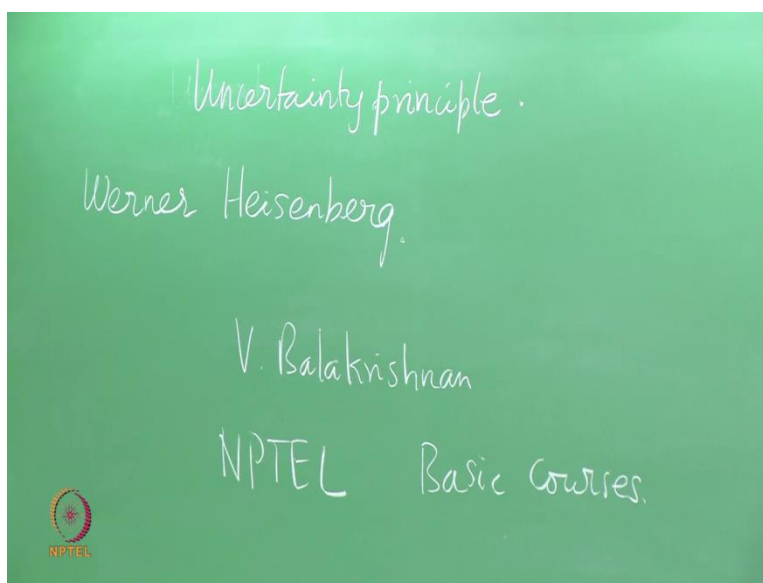


Introductory Quantum Mechanics and Spectroscopy
Prof. Mangala Sunder Krishnan
Department of Chemistry
Indian Institute of Technology, Madras

Lecture – 4
Part II
Uncertainty principle

(Refer Slide Time: 00:28)

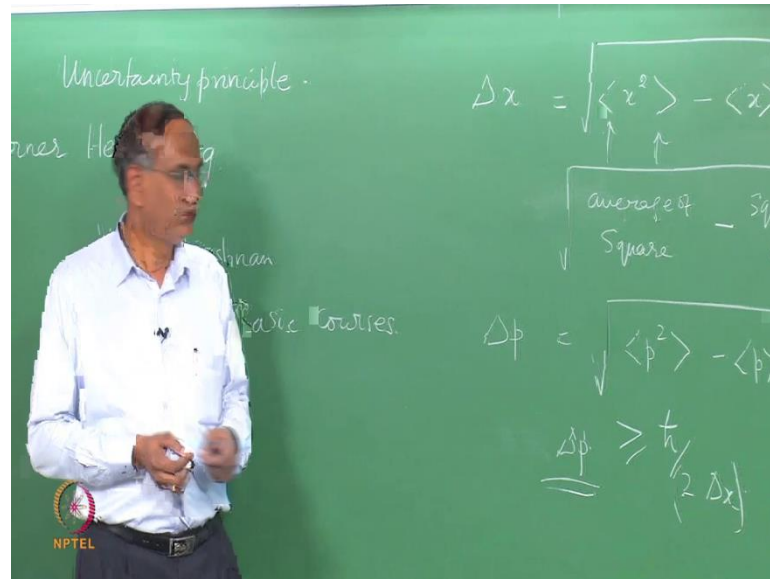


So, we shall continue the particle-in-a-two-d-box, but for the moment let us consider a little bit on this famous principle, called the uncertainty principle, which was first put forward by Werner Heisenberg.

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

(Refer Slide Time: 01:40)



Now, uncertainty, delta x in any measurement, 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, square of the average of that variable and this whole thing is under a square root.

This is the angular brackets, tell you 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 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, that is the, 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 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.

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 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 yes, in the denominator, therefore the uncertainty in Δp is very large, 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.

What it also means is, that position and momentum cannot be simultaneously used as variables for describing the state of a particle as, 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. 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 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 cannot 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's lecture tells you how to generalize the Heisenberg's uncertainty states in using other classical formulations and eventually, what is known as the commutator.

(Refer Slide Time: 06:41)

The image shows handwritten notes on a green background. At the top, the wave function is given as $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$ with $n=1$ to the right. Below this, the average value of position is written as $\langle x \rangle = L/2$, with the word "Average" written above it. To the right of this is a graph of the wave function, showing a single positive half-sine wave from $x=0$ to $x=L$, with a vertical line at $x=L/2$ and the label $L/2$ below it. In the center, the expectation value formula is written as $\langle A \rangle_\psi = \frac{\int \psi^* \hat{A} \psi d\tau}{\int \psi^* \psi d\tau}$. To the right of this formula, the word "Postulate" is written and underlined. In the bottom left corner, there is a small circular logo with the text "NPTEL" below it.

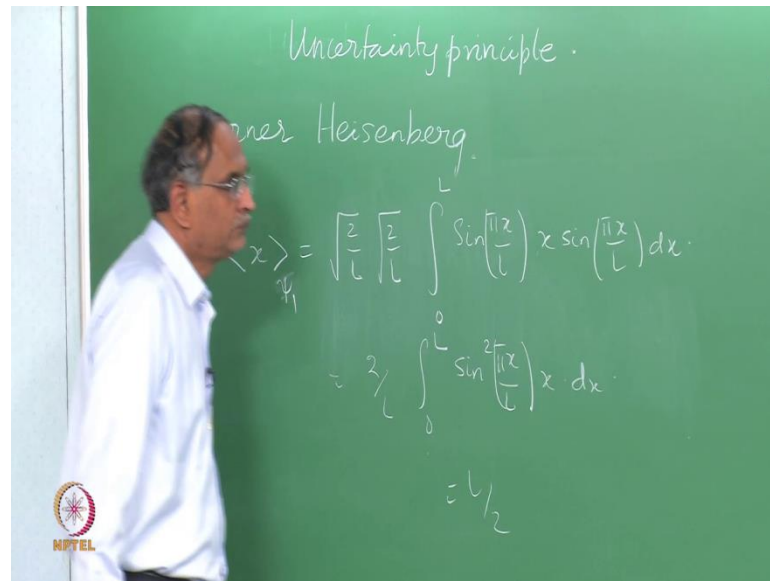
Now, let us use the wave function ψ of x for the one-dimensional box, $\sqrt{2/L} \sin \pi x/L$, we will take the n equal to 1 case quantum number. And if we try to calculate the average value x for the particle in this state whose wave function and the probability of the particle at various points is symmetrically the same on either side of $L/2$, 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 is also the expectation value or the average value, this is called.

The average value in quantum mechanics for any variable A in the state ψ is given by $\int \psi^* \hat{A} \psi d\tau$, 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 three-dimensional divided by the integral $\int \psi^* \psi d\tau$. This is a postulate.

I do not 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 \hat{A} , and the \hat{A} is between the wave function ψ and the complex conjugate ψ^* , if ψ is a complex function, otherwise both of them are ψ .

This prescription must be kept in mind. This is introduced as a postulatory form.

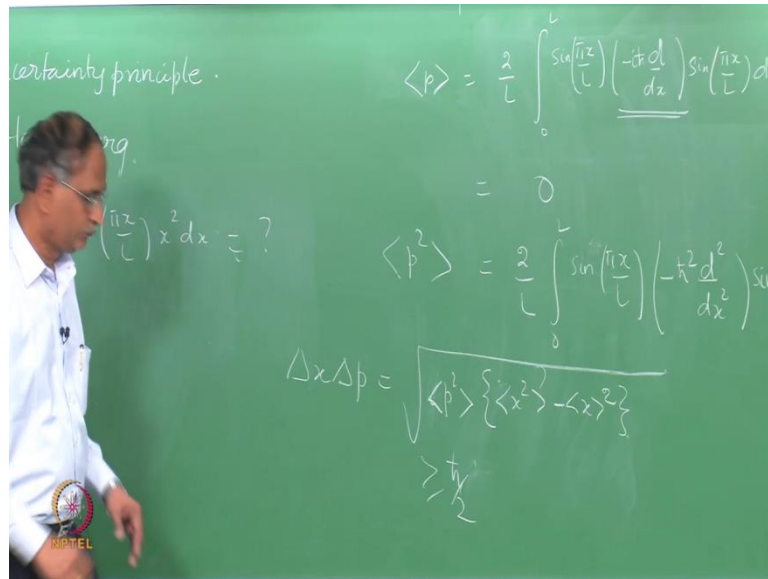
(Refer Slide Time: 09:35)



And let me calculate the x for the particles, it is very easy now. Therefore, the average value x is given by the integral $\frac{2}{L} \int_0^L \sin^2\left(\frac{\pi x}{L}\right) x dx$, because it is $\psi^* \psi$ and you have $\sin\left(\frac{\pi x}{L}\right) x \sin\left(\frac{\pi x}{L}\right) dx$ between 0 and L for the particle in the quantum state with the quantum number 1, which is what we call as ψ_1 . And x , of course, does not change anything. I mean, it simply multiplies to this, therefore this integral is $\frac{2}{L} \int_0^L \sin^2\left(\frac{\pi x}{L}\right) x dx$.

Calculate this integral, and show that the answer is $L/2$; that is for you to do the exercise.

(Refer Slide Time: 10:41)

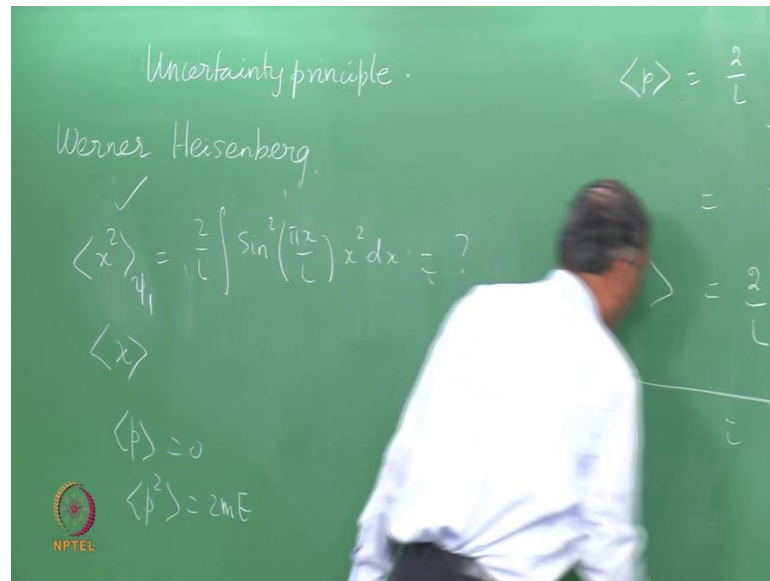


What about the momentum? You have to be careful in ensuring, that the momentum operator, which is a derivative operator is placed as written here, namely, 2 by L , that comes from the two constant ψ star, ψ . Then, you have sine πx by L between 0 to L and the momentum operator is minus $i \hbar$ bar d by dx acting on sine πx 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 sine \cos will give you here sine $2 \pi x$ 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 sine square sine πx by L . And now, you remember it is minus \hbar bar square d square by $d x$ square for the operator p square sine πx 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 one.

This, of course, you know is nothing but $2mE$, 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 $2mE$. Therefore, you see, that p square is immediately given by the energy that we know, you can write that.

(Refer Slide Time: 12:58)



What about the x square? If I have to do x square all I need to do is the same thing, write x square ψ_1 and I have the integral, that needs to be evaluated is integral 2 by L sine square πx by L times x square dx . Therefore, you know the value of x square, you know the value of x , you know the value of p as 0 , you know the value of p square as nothing but $2mE$.

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. 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 \hbar by 2 . 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, I mean, it can be extended to particle in the two-dimensional box except, that now you 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, namely, x and y are independent coordinates. Therefore, x and p_y can be simultaneously measured or 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 the Δx I gave you, and the definition for the Δp I gave you; those are fundamental. I have not told you where they come from, may be in a separate lecture or in the class when we discuss these things through elaborations. I will tell you about the origin of the Δx and Δp , but these are definitions, which you have to start with, working, and then feel more comfortable and 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, 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 the 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.