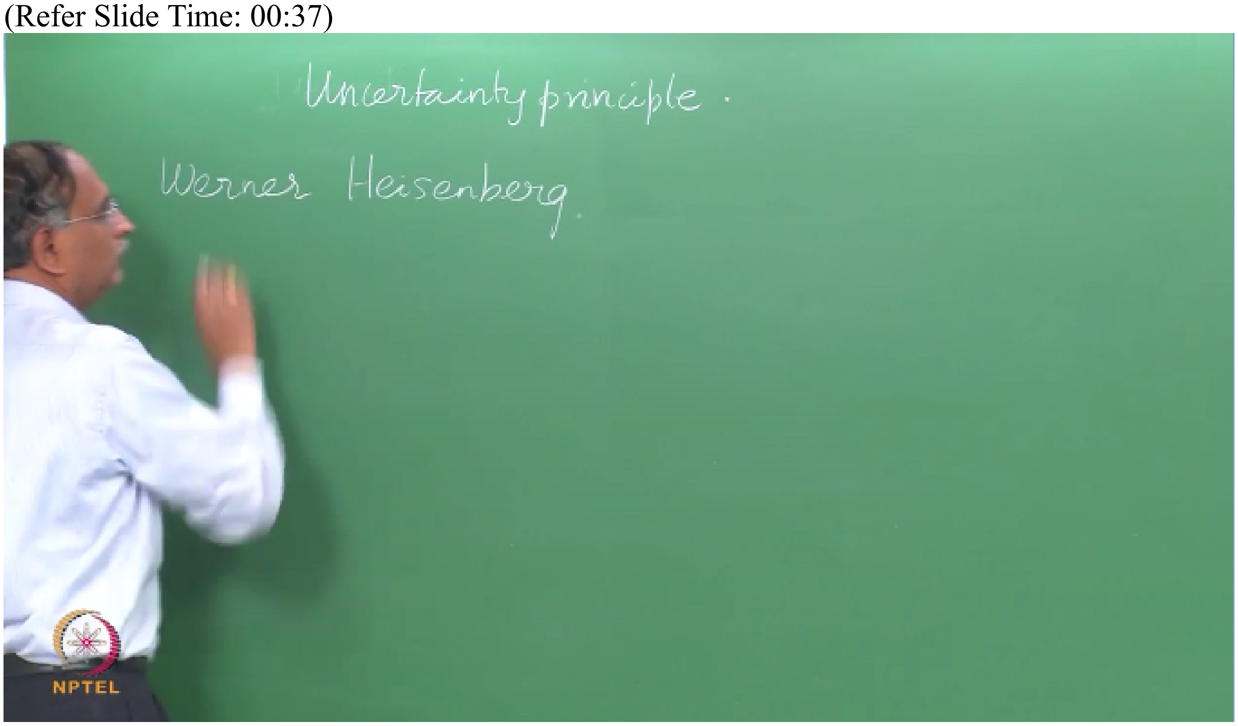

Now there's a very beautiful lecture on the Heisenberg's uncertainty principle by Professor V. Balakrishnan and its there in the NPTEL website under basic courses or in physics, this is on quantum mechanics.

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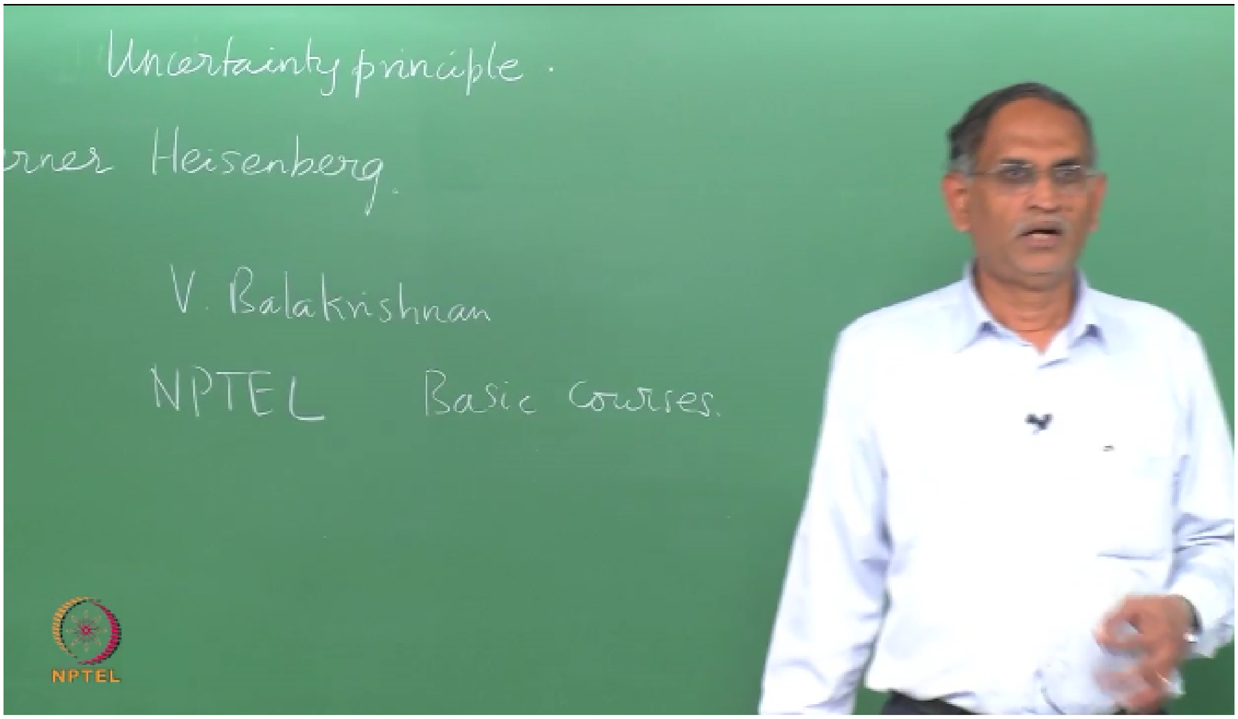

The very first lecture is on the Heisenberg's uncertainty principle, I would like everyone, I would like to recommend that to every one of you to go through that lecture, but this is very very preliminary it's not anything like what was there, but you would appreciate that lecture far more when you listen to professor Balakrishnan account of how the Heisenberg's uncertainty principle is to be understood, we will do a much simpler exercise since you are beginning, this is meant for the introductory very first year students.

Now uncertainty delta X in any measurement quantity X is given by this simple statement that it's the difference between the average of the square of that variable minus the square of the average, square of the average of the variable and this whole thing is under a square root, okay, this is the angular brackets tell you that the average value,
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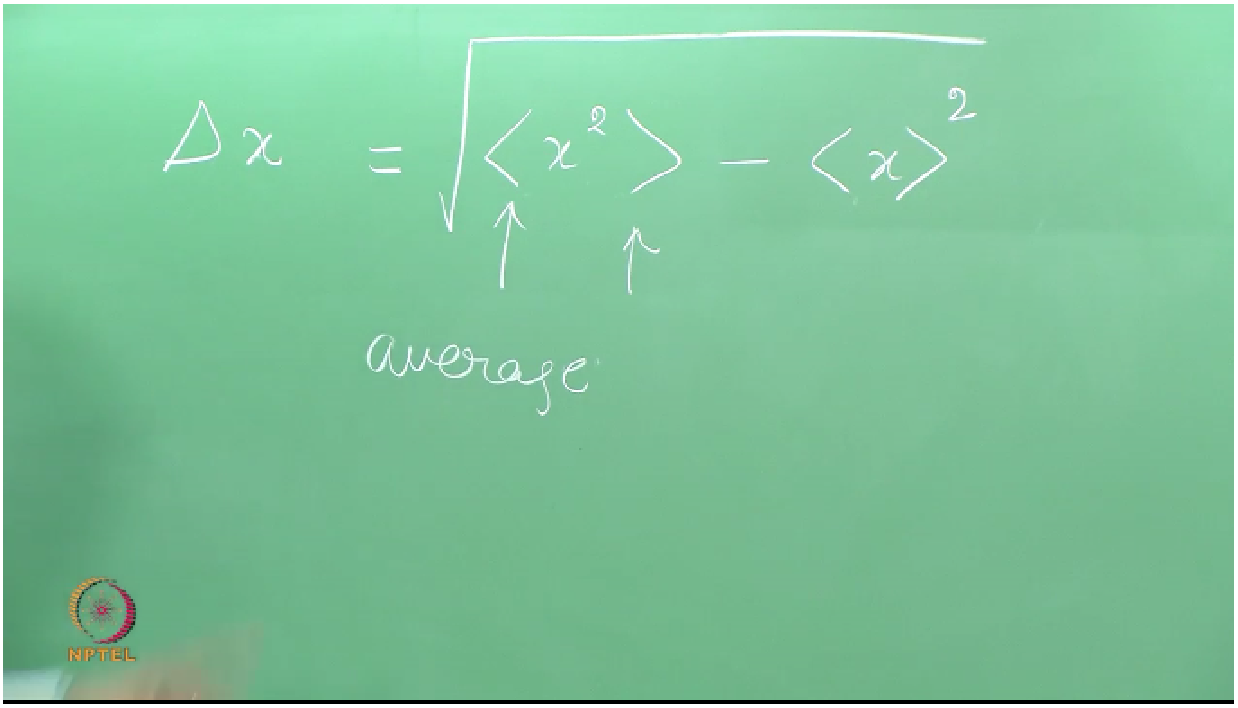

what is inside is the one for which the average is taken, therefore the average is taken for the square of that value X, here the average is taken for the value itself and then it is squared. The difference between the two, the square root of this is called the uncertainty average of the square minus square of the average, this I don't know how to say it in English, it's the square root okay or you can write with in bracket square root.

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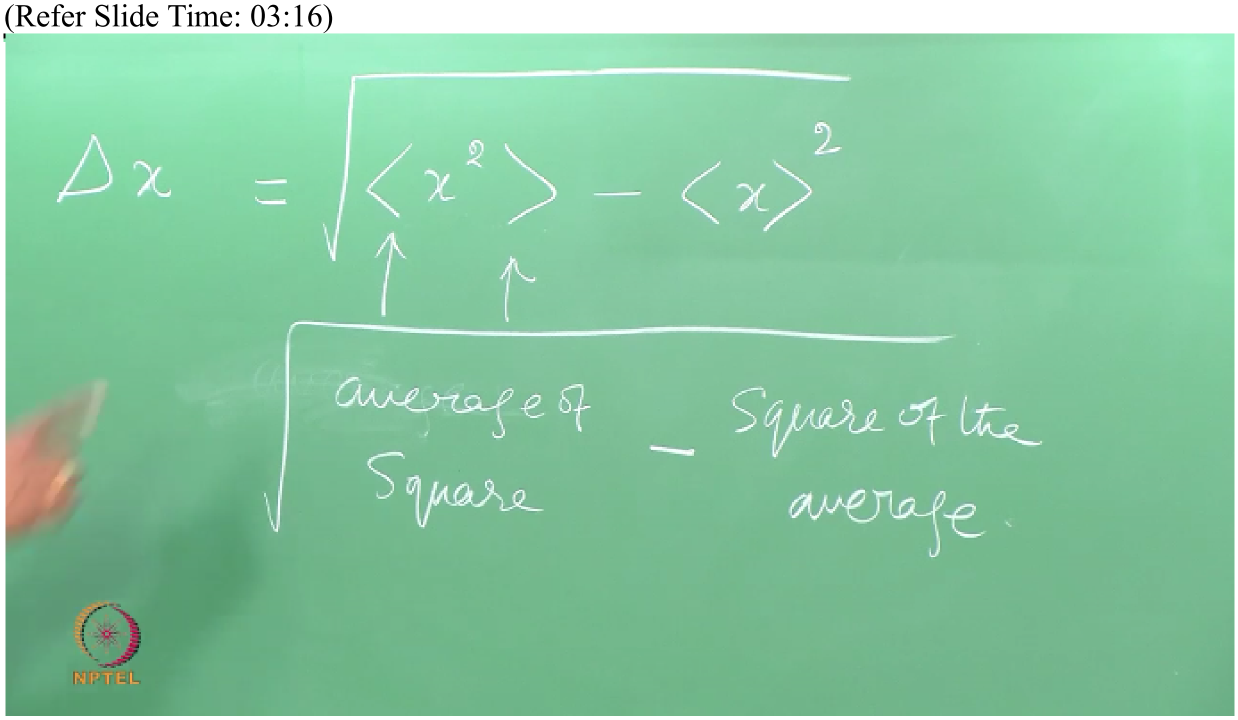

Likewise the uncertainty this is for the position variable, and this is for the momentum variable I have introduced this in a separate account I might tell you how this formula comes about and so on, but let us just introduce these things as defined in textbooks the delta P is again the average of the square of the momentum minus the momentum square, okay.

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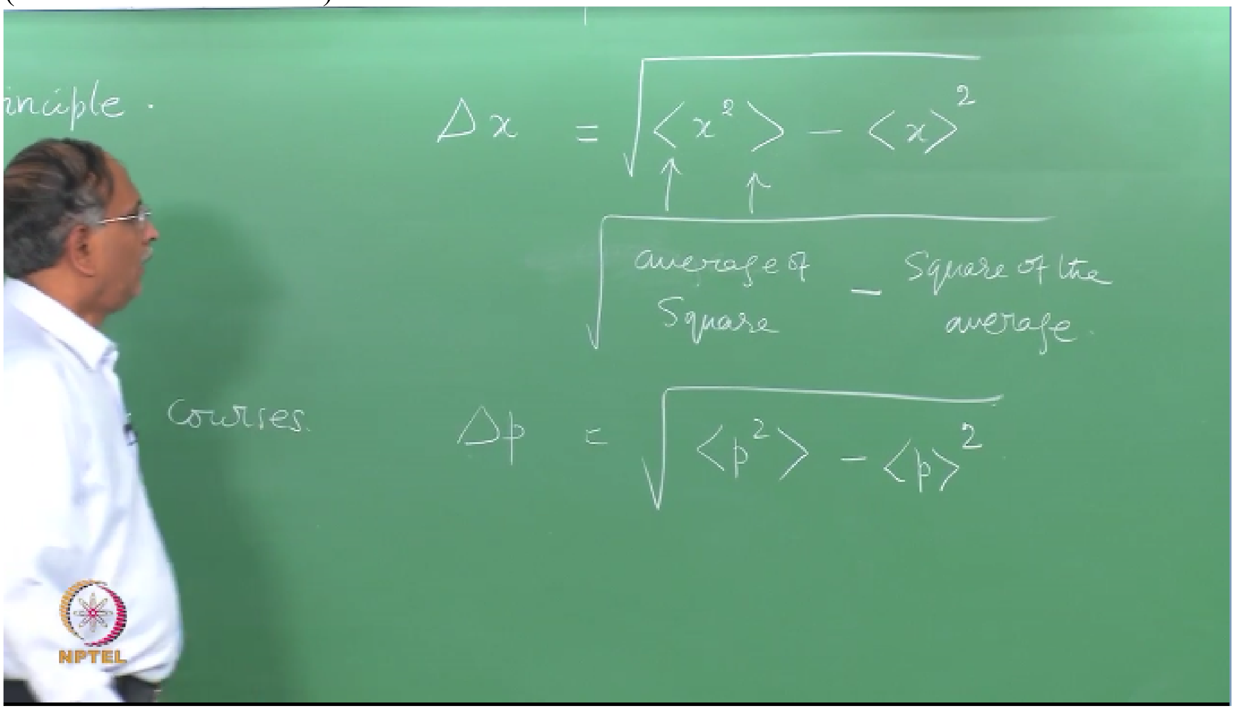

Delta X, delta P the product of the two is greater than or equal to H bar/2 okay,

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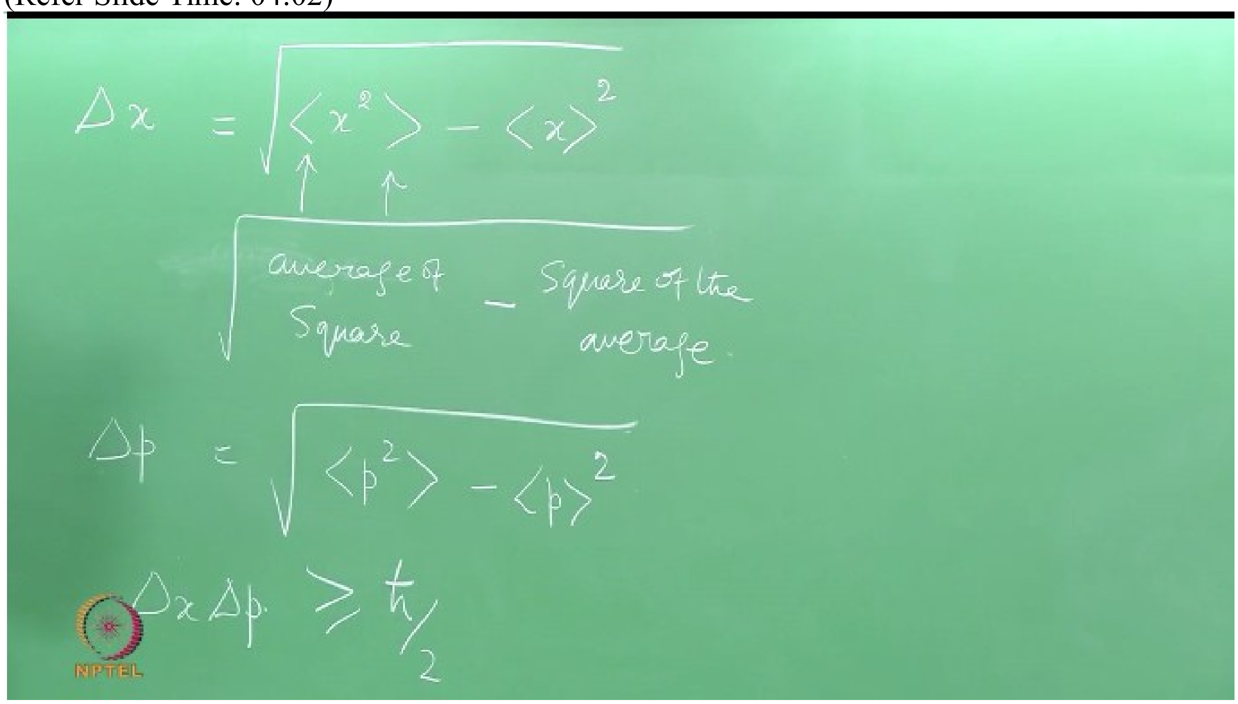

this is the Heisenberg's statement about the uncertainty between X and P, what it means is that if for some preparation of the states we are able to minimize this by making sure that this average and this squared average are very close to each other, therefore we are able to measure the position very, very, very accurately, if we do that what uncertainty principle tells you that is in the denominator, therefore the uncertainty in delta P is very large, it's 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, what 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 both but 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 velocity of a particle at one instant of time and be able to solve, therefore if you can specify the velocity obviously you can also specify the momentum of the particle therefore position and momentum can be simultaneously used as descriptors for defining the state of a classical particle but they can't be used as descriptors for the state of a quantum particle.

And the relation between the two is given by this famous Heisenberg's uncertainty principle and professor Balakrishnan lecture tells you how to generalize the Heisenberg's uncertainty states in using other classical formulations and eventually what is known as the commutator, okay.

Now let's use the wave functions sai(x) for the one dimensional box root 2/L sine pi X/L, we will take the N = 1 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 particle at various points is symmetrically the same on either side of L/2, okay,
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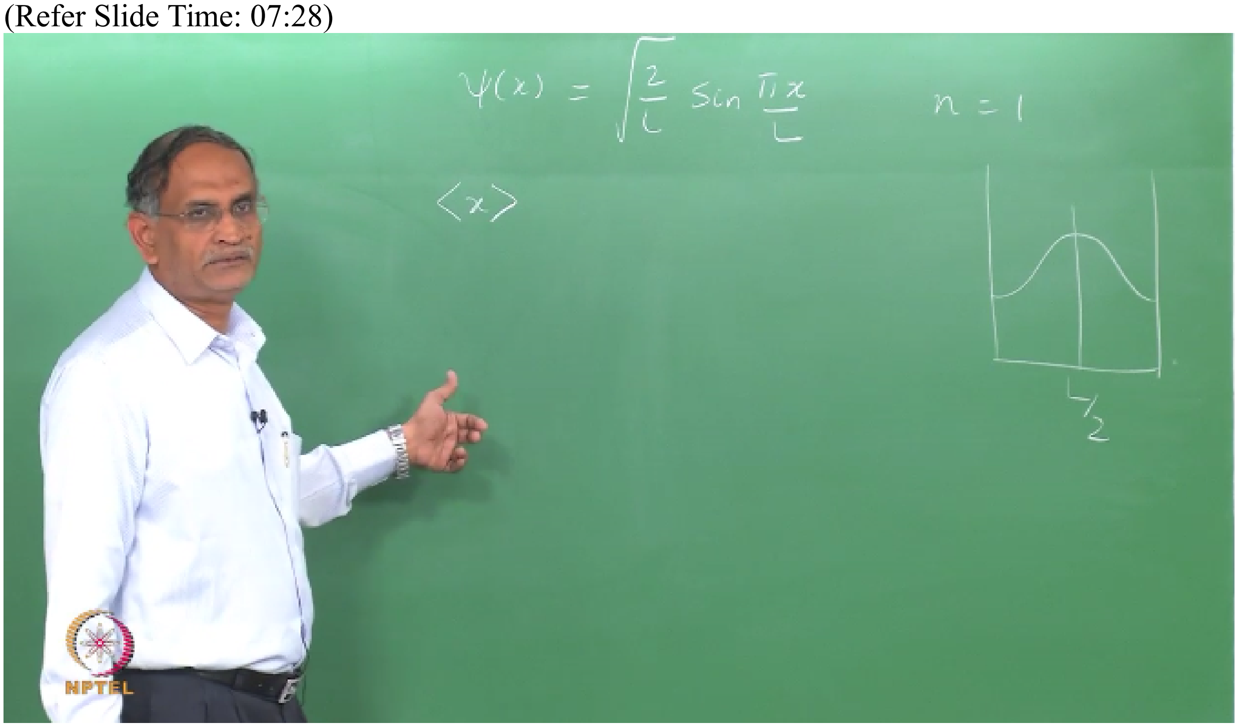

it should be immediately clear that the average value for the particle position given that these are the probabilities for the particles position being here or here or here or here by looking at this being a symmetrical graph you can immediately say X should be L/2, but that's also the expectation value or the average value this is called.

The average value in quantum mechanics for any variable A in the state sai is given by sai star A on sai D tau which is the volume element or the area element or the length element similar to whether it's a one dimensional box or a two or three dimensional, divided by the integral sai star, sai D tau okay this is a postulate,

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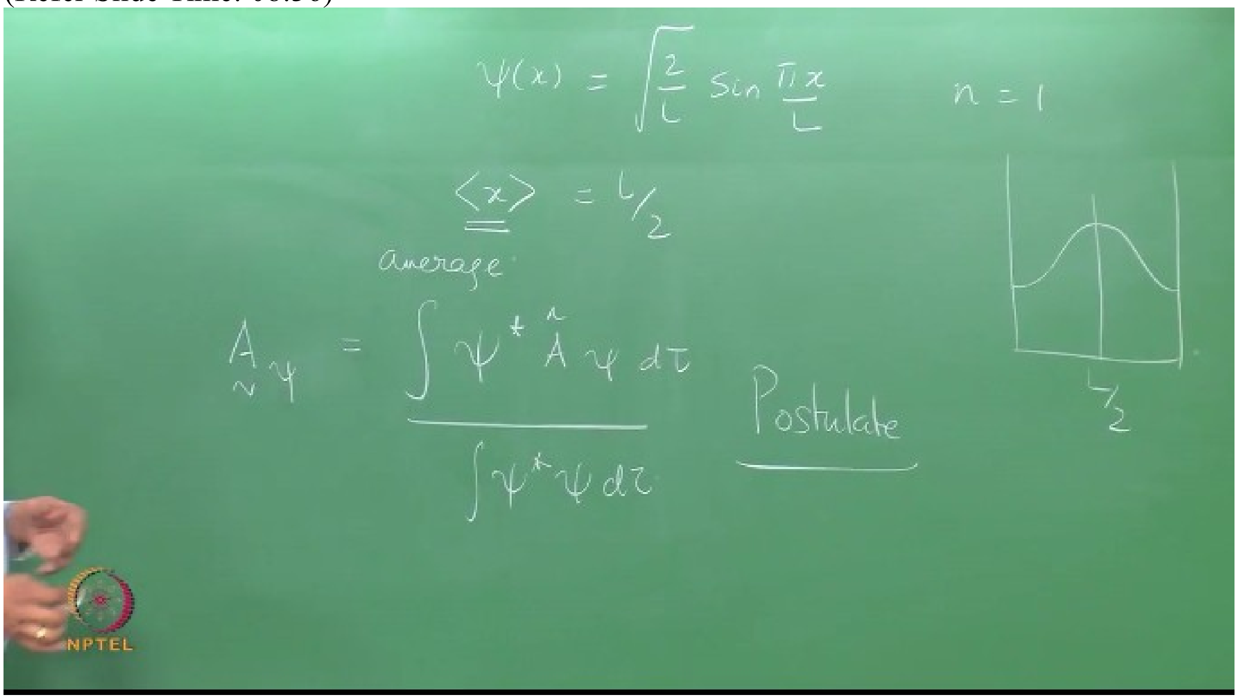

I don't want to tell you how this can be arrived at using arguments you will find such things in physics books, but for the particular course that you have started taking this is the postulatory introduction for the expectation value of any variable A whose corresponding representation as an operator is given by this A hat, and the A hat is between the wave function sai and the complex conjugate sai star, if sai is a complex function, otherwise both of them are sai.

This prescription must be kept in mind, this is introduced as a postulatory form, and let me calculate the X, for the particulates very easy now, therefore the average value X is given by the integral root 2/L root 2/L because it's a star sine and you have sine pi X/L, X sine pi X/L DX between 0 and L for the particle in the quantum state with the quantum number 1, which is what we call as sai 1, okay.

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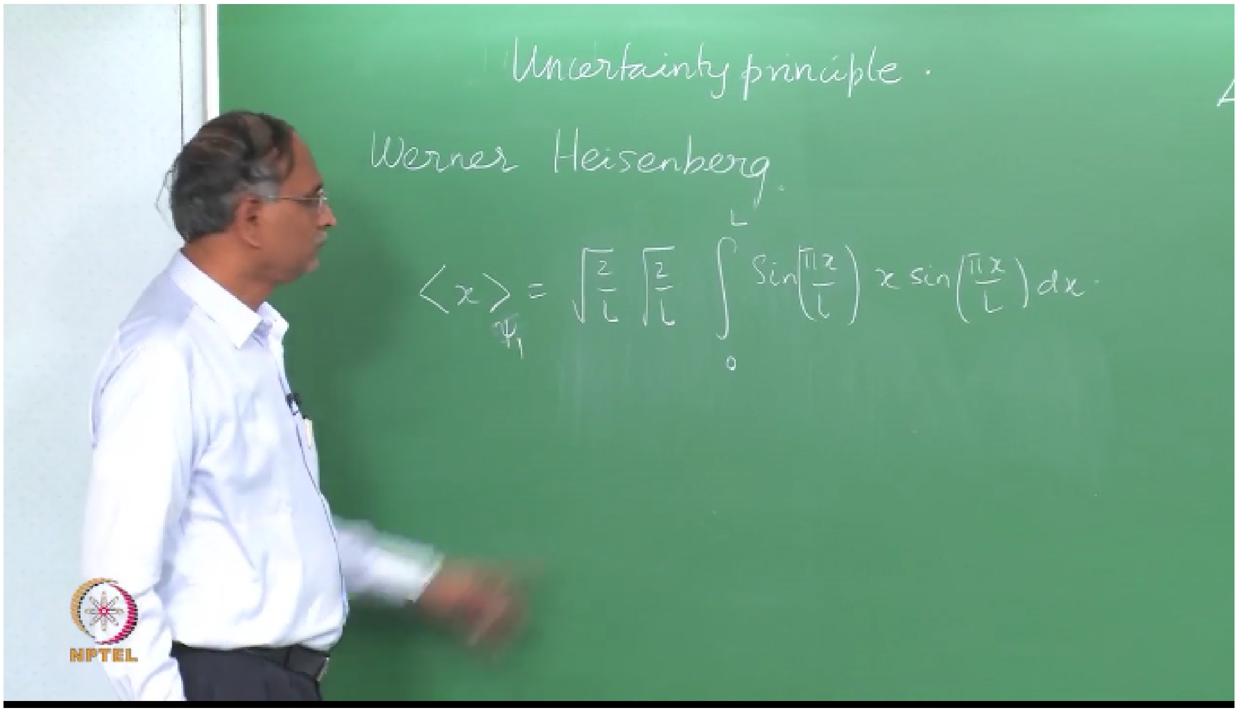

And X of course doesn't change anything I mean it simply multiplies to this, therefore this integral is 2/ L 0 to L sine square pi X/L multiplied by X DX, calculate this integral and show that the answer is L/2, okay, that's for you to do the exercise.

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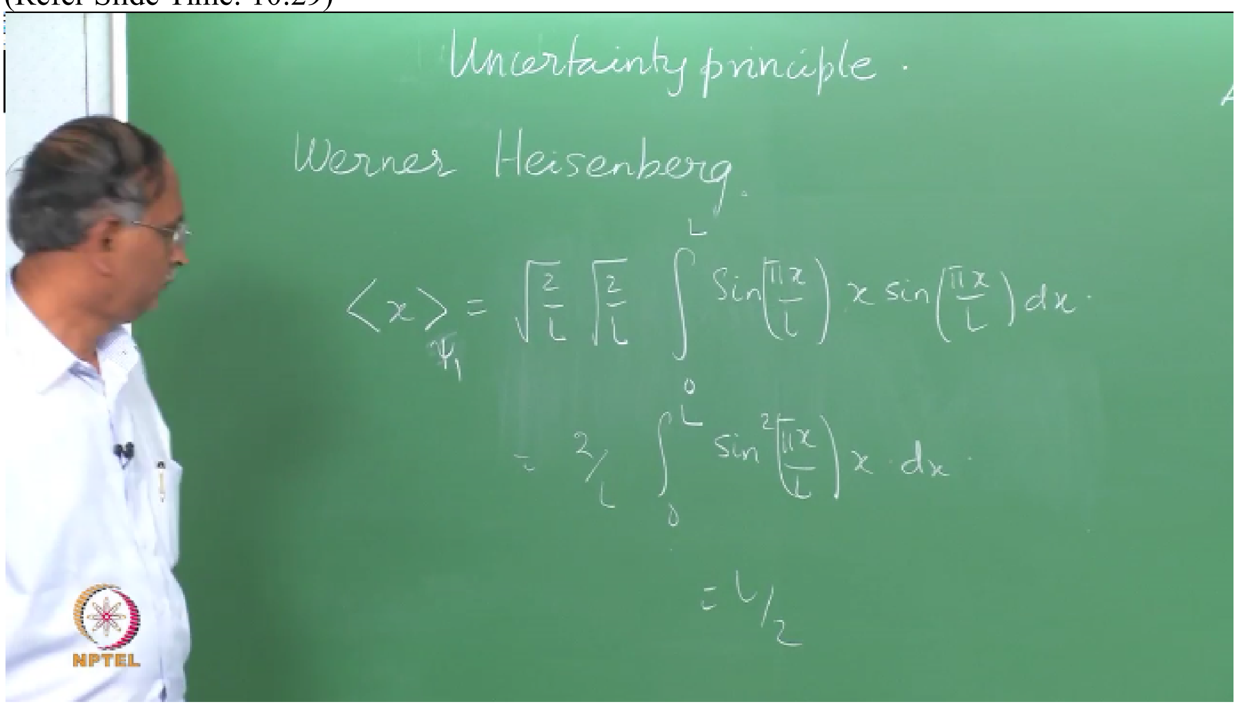

What about the momentum? You have to be careful in ensuring that the momentum operator which is a derivative operator is placed as written here namely 2/L that comes from the two constants sai star sine, then you have sine pi X/L between 0 to L, and the momentum operator is -IH bar D/DX acting on sine pi X/L DX,

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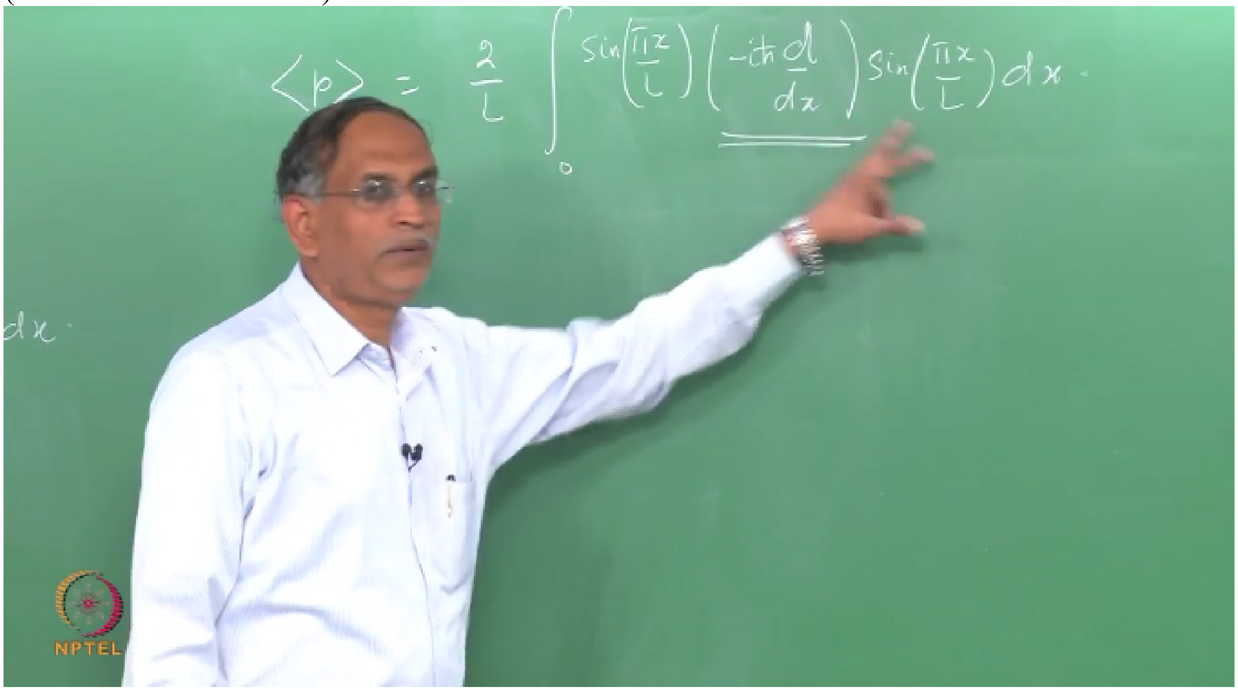

see that the operator is sandwiched between the wave function and the complex conjugate of the wave function, but here the wave function is real therefore you don't see the difference between the two.

What is this? It's very easy to see that this will give you, the derivative will give you a cost and a sine cost will give you a sine 2 pi X/L and that in this interval is actually 0.

What about the average value of P square? The average value of T square is given by 2/L again sine square, sine pi X/L, and now you remember it's -H bar square D square/DX square for the operator P square, sine pi X/L DX, and it's between 0 and L,

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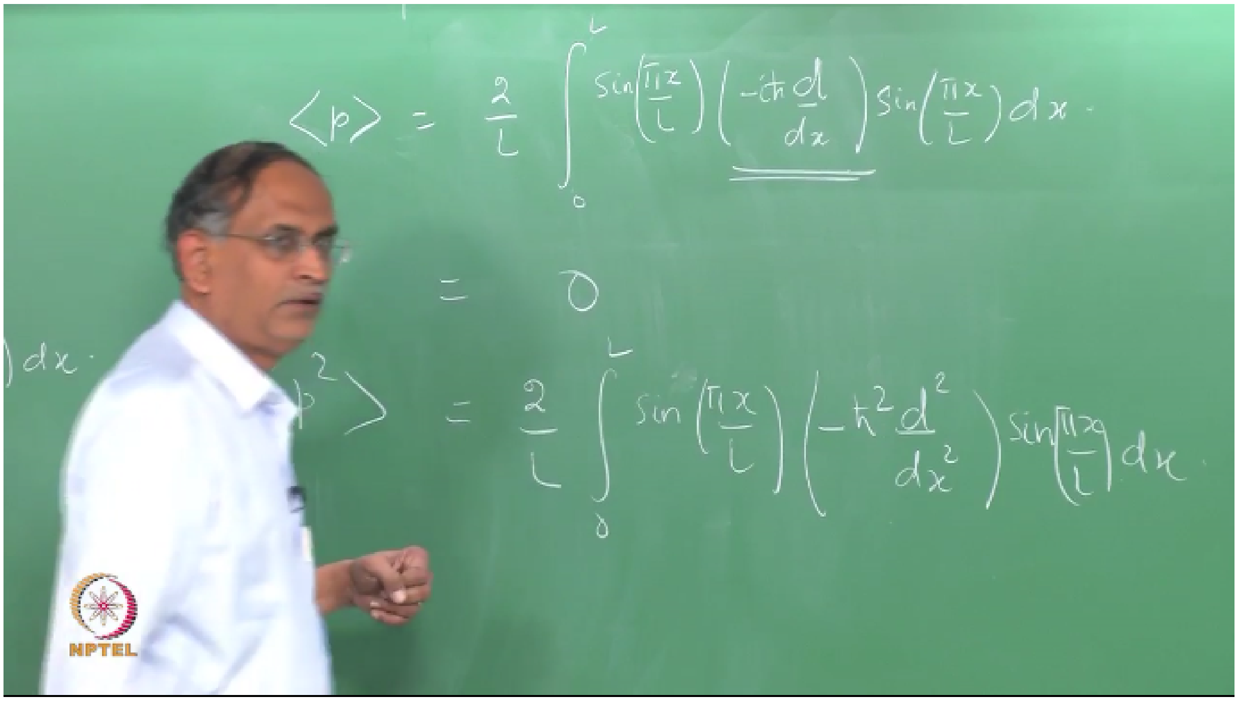

I didn't write the denominator because we have chosen the wave function by ensuring that the wave function is the integral of the square of the wave function is actually 1 in the entire region, therefore I didn't write the denominator that's 1. This of course you know is nothing but 2M E the total energy, this is P square on the wave function you remember P square by 2M on the wave function gave you the E therefore this is 2M E, therefore you see that P square is immediately given by the energy that we know, you can write that okay.

What about the X square? If I have to do X square all I need to do the same thing, write X square on sai 1, and I have the integral that needs to be evaluated is integral 2/L sine square pi X/L and X square DX, therefore you know the value of X square, you know the value of X, you know the value of P and 0, you know the value of P square as nothing but 2M E,
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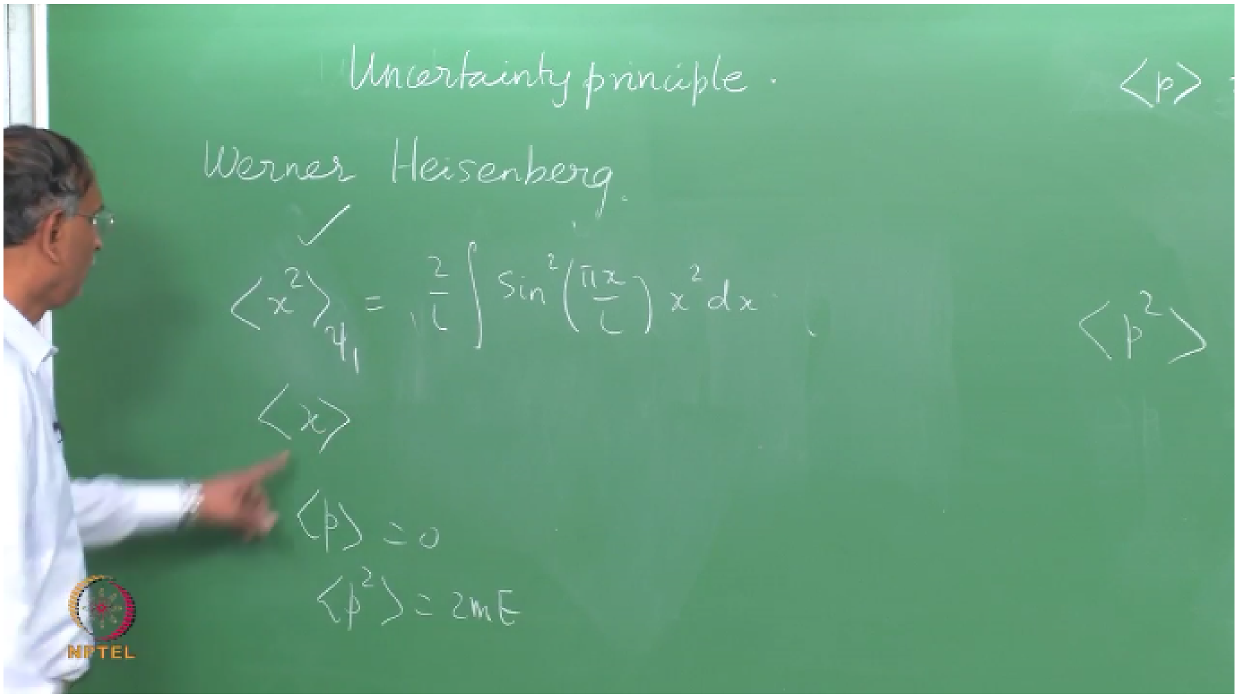

this is the only integral that I have not calculated once you have done that you can calculate delta X, delta P as nothing but the square root of P square, -P of course you know that's 0 times X square -X whole square okay.

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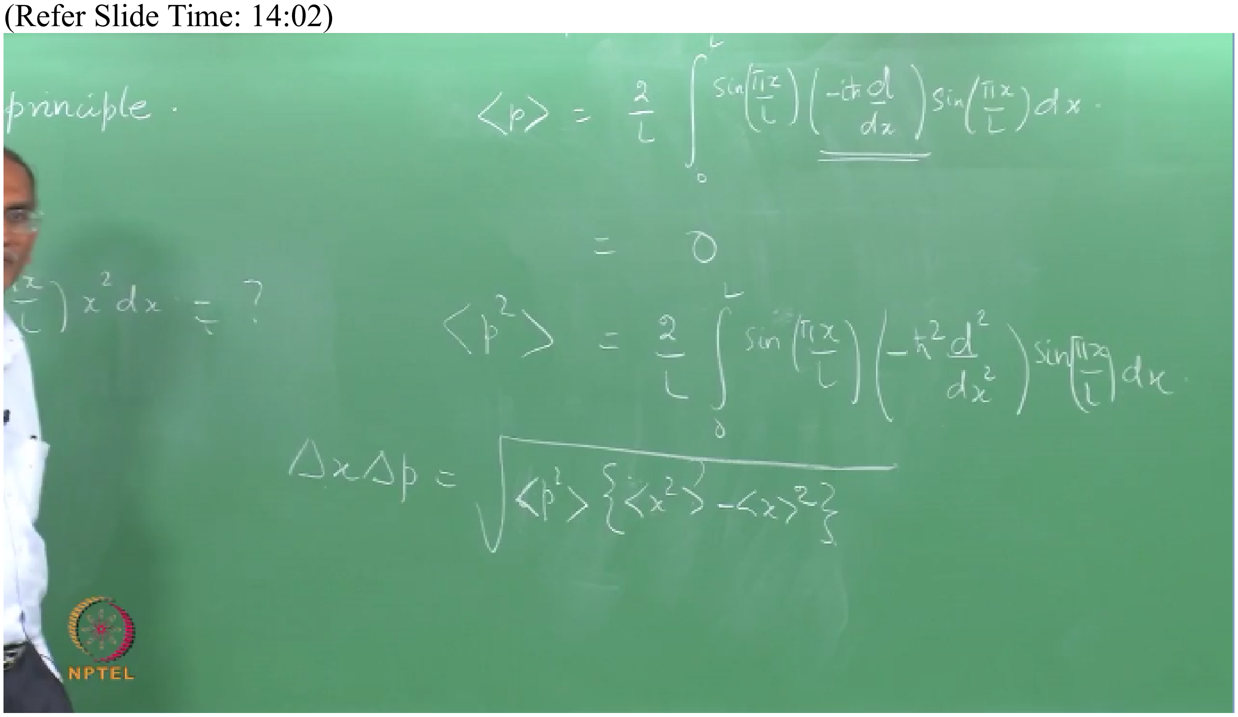

And you should be able to verify that this answer is greater than or equal to H bar/2, okay, so this is the statement of the Heisenberg's uncertainty principle for the particle in a one dimensional box.

Now exactly the same statement can be extent, I mean it can be extended to particle in the two dimensional box except that now you have X and Y 2 two independent coordinates, PX and PY as two independent coordinates, therefore you have a corresponding uncertainty relation in 2 dimensions with one exception namely X and Y are independent coordinates, therefore X and PY can be simultaneously measured or can be ascribed as a property to the system, Y and PX can be simultaneously specified for the particle, X and Y can be specified, PX and PY can be specified, but not X and PX and Y and PY, that's 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 more permutation that would 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 the delta X I gave you and the definition for the delta P I gave you those are fundamental, I've not told you where they come from maybe in a separate lecture or in the class when we discuss these things through the 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 postulatory basis of quantum mechanics for this course in the next part of this lecture which is the third part for the particle in a 2 dimensional box. With that we will complete the two simple modules particle in a 1D and a 2D box.

We will meet again for the last portion of the particle in the 2D box lecture the next time. Thank you.

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