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Chemistry I
Introduction to Quantum Chemistry
And Molecular Spectroscopy

Lecture – 10
Schrodinger Equation
Particle in a One-dimensional Box: Part II

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So let us continue from where we left, namely the wave function sai N(x) as root 2/L sine N pi X/L, and the energy EN as H square N square/8MLsquare,
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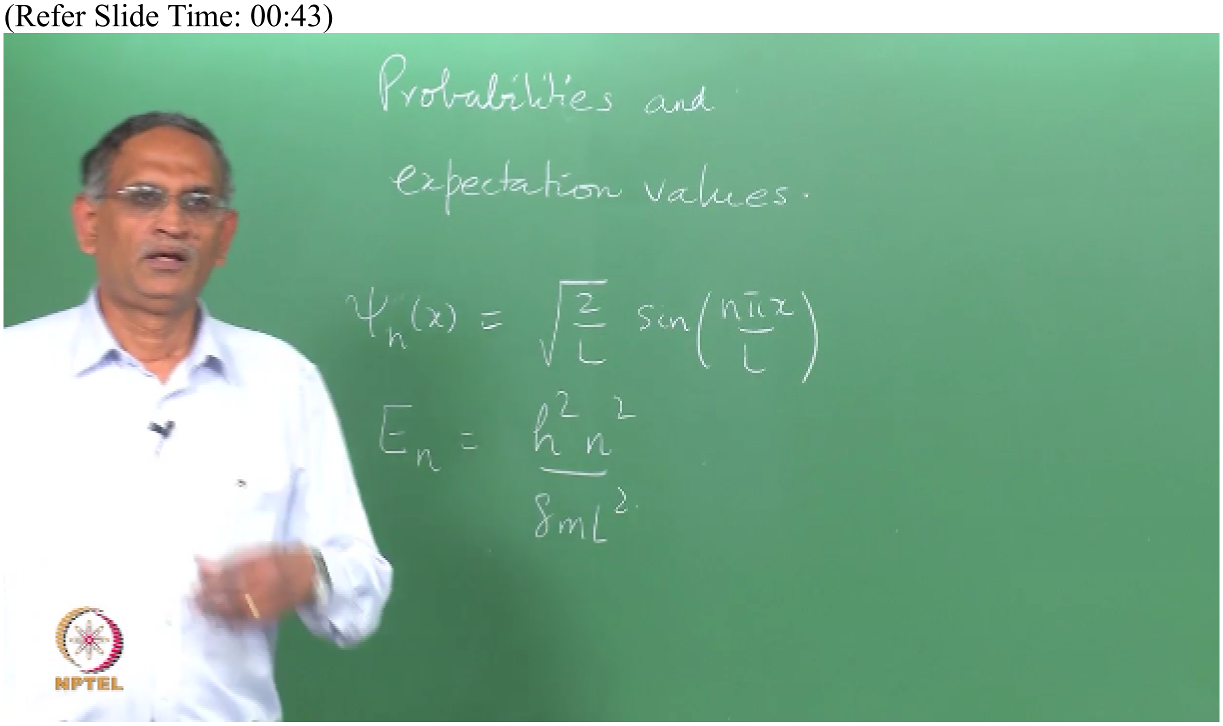

since sai star sai is the probability density at any point X, and sai star sai at the small interval DX around X gives you the probability that the particle is in that small region.

If you plot sai square(x) as a function of X
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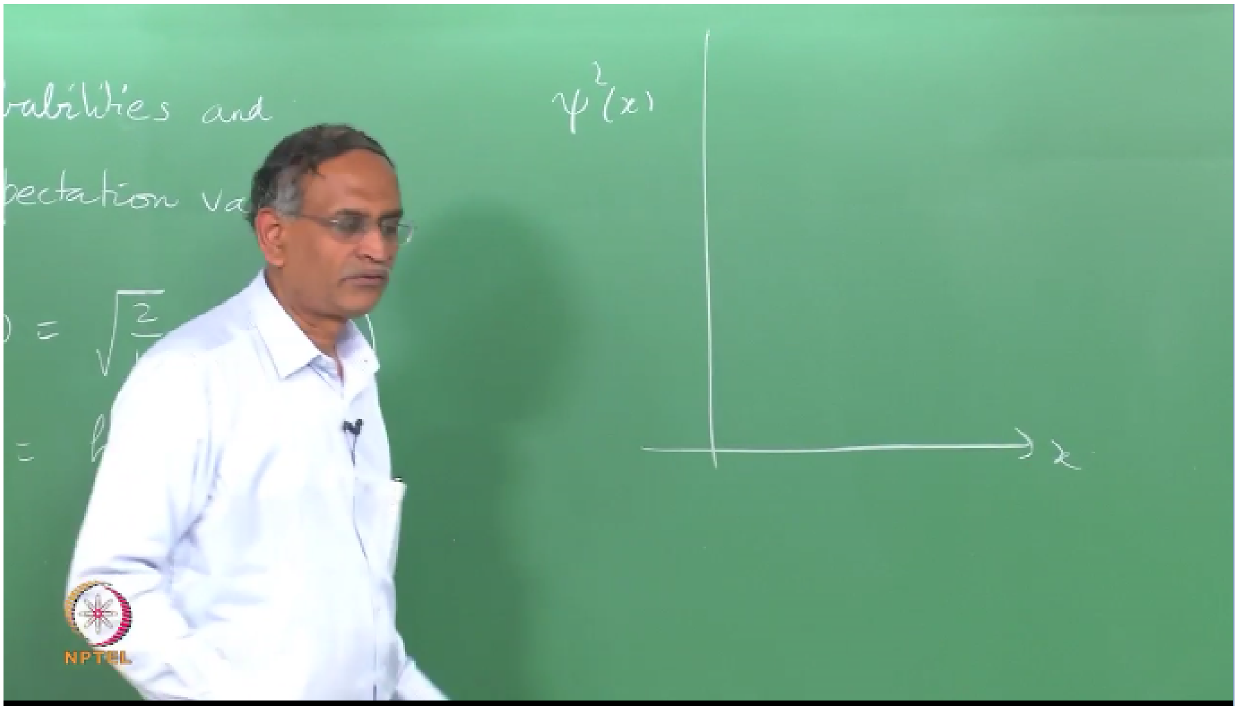

you get some ideas about what these probabilities mean, so let me show this graph for some value of the box length L,
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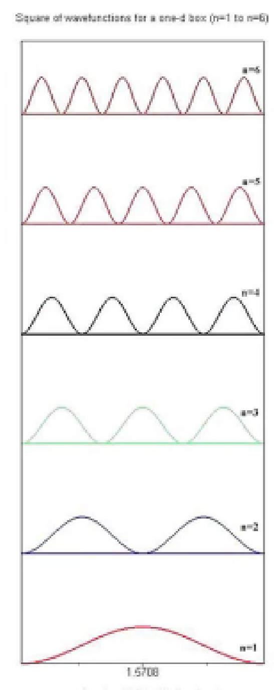

okay, and we have a root 2/L which is a pre-factor for the wave function, so the wave function has a dimension, it has a dimension of 1/square root of the length, okay, and then you see that sai star sai DL takes care of the probability being a number, okay.
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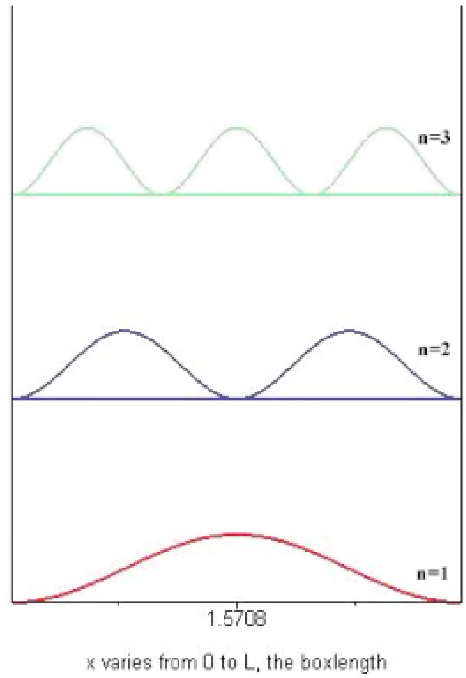

Now if you plot the sai star sai for the first wave function namely N = 1, you see that this is nothing but the 1/2 sine wave with a little bit of tapering on the edges, when it is N = 2, please remember that the expression if you look at the wave function, here is the wave function itself if you look at the wave function N = 1 is a 1/2 sine wave, N = 2 is a full sine wave, this is a 3 1/2 sine wave and so on, therefore if you take the square of this wave obviously the picture that you get is the picture that I showed you now.

So this is the square of the N = 2 wave,
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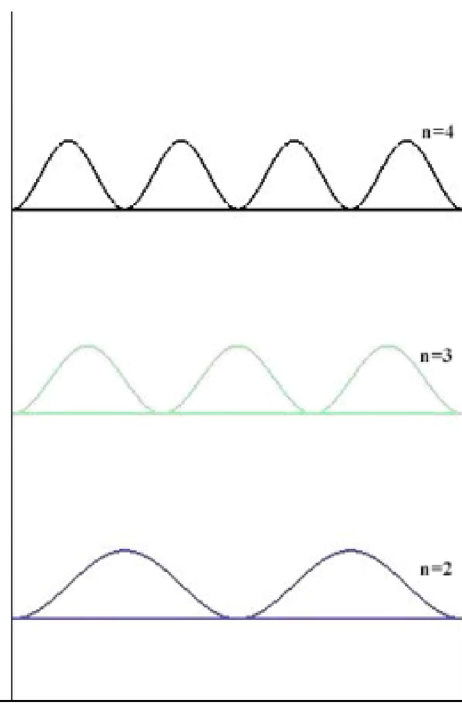

and this is the square of the N = 3, sine 3 pi X/L, since it is 0 to L you have that shape, and also the shapes for N = 4, and as you see that as N increases these oscillations become so close to each other that for very, very large N it looks like that the probability density is uniformed, okay.

What does that mean? If we have to do this exercise for a classical system, let's assume that the particle is moving in the box in some way and let's not ask the question how does it get deflected from one end to the other end, there are questions for which we don't have any answers, and questions which are also meaningless, let's assume that we are looking at the particle at a given instant of time and using a small window, if the particle is moving at constant speed because it's kinetic energy is a constant energy E and if it is a constant then the probability of locating the particle in every small region of the same size is uniform, it's the same value that's what is meant by this particular flash movie telling you that the probability P1
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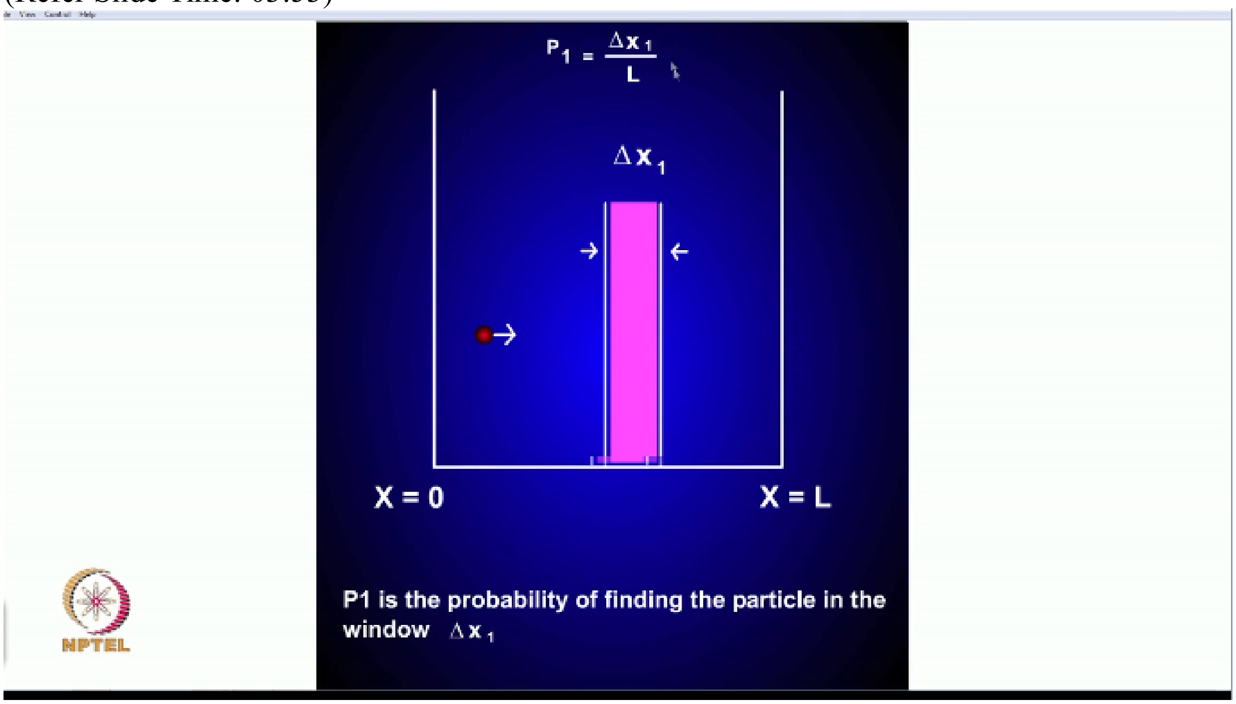

for an interval of delta X if you are locating the particle in that interval across this, it's uniform.

Now if the delta X is different it's going to be different by that corresponding ratio namely delta X2/L,
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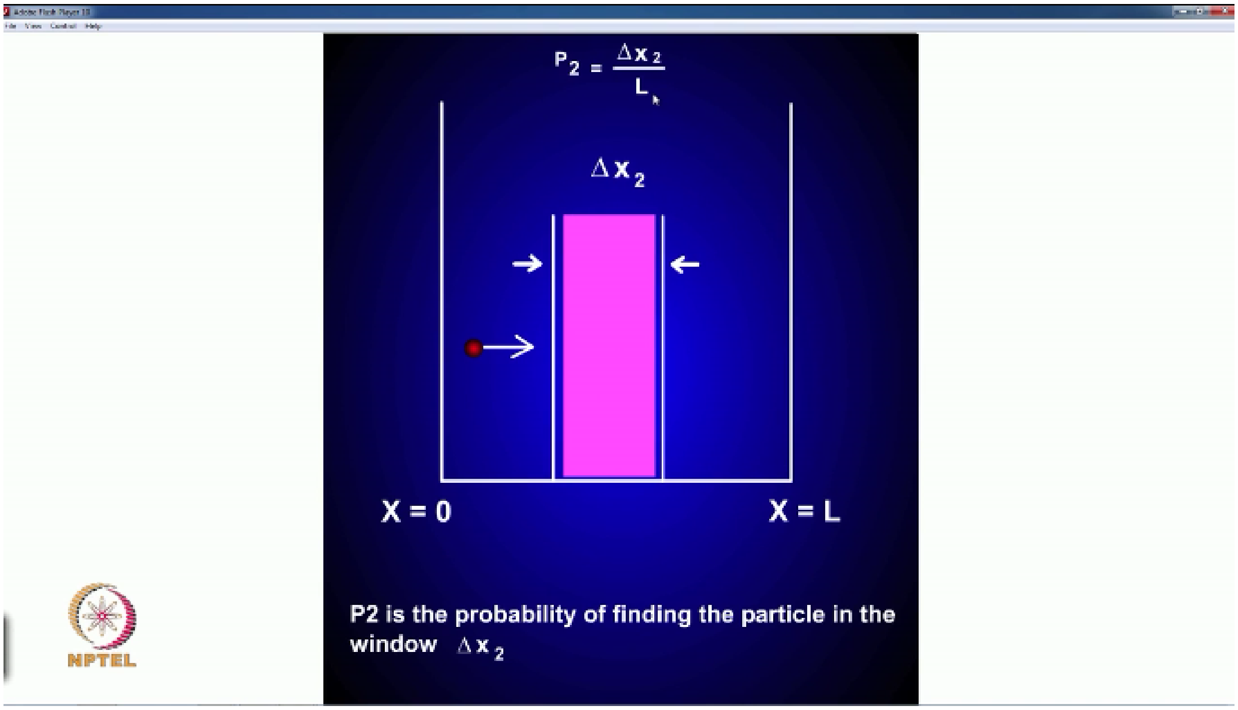

this is what we expect the particles position and its probability to be associated with, but in quantum mechanics we don't see that in this particular case we see a slightly different result,
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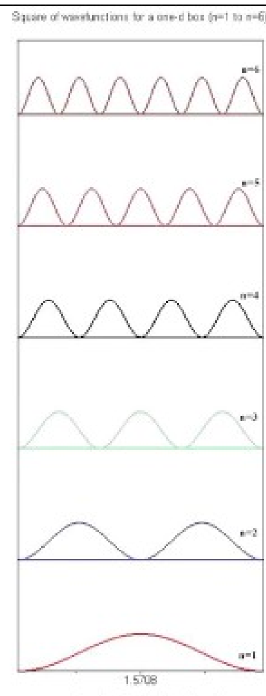

you see that the probability is not uniform and the probability is also not the same for different energies at any given location.

So let's look at this particular graph here, let's look at this region right in the middle for N = 1
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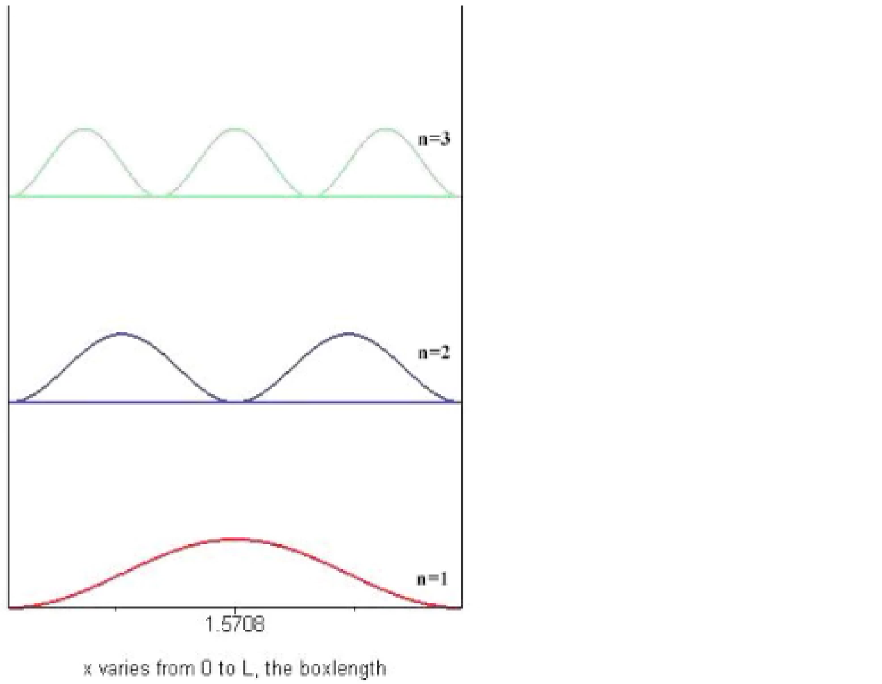

the red line, you see that near the middle if you are looking at a probability of this kind, the way to represent this is using this simple picture, and if we have the function in this finite region, the probability in the middle region for a small interval DX if you are looking at it, it's the area here DX, okay,

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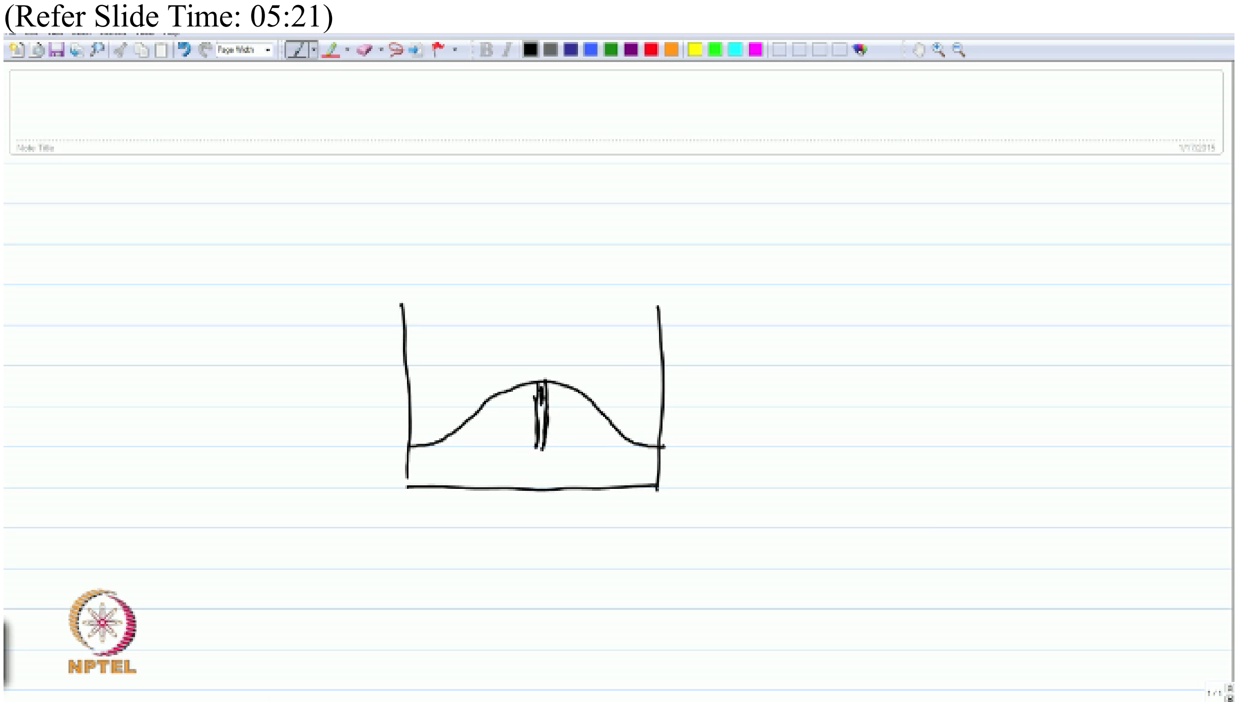

such small this sai square calculated right at the middle value of the interval, and likewise if you have a particle with a slightly different energy, this energy is E1 and that's H square/8ML square.

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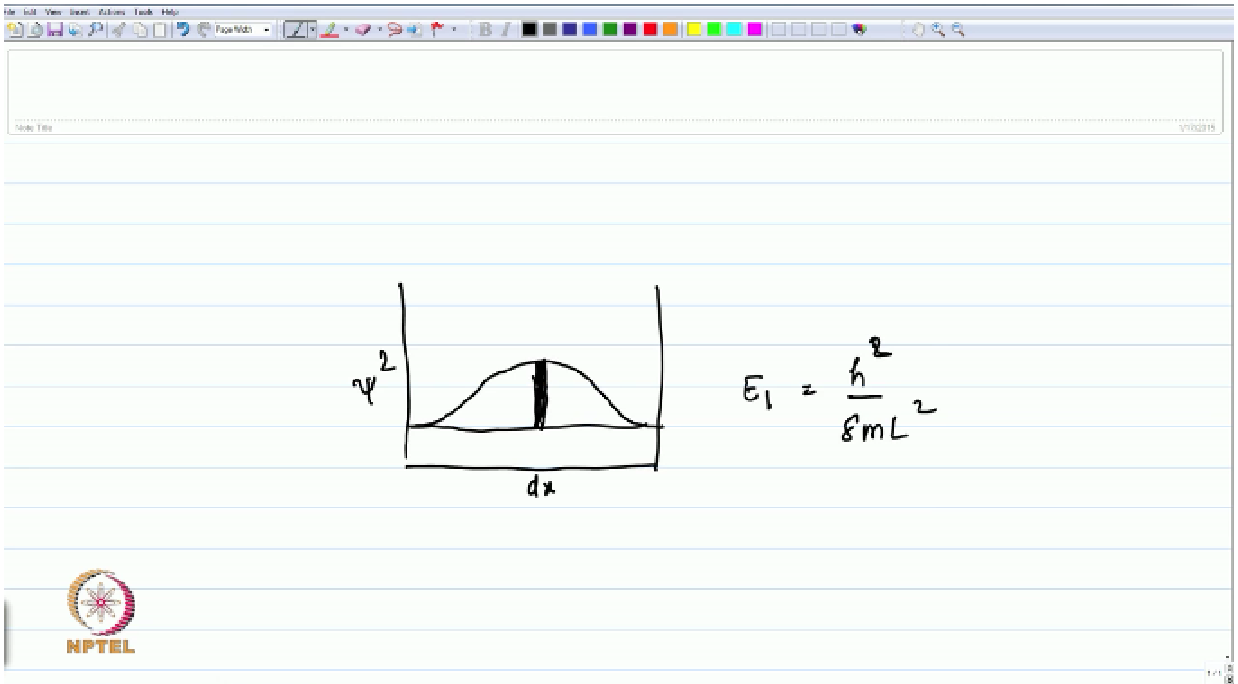

If the particle has energy E2, now you see that the sine wave gives you for the same thing a two components, a maximum at this point and again a maximum this is L/4, this is L/2, this is 3L/4 and this is L, and this is 0, okay,

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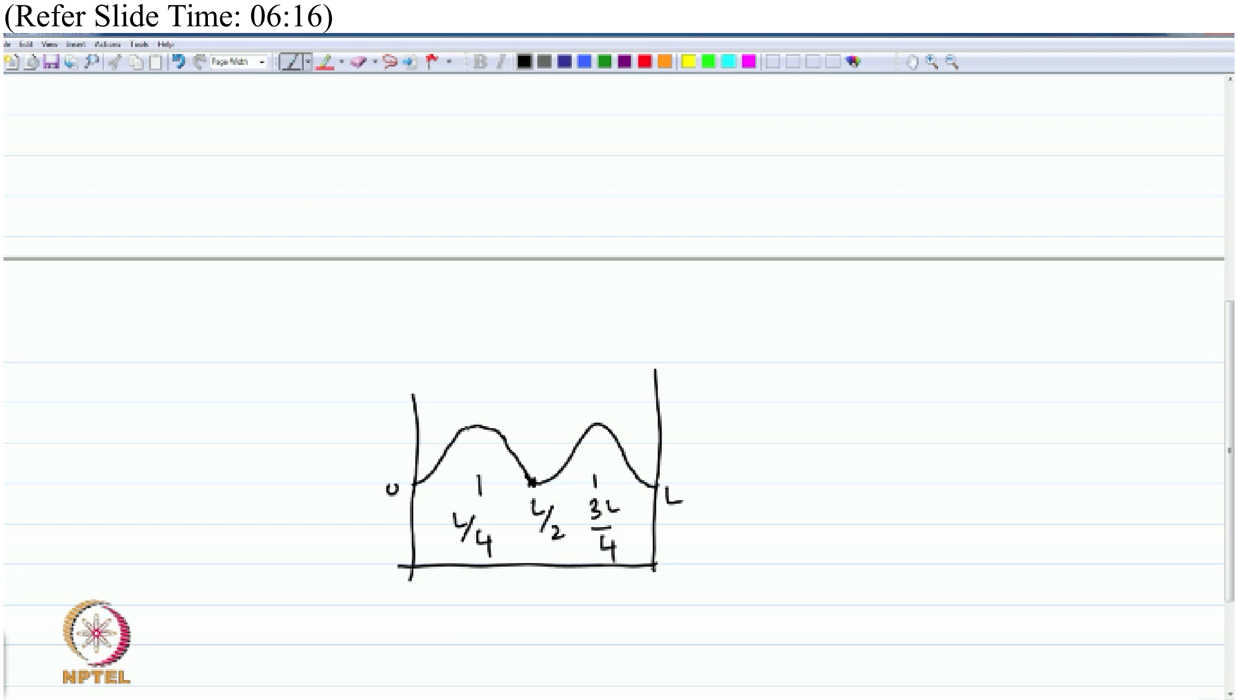

so you see that the probability maximizes in the intermediate regions L/4 and 3L/4, but its minimum in the middle, and also the probability is not uniformed, the probability of locating the particle in a certain region is dependent on what that region is, and also what the energy associated with that particular wave function is for that particle, so this is something very unique and very special with quantum mechanics, and it's not something that we can immediately accept as a, I mean something that makes sense, that's a way it is if you write the Schrodinger equation and if the interpretation of Max Born as the most meaningful interpretation for the wave function is to be accepted then these are consequences with that accepting those, what are called the cornerstones.

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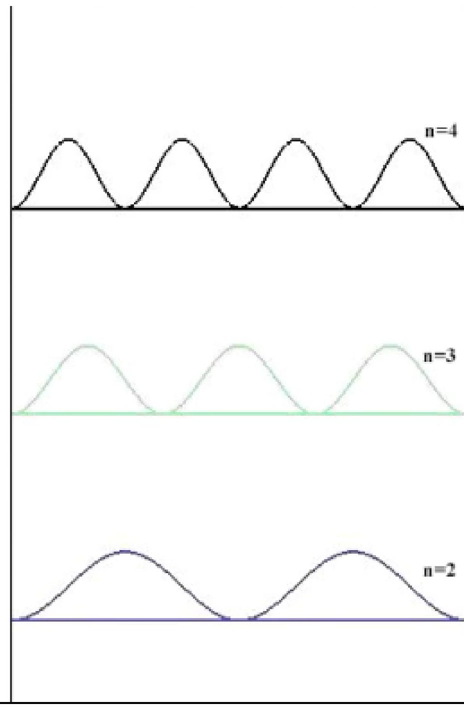

And the probability varies depending on what the energy is as you see in this particular graph, you see that the probabilities according to the square of the wave function plot that you have here, for example in the 1/4th length of the box or the 3/4th length of the box is different, and you have a little bit of a different energy then you see that at that point it's actually very nearly 0, and then it varies but what happens when N becomes extremely large you see that all these things become more or less uniform, I mean there's so many oscillations that if you take any particular small region if the N is extremely large the probability of locating the particle in that region is nearly the same as locating that particle in any other, but the same extent of that region, therefore the classical idea gets closer and closer to the reality of a quantum equation when the energies of the particles become extremely large.

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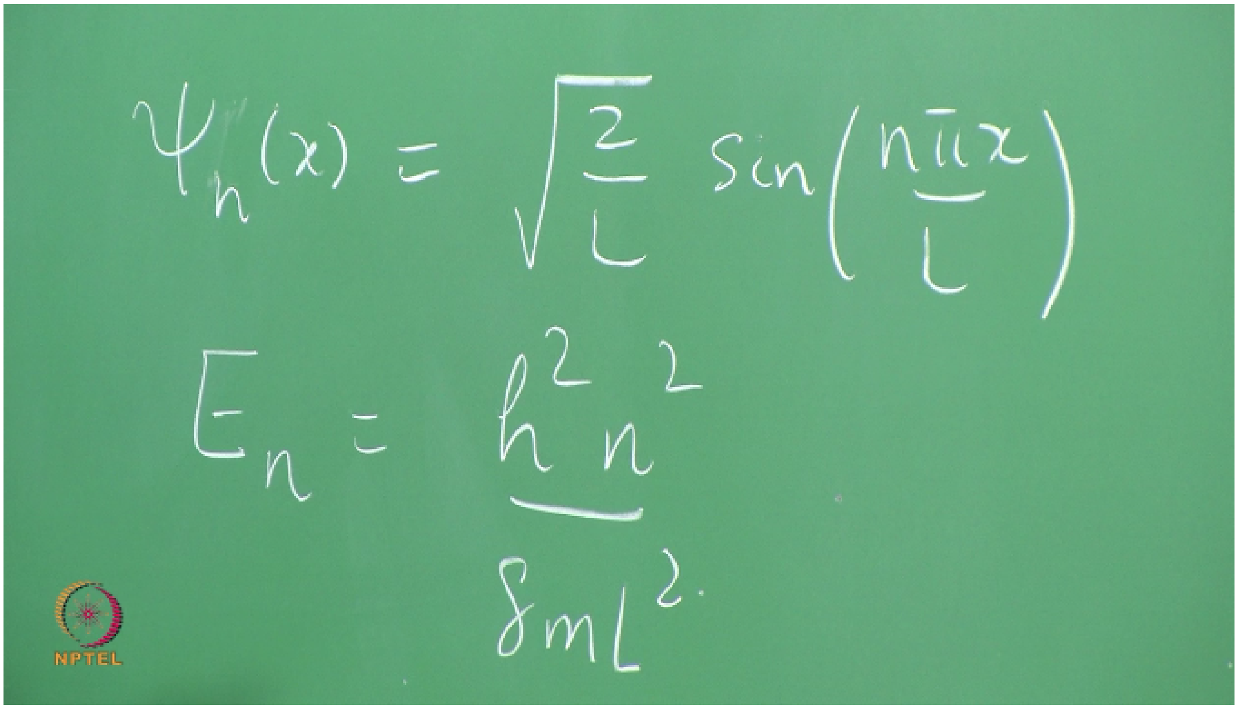

Now there are two conditions namely in the energy expression that you have here, you remember H square and the N square, the mass of the particle is M and the length of the box L

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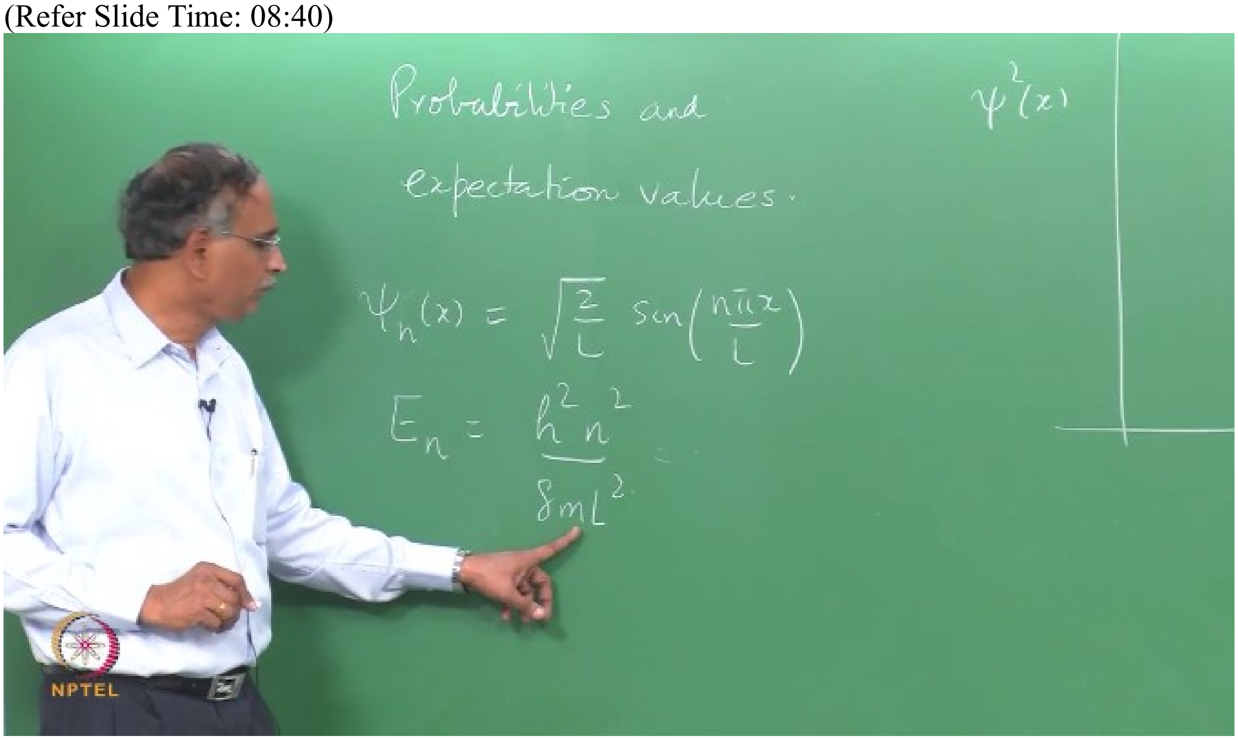

both of them determine what is the spread between different energies, so if you plot E1, it's 1 times H square/8 ML square E2 is 4 frames that unit E3 is 9 times that unit E4 is 16 times that unit, and as you increase this energy you see that the gap between the energies increased,

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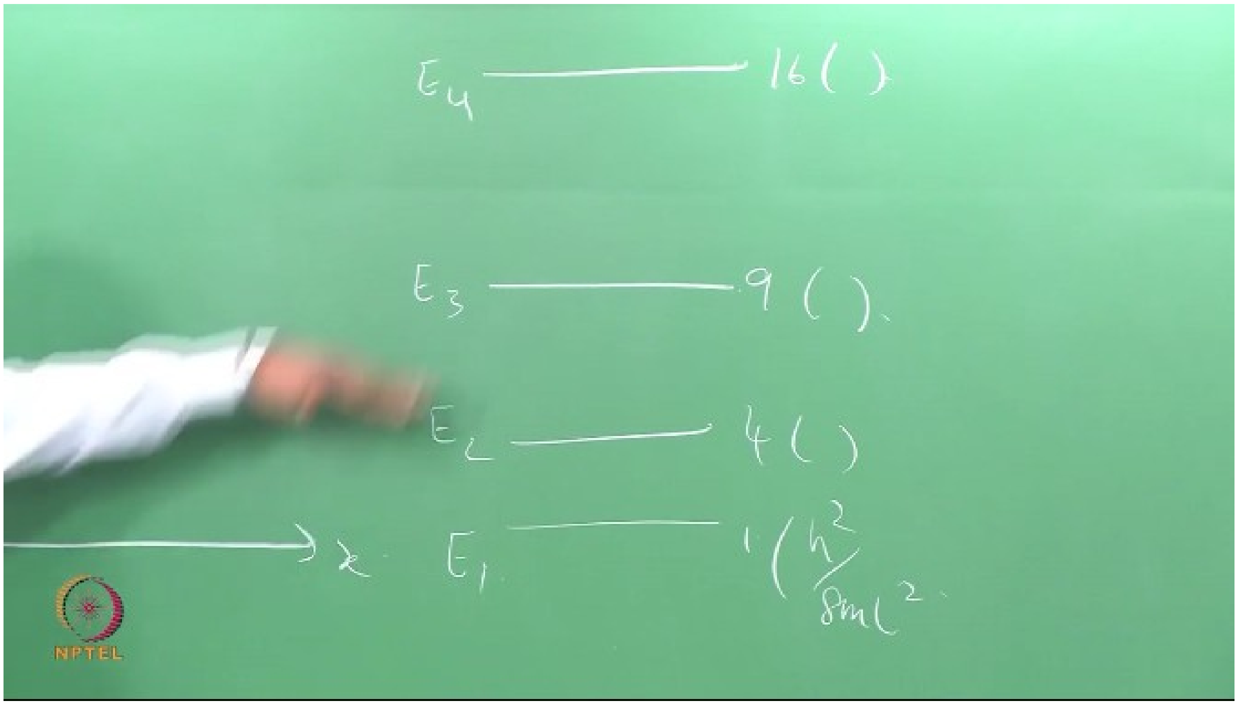

but you can also see the following namely as you increase these energies the probabilities of finding the particle in any given region more or less approaches a constant value, which is proportional to the extent of that region divided by the total length of that region for very, very large values of N, that's the classical limit and that classical limit can be obtained by doing some manipulations here by choosing a heavy particle so that the gaps are smaller, and therefore the larger energies are reached very quickly or the length of the box is very large.

Macroscopic dimension, macroscopic particle you see that the quantum conditions are becoming less and less important but smaller particles narrow region the quantization results are somewhat unique and that's where we have to spend a lot of time trying to understand why quantum mechanics is important for atomic particles in atomic dimensions, when L is very large, when M is very large you see that these quantization energies the gaps between them are not very important and a very large amount of energy that is very high values of the quantum number or easily reached, and the particle behaves more or less like classically, so this is an important, what is called the correspondence limit as one would call it.

And this was first considered by Niels Bohr, the correspondence principle is that quantum mechanics approaches classical predictions, classical mechanical predictions for very very large values of the quantum number as in this case, very large particles of macroscopic dimensions, and particles of microscopic size then quantum is less and less important, and that's how we were never able to discover quantum mechanics until we started looking at the atomic details more and more closely, okay, so this is the association that I would like you to have with the particle in a box model, we will look at the particle in a 2D box and some other simpler models, before we discuss what are called the expectation values or the average values to be seen or to be calculated using quantum mechanics as we will see in the experiments.

We will protect for a later lecture, but remember the message that we have here quantization of energies, probability descriptions, and the probability descriptions being very different from classical expectations, and when the system becomes more and more classical with larger and larger energies, these are the pointers that you have to have in order to understand things better.

In the next lecture we will start looking at, not one dimension but motion in a plane that is there are 2 coordinates X and Y or even 3 X, Y and Z and look at the particles and we'll see one more unique result namely the degeneracy.
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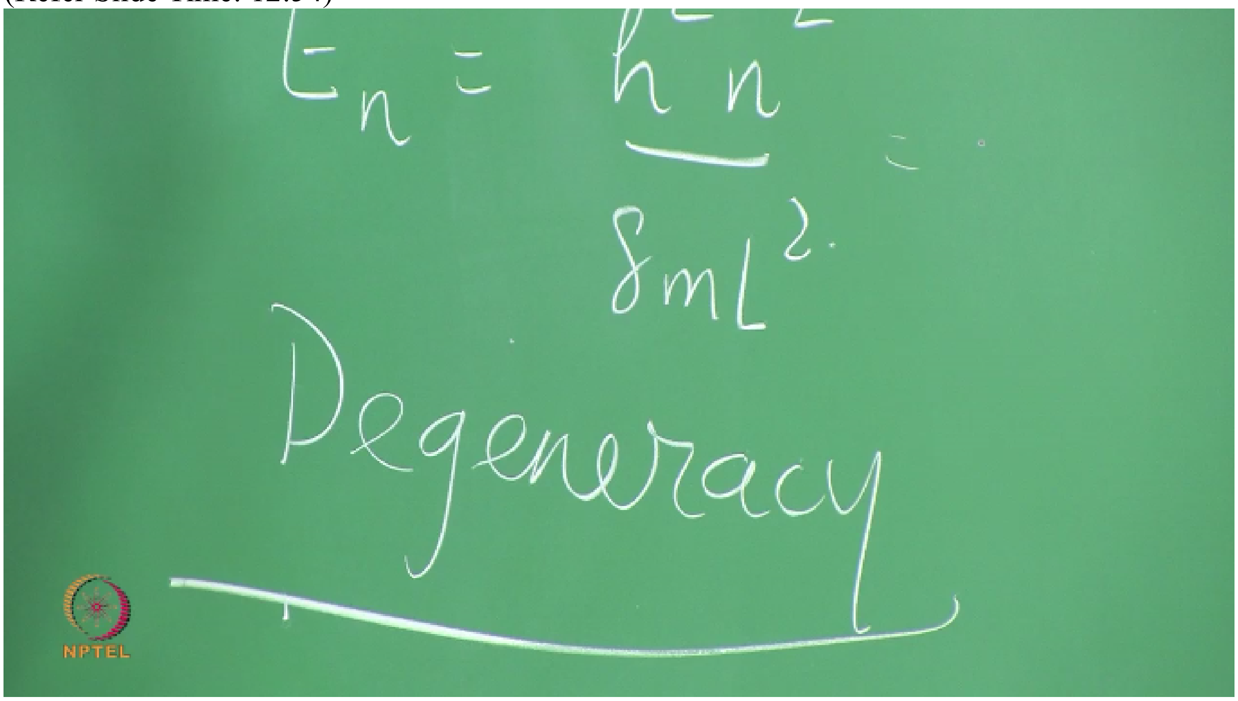

We will look at that in the next lecture, okay. Thank you.

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