Quantum Mechanics
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Lecture – 04
Review of Particle in Box, Potential Well, Barrier, Harmonic Oscillator-II

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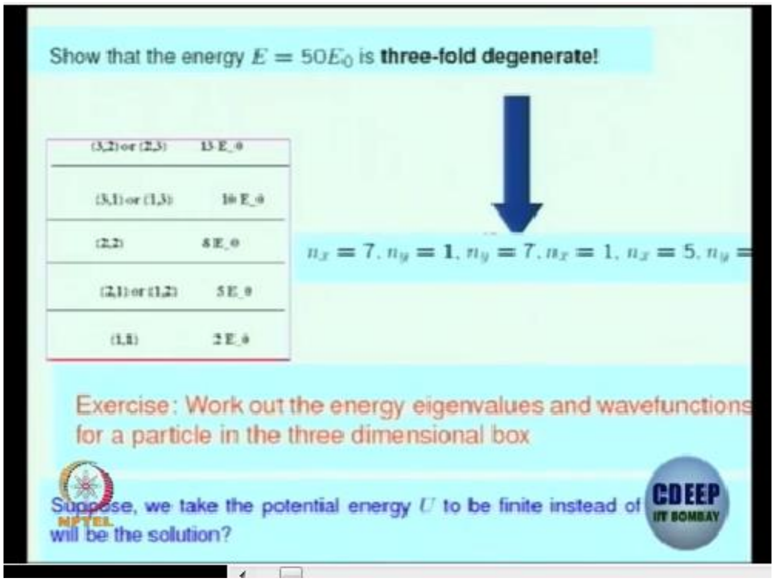

So far we looked at a particle trapped inside a box due to this potential which is infinity at some boundaries. If you make that potential energy to be finite, what are the new features you start seeing?

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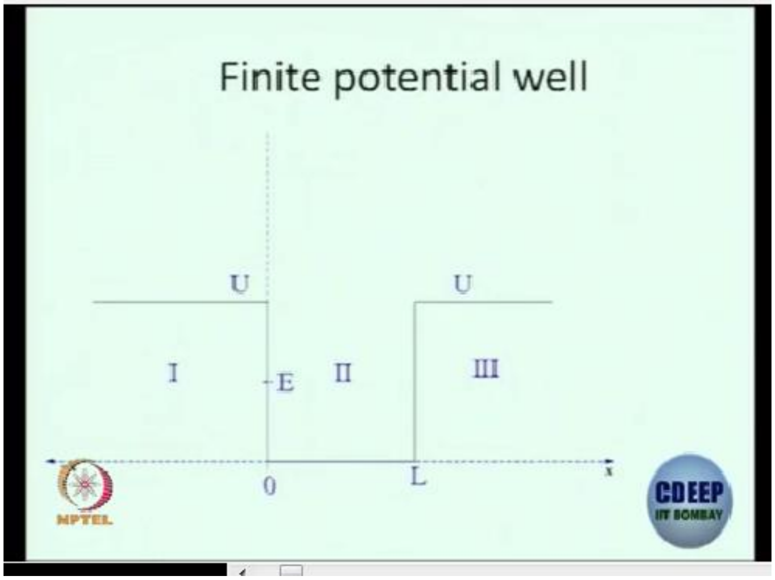

And what is the new solution? These are questions you can ask. This also you have done in the context of 1-dimensional potential wells, right. What do you do? You break it up into region I, region II, region III. Region I and region III are almost similar. And region I goes up to -infinity. Region III goes up to positive infinity and you have an intermediate well region. And if the energy which I have marked as E is < U, then you can have a kind of a classically, it would have been, if the particle was inside, it would have been inside, right. Why?

Because the total energy has to be, cannot become less than the potential energy. So as the thing happens classically, you get kinetic energy to be negative. Kinetic energy negative in classical physics is it allowed? No, not allowed.

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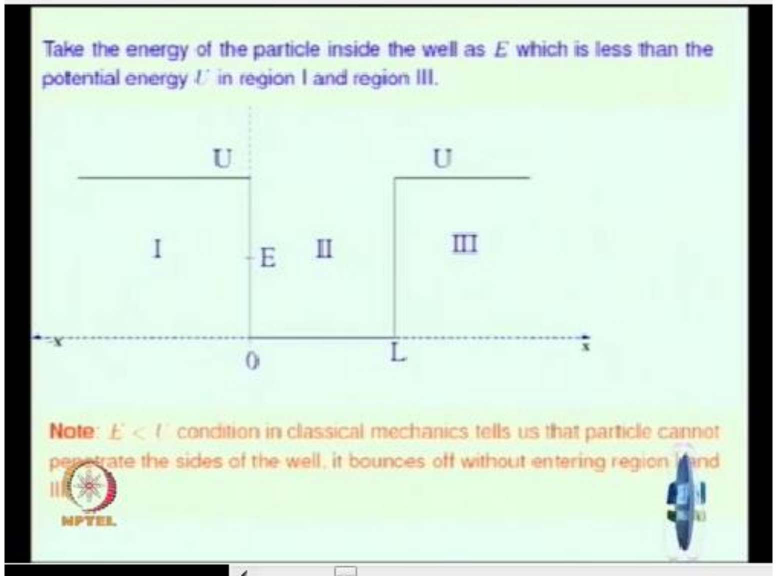

But in quantum mechanics, because we are going to take this to be like it is inside the well with energy less than the potential energy and it is like a wave, there are chances of the wave trickling out into region I and region III, okay. So this is what I am saying here. Take the energy of the particle inside the well as E which is less than the potential energy which is seen in region I and region III.

And now we would like to see this in classical mechanics, particle cannot penetrate the 2 walls, x=0 and x=L because of finite energy. The earlier problem particle in a box is you made U tending to infinity. Now I made U to be finite. But quantum mechanically, you will get non-0 wavefunction in region I and region III. You all agree? Pictorially, okay?

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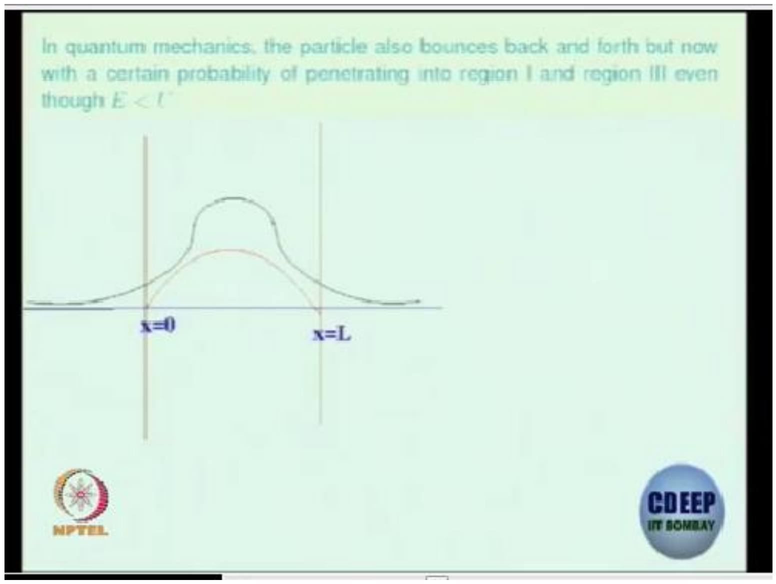

So this is what I said quantum mechanically, there is a certain probability of penetrating into region I and region III even though the total energy of the particle is less than the potential energy, okay. So you can plot the wavefunction. The red line which I have plotted, the red is actually the, what is the red line? Particle in a box with infinite potential energy, ground state wavefunction, right. Everybody agrees?

Sin function, it goes to 0 at x=0 and x=L and what happens, so this is just to be taken as not an accurate answer to the differential equation. The trend of the wavefunction, once you make U to be finite, is that it tapers off in region III and region I and it is not 0 at x=0 or x=L. And it takes care of what all properties? Continuity of wavefunction and derivative of wavefunction to be continuous. It will take care of that. Earlier when we did the particle in a box, we did not need to worry about it. Is that correct?

So some of these things when you see visually, some of these plots, it will register in your mind much better rather than mechanically solving equations. So suddenly the particle in a box has suddenly reduced the barrier from infinite barrier to a certain height. And what all can happen to plot the ground state wavefunction, start showing some tails in region I and region III, okay. What happens to the wavelength?

You can start looking at what will be the de-Broglie wavelength of the particle in an infinite dimensional box. Take a ground state of the particle. What will happen to the wavelength of this? Pictorially you can see wavelength what happens here? Increasing, right. This periodicity of becoming 0, it is L in the context of the particle in a box but it is no longer L, it is more than L. So wavelength starts increasing.

If the wavelength starts increasing, what will happen to the energy? Energy will start decreasing. There you can start arguing without even, can get a quality to be a feel of what happens in realistic situation, okay.

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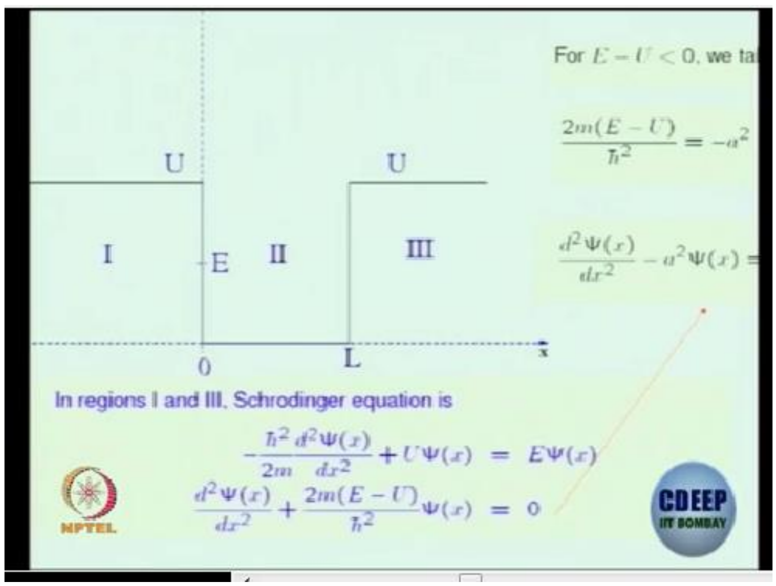

So then that math, formal math which you have all done, region I, region III, you put E<U, right. I am sure you have done this? And you take then since E<U, E-U is negative. You call it as a negative a squared and then you can solve this differential equation. The solutions are exponentially growing and exponentially damping solution in region I and region III.

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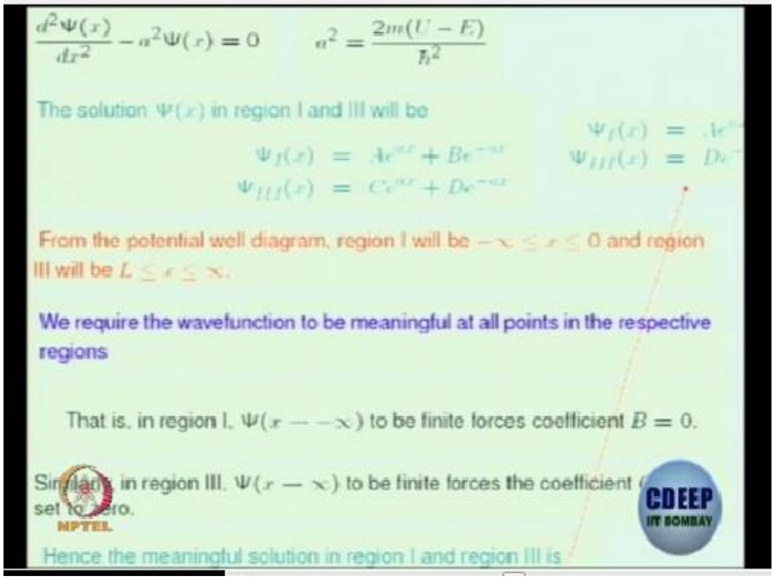

Formally , I am going little fast because the assumption is that you have done these things. It is for you to recall I am going, okay. It is not that this is not the theme of quantum mechanics 1, but you need to know this if you want to do upon in mechanics also. So I do not want to forget. So that is why I am going through this, okay. So region I and region III, formally this is a solution to the differential equation.

But you will start putting in condition that the wavefunction cannot blow up in these regions, right. So that comes from physics. So once you put in the condition that the wavefunction cannot blow up, which coefficients will vanish? In region I as extends to -∞, the one which will kind of blow up is the second term. So you can make the B coefficient to be 0. Similarly, for the region III, which one should be 0? C should be 0, okay.

So this is the physics input. The solution which you wrote in the top, this is blindly looking at a differential equation, you will write the solution, okay. But the physics input is that you needed to be well-defined in the appropriate region which tell you which coefficient can be put to 0? B will be 0 in region I and C will be 0 in region III, okay. So the meaningful solution for region I and region III is $\psi_I(x)$ is $Ae^{ax}$and $\psi_{III}(x)$ is De^{-ax} .

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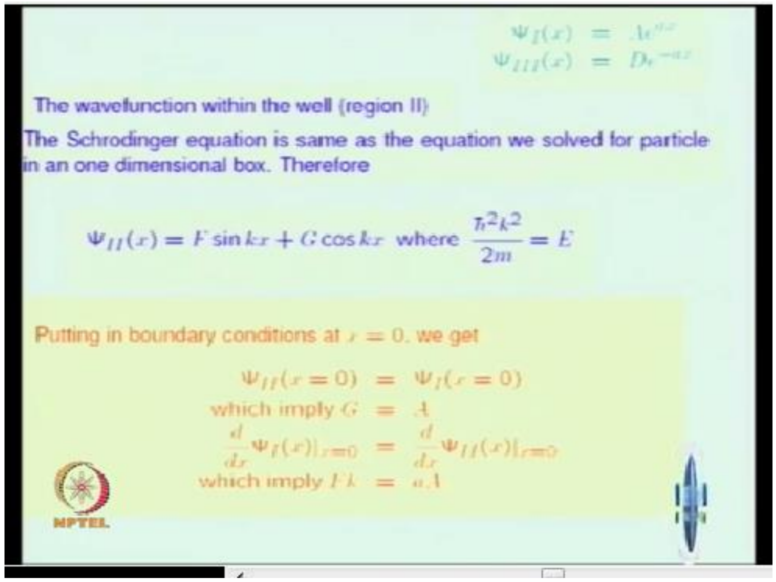

What about region II? Region II is exactly similar to what you did for a particle in a box. Because inside the box, U is 0. So you can solve them which is the sinusoidal function. But since the wavefunction is not vanishing at x=L and x=0, it will be in general a linear superposition of the 2 solutions. You cannot make G to be 0 in this case. G can be arbitrary. Agree? And then you put in boundary conditions, continuity of wavefunction.

What are the 2 boundaries? x=0 and x=L. At x=0, I and II should match. And at x=L, II and III wavefunction, in the region II and region II have to match.

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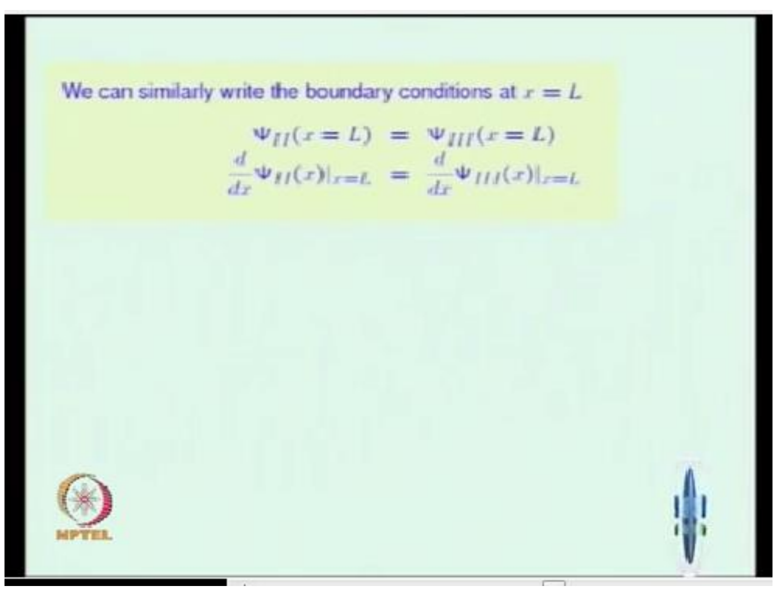

So at x=L, region II and region III wavefunction and derivative of the wavefunction, because the potential energy is finite here. When the potential energy is finite, both wavefunction as well as the derivative of wavefunction should be continuous, okay.

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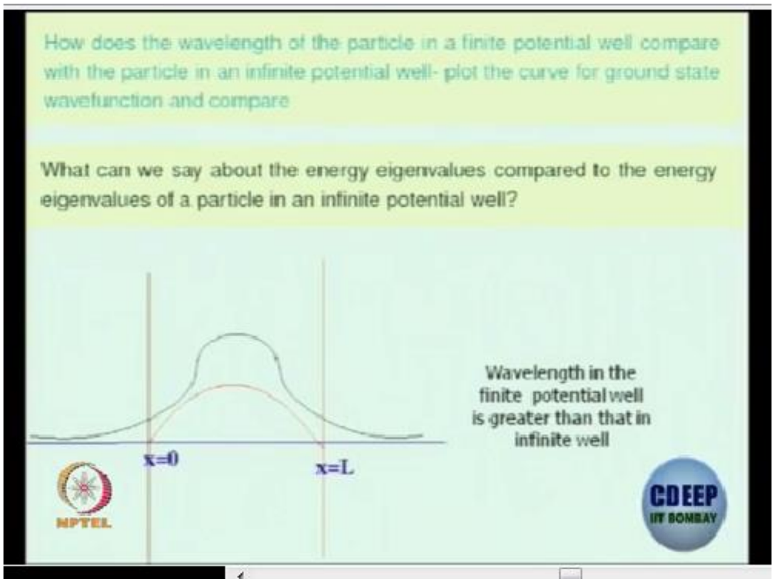

So this I have already said how does the wavelength compare with the particle in an infinite well. You have already plotted here and you can make out that the energy eigen values, how will it be in comparison to energy eigen values, okay. So this is all clear from the picture.

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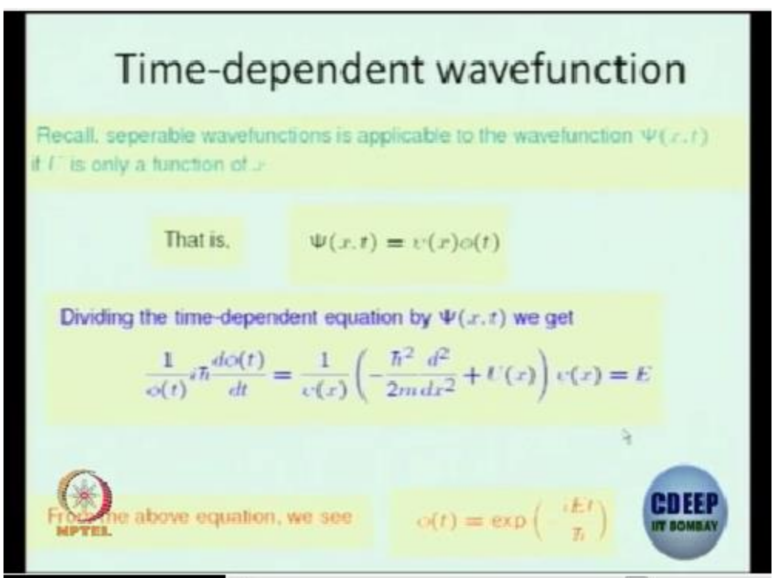

Just for completeness, time-dependent wavefunction, how does one do it? You try to write, we will take only potential energies which are functions of only x, okay. This is the kind of problems you are going to look at in this course. But you could have time-dependent potentials also. We will see it in the next course, okay, the next level course. In this course, U will be only a function of position and in 1-dimension, we will take it to be a function of x.

Wavefunction can be in general a function of x and t because potential energy is only a function of x looking. At the differential equation, you can separate the operators which are dependent on time-dependent operators from the space-dependent operators. So you can write a wavefunction as a $\psi(x)\phi(t)$. Exactly like what we did in a 2-dimensional box, I just want to mimic here for a time-dependent wavefunction.

So you remember the time-dependent wavefunction, the time-dependent Schrodinger equation. We can rewrite it in this fashion, right. This part is the $i\hbar\frac{\partial\psi(x,t)}{\partial t}$ will become dependent only on $\Phi(t)$. So you can write it as the partial derivatives as total derivatives of $\Phi(t)$ and you can divide it by the wavefunction and write this as 2 separate operators, operators which depend only on t, operators which depend only on x and you can equate it to energy E.

So from the time-dependent Schrodinger equation, show the step. Please work it out and show the step. And from this equation, you can solve this to be equal to E. This equation, the extreme left to the extreme right. You will get the time-dependent piece on the wavefunction, okay, which is dependent on the energy of that, energy E, okay.

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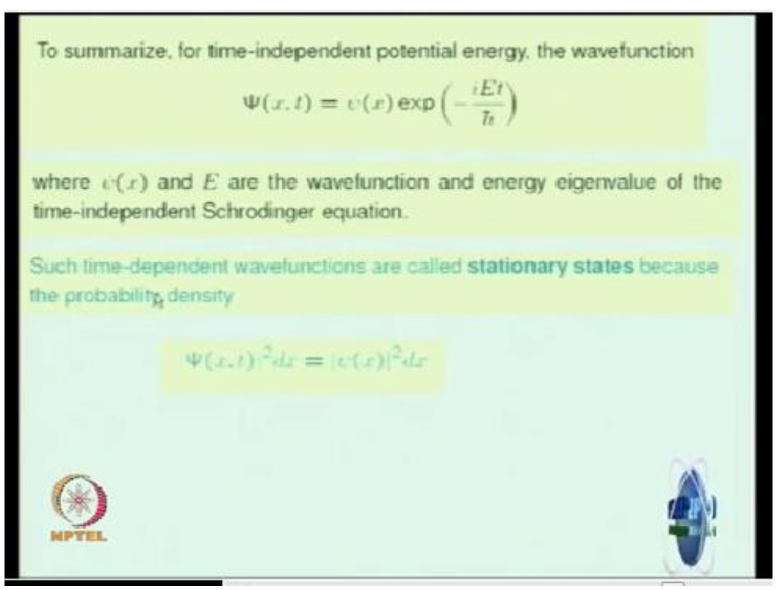

So what will be the total wavefunction? For potentials which are only position dependent, the total wavefunction can be written as psi of x, that psi of x is the solution for the time-independent equation, and the time-independent equation will also have, the state will have a specific energy E, right. And for that energy, you will have an exponential factor which is time-dependent, multiplying that piece.

This is the most general solution for time-independent potentials. Yes, and these, psi of x satisfies time-independent Schrodinger equation and you can show for such cases where you have, they are called stationary states. If you do $|\psi(x,t)|^2$ here, it is same as $|\psi(x)|^2$here. Is that clear? Because this is just a face factor. So such state which satisfies this property, they are called stationary states. And superposition state stationary states, suppose I take a particle in a box and take the state to be a position of ground state and first excited state. Are they stationary states? No. They are not stationary states. Particle in a 2-dimensional box, if I take the superposition of degenerate states, what happens there? Will that be stationary states? Think about it? So the energy will be the same. So it will be looking like a stationary state, okay.

So some of these things if once you go to 2-dimensional, the stationary states can also be in the subspace where it can be in the superposition of degenerate states, okay. So this is also one of the important feature which happens in experiments which is called tunnel effect which requires quantum mechanics. You cannot work with classical mechanics to explain tunnelling which is seen in the lab.

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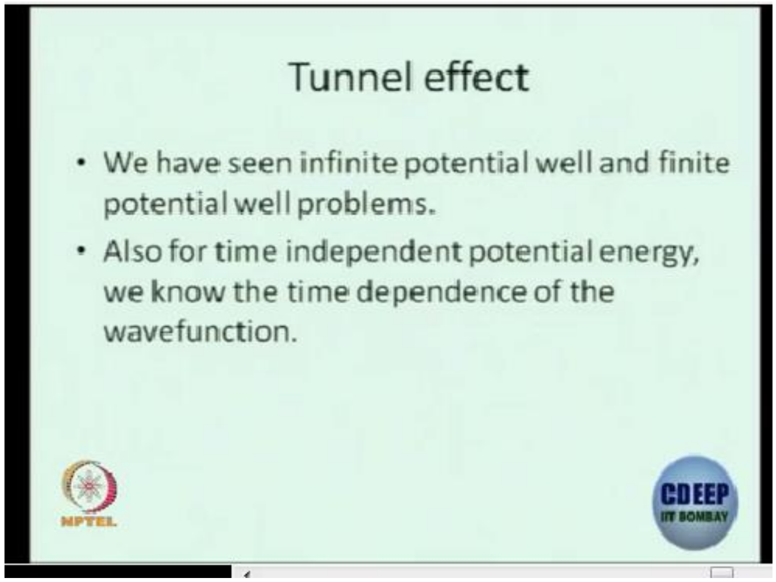

And we have seen infinite potential well and finite potential well problems so far. Also we have seen time-independent potential energy, how to write the time-dependence for them is to summarize.

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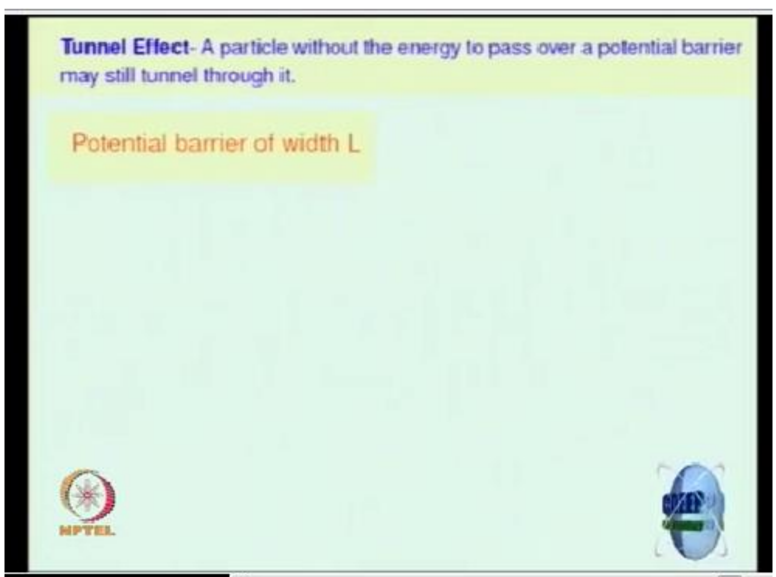

So now what do we want to see? Even if the particle has, does not have enough energy to cross the barrier, you can still tunnel through this. So this is what I showed for your finite, for the finite well I showed you.

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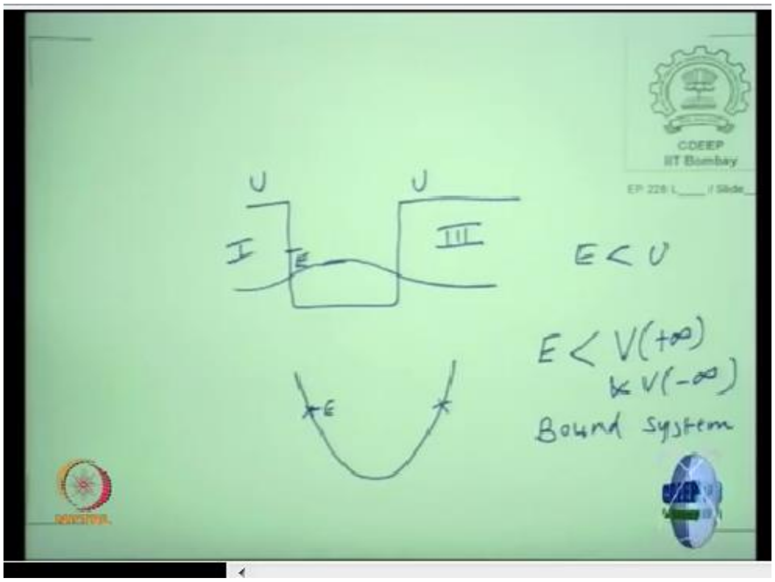

If suppose the energy of the particle is E and U where E<U, the wavefunction can actually cross, you know. It can tunnel into region I and region III, okay.

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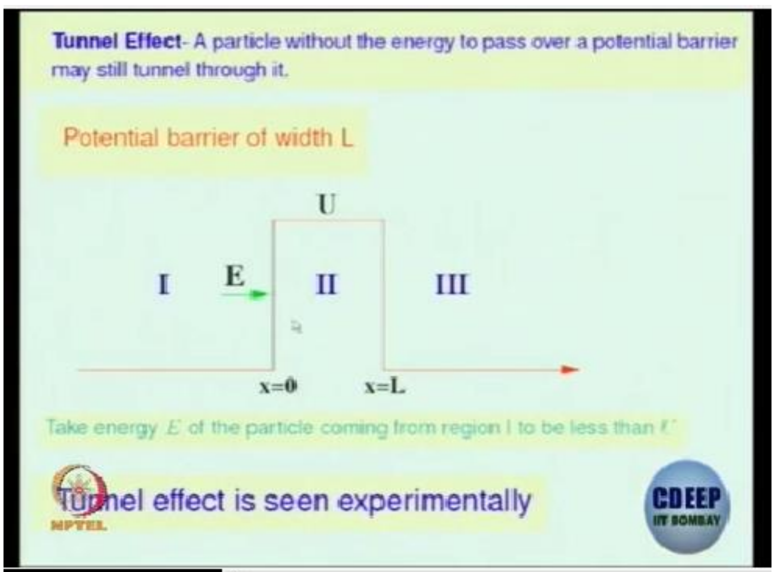

You can also have a similar situation in the context of barriers where the energy of the particle is less than the energy of the potential barrier. Suppose you want to climb a mountain, okay and you do not have that much of energy to climb the momentum, you know, you do not have that momentum or energy to climb the mountain. Classically we cannot. Only if you have that much of energy to go against the potential energy then you can go.

But quantum mechanically, there is a microscopic particle, it can start showing signature going into the other side, okay. So this is what will happen in microscopic world. Not for microscopic world as I already said, the wavelength is so small that those signatures are not going to be seen, the wave like nature is not going to be seen, right, okay. So take an electron with energy E<potential energy and then tunnel effect is seen experimentally that what is that mean?

Classically, if I shoot in a particle or a beam from region I, will I see it in region III? No. Classically I cannot see. Quantum mechanically we do get some kind of a signal coming out of region III. Even though the energy of the beam which I sent in is much less than the potential energy of a region which I have put in, okay. How do I put in such kind of a potential energy region?

I can try and make a constant electric field, you know, we can put in some region between x=0 to x=L. I can make it, I can make a non-trivial potential energy region, okay. So is this particle which is coming here or a beam which is coming here, will not be able to cross that region because of the, you know, it will not have that enough energy but quantum mechanically, it can tunnel through it because there will be a damping wave function and it can come out of it.

Once it comes out of it, it is like the free particle again. It can be, okay. So this is the (()) (18:47) qualitative.

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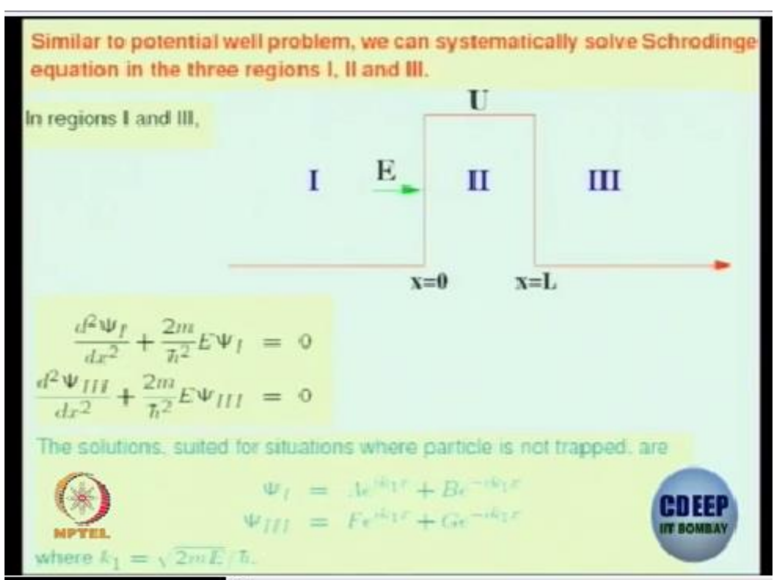

So similar to what we did in the case of potential well, you can solve region I, region III. Region

I, region III is like a free particle, U=0 situation. So you can write the solution as a linear combination of the free wave which is oscillatory solutions.

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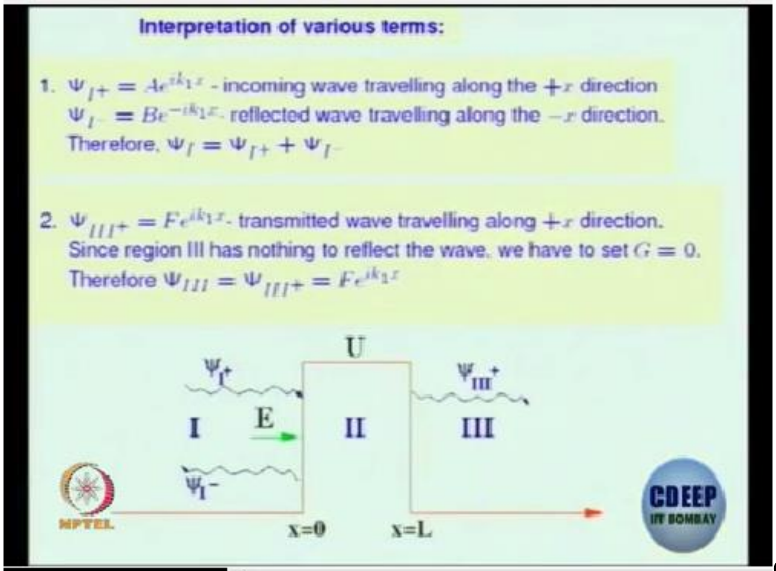

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And what are the interpretations of those terms? In region I, the incoming wave S going along positive x direction and the reflected wave is going in the opposite direction, right. So B is the factor multiplying the reflected wave and $Ae^{ik_x x}$ is the incoming wave. And region III, what is your expectation? The incoming beam goes in even though the intermediate region has potential energy higher than its energy, it kind of exponentially tapers inside.

After that, there is nothing to reflect it back. It has to keep going, okay. So you will have only a forward wave which is what is called as a transmitted. Mathematically you can write a linear superposition but looking at this qualitative situation of an incoming beam coming from the left facing a barrier whose potential energy is greater than the energy of the incoming beam, kind of exponentially dampers down in region II and when it comes out, there is nothing to reflect it back. It keeps going. So that is the transmitted wave, okay.

So I have shown it pictorially also here. So there is an incoming beam. When it faces this barrier, there can be a reflected beam but inside this region, it keeps exponentially damping and again when it comes out here, it goes in the forward direction which is the transmitted beam. Is the picture clear?

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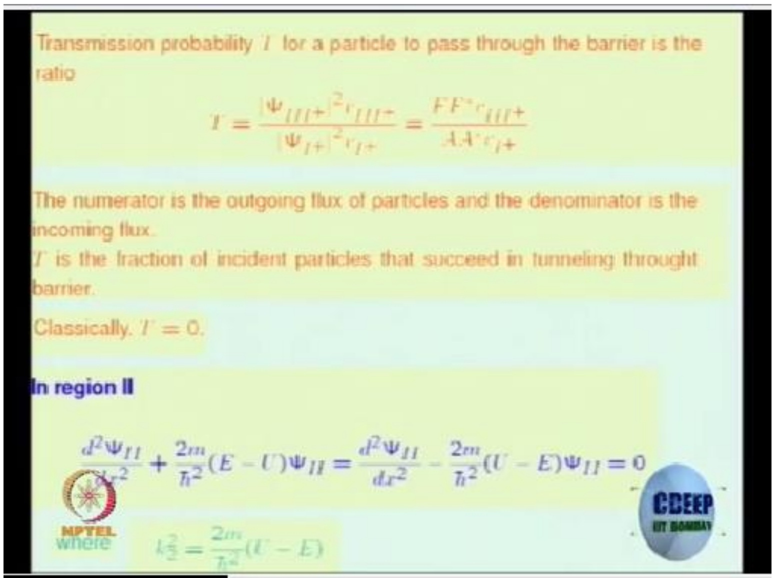

And what is the experimentalists want to see? They want to see the signal in region III and they define a quantity called the transmission amplitude or transmission coefficient or transmission probability, T which will have information about the probability of the particle seen in region III and it should be explicitly the flux which is seen. We will define what is the flux? And that ratio with respect to the incoming beam which is just the forward incident beam which depends on the coefficient A, okay.

So that ratio is what is called as the transmission coefficient. Conservation will tell us if the transmission coefficient T is found, there will also be an equivalent reflection coefficient. There is a reflection beam. If a detector is placed in this region also, you can get a reflected flux and that will give you a reflection coefficient or reflection probability R and total probability has to add up to 1, conservation which means R+T should be equal to what?

So that is the way to understand and tunnel effect is there, is proven because T was non-0 and they said that tunnelling happens in quantum mechanics and not in classical mechanics. Classically T is 0. In region II, you will have a non-trivial potential energy in the barrier and you will have a kind of solution I have already said which will be an exponential damping or growing because it is in a compact region.

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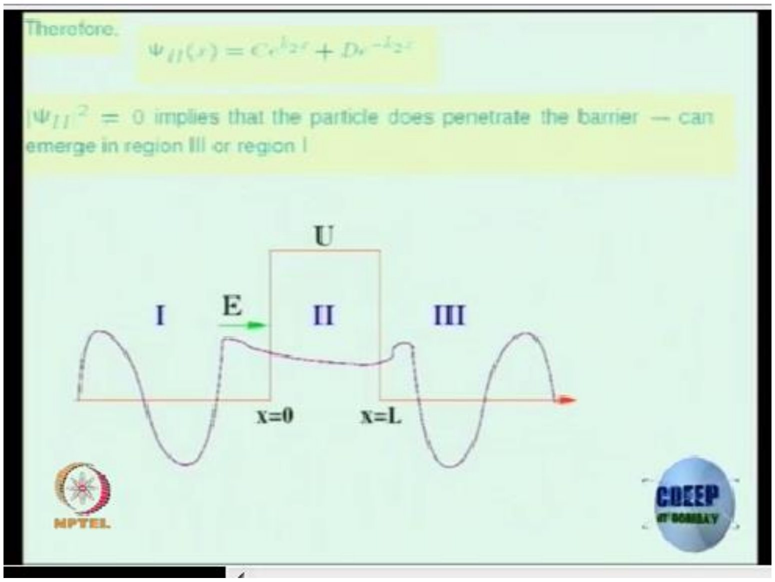

So you can rewrite it as an exponential solution and the particle dust penetrate the barrier, can emerge in region III or region I. You can plot the curve which is of this type, okay. So this is just a linear superposition of exponentially growing and damping. You can have both the linear combination and you should have, at this point, continuity of wavefunction and differentiability of wavefunction.

Similarly, here, continuity of wavefunction and differentiability of wavefunction and this is a plot of the trend of how the; it will be oscillatory on region I and region III and it will be exponentially damping or growing in region, okay.

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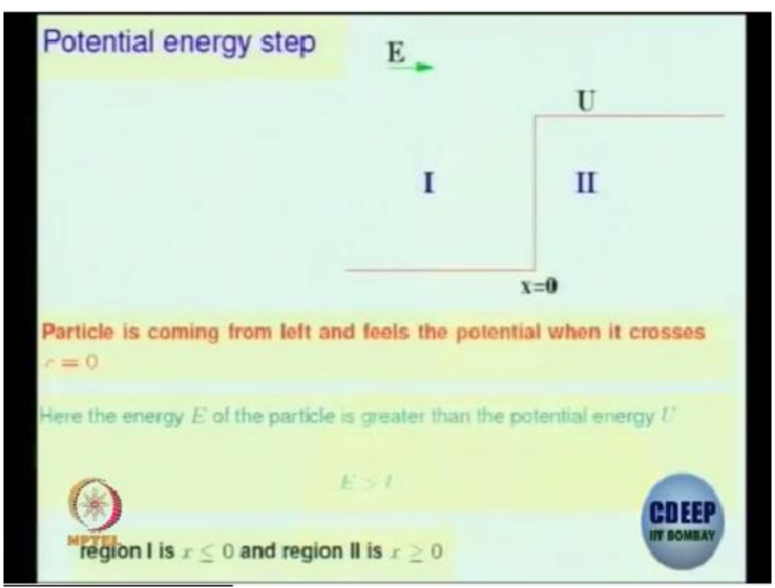

So this is just a part of the earlier one. You just have a potential step and you can, particle is coming from region I. If the energy I have shown in the diagram as E about U which means E>U, okay which means, what does the type of solution in region I and region II? Sinusoidal. You will have it to be an oscillatory solution and you will have 2 solution in 2 regions will be oscillatory.

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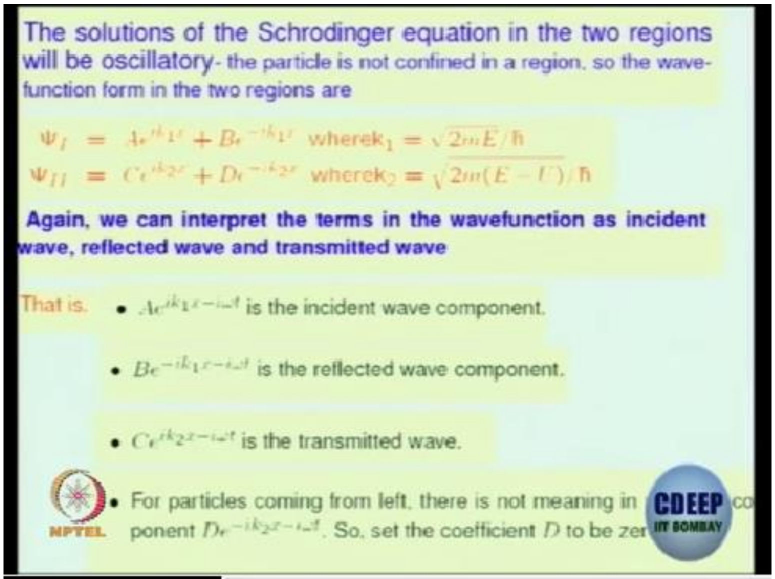

And the particle is not, there are so confinement. Particle in a box, the particle is confined to region I and, inside the box. Here the particle is free, it keeps moving freely. Once it cease this potential energy, it will show a slight deflection because its energy-, the kinetic energy will decrease, right. That is all will happen. Otherwise, they are free particles and you have region I and region II and you can interpret these terms as the incident wave, reflected wave and transmitted wave, okay. Can we have D? Is D allowed?

D is not allowed if you take the incident beam coming from the left. Similarly, if you take the incident beam coming from the right, yes. So you have to make sure that this appropriate coefficient is set to 0 depending on the problem, okay. So these 2 solutions which are given are 2 solutions of the differential equation. But which one will be dependent on if I say the incident beam is coming from the right, then you have to appropriately put the, only the transmitted beam will be allowed in regions, okay.

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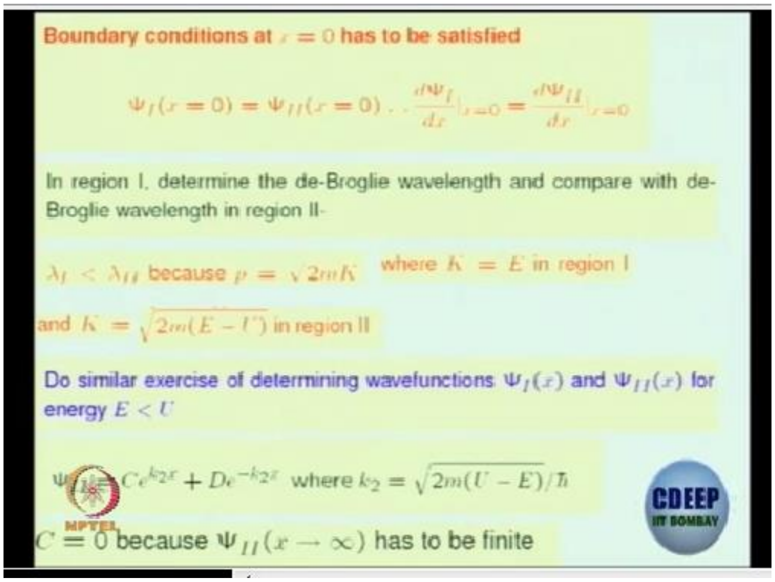

And boundary condition, derivative of boundary condition, see how the de-Broglie wavelength compares in region I and region II, okay. And do a similar exercise for E<U, okay. You will have a, if E<U, then in region II, it will be an exponentially growing and damping but because region II goes up to +∞, you have to put C=0, right. Very systematic. Nothing, it is not that today this will be the answer, tomorrow it will be a different answer. It is the same, going to be. It is logically argued and fixed, okay. So what is the bound system?

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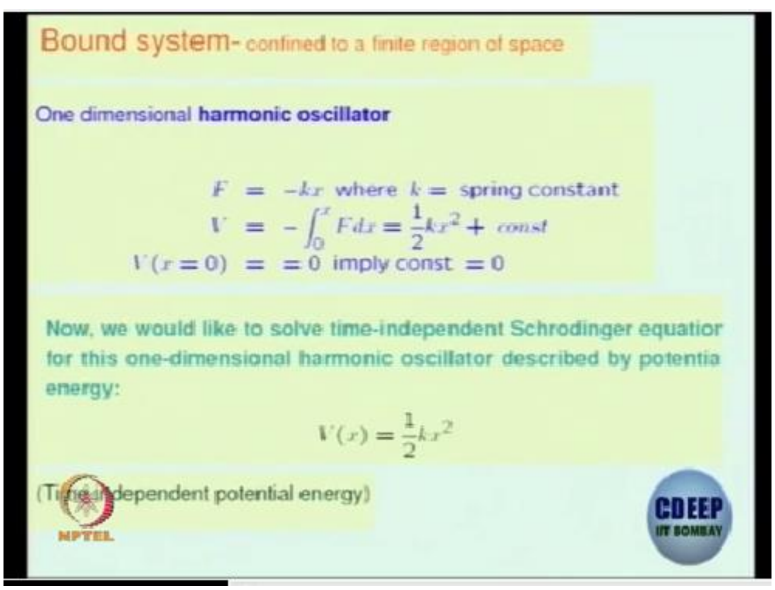

Bound system means what? It is kind of constrained into a region. Like particle in a box is a bound system. What about harmonic oscillator? Harmonic oscillator has some kind of potential like this, right. If there is a particle with energy E, okay. Classically these 2 are turning points. You all agree, right? Beyond that point, it cannot go because its kinetic energy will become negative, right?

So typically it is going to be some kind of a bound system where the formal definition of a bound system is if E<V, at +∞ and V at -∞, we call it to be a bound system. Particle is a box satisfies this. Harmonic oscillator satisfies this. They are all bound systems. What about hydrogen atom? Hydrogen atom, what is the potential energy?

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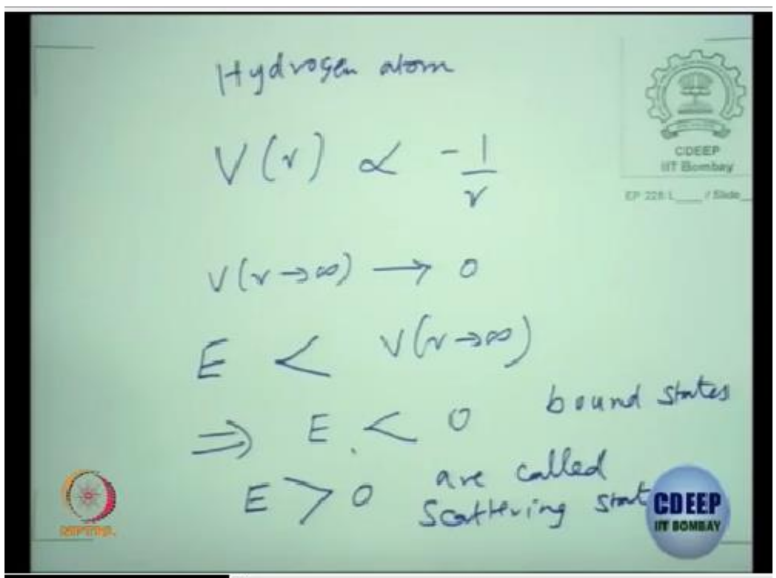

Is that right? What happens for r tending to infinity? So condition for bound state is E<V at r tending to infinity which means E<0 are bound states. All your hydrogen atom spectrum, energies are negative or; negative right. Suppose I make E positive, what are those states called? Louder, scattering states. E>0 hydrogen atom are called scattering states, okay. What is the condition for scattering states?

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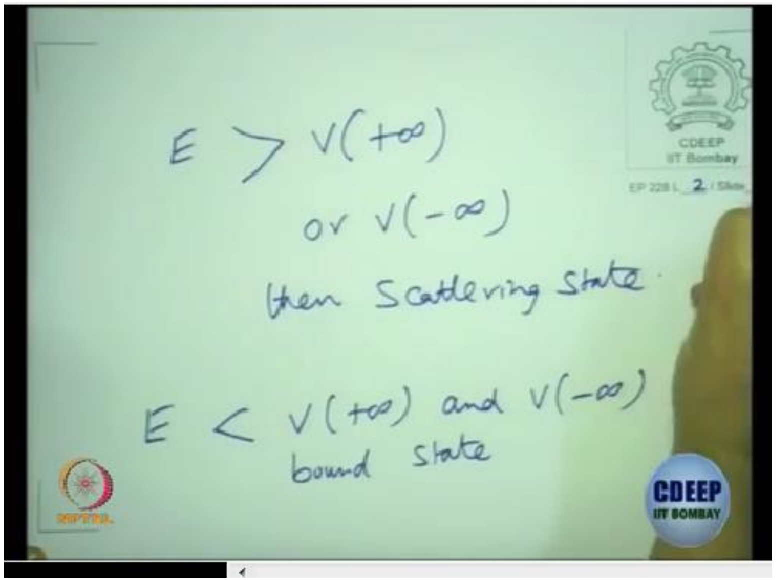

General, if E>V at +∞ or V at -∞, then scattering state. What are the condition for bound state? E<V at +∞ and V at -∞ then we call it bound state. You can also see it by drawing a barrier.

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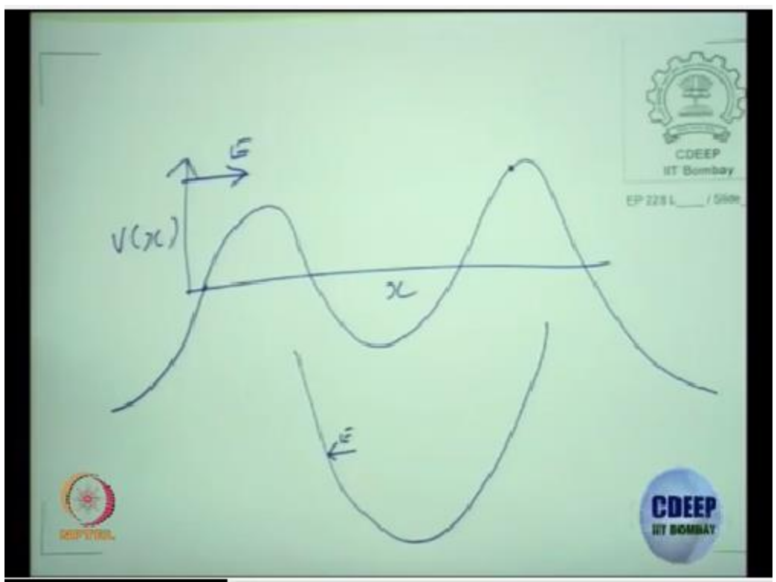

You can draw barriers like arbitrary, you know, something like this and see if you have a particle with energy, let us say this one, okay. When it comes to this point, it may not be able to, if it is really a big peak, may not be able to climb but it can still come out, okay. It is not getting trapped. So this is why it is a scattering state. And if you have a particle in infinite like things and you have a particle here, you know, it gets trapped and it is coming here with energy E.

It cannot climb up and it is going here, you know, it is also, it cannot climb up. So it is kind of trapped. That is the bound state, okay. This picture is very nicely given in Griffiths chapter 2, you should see it, the turning points and how to get it. So once you have things in the picture form, what is the bound state, what is the scattering state, why E<0 for hydrogen atom is a bound state, why E+ will be a scattering state? Nice to get a picture of this.

So far you did only step potential with constant potentials and so on. But harmonic oscillators are first one which is going to be a non-trivial. So this is a plot of V of x versus x, okay. So such kind of potentials are also possible. V not be sinusoidal. Would have all kinds of potentials. So if you have these potentials, the way to see it is first look at how the potential goes at + or -∞ if you are doing a 1D problem.

If you are doing in a spherical coordinates, then you can look at how the trend is at r=0 and r=∞. And see what is happening. Then decide whether the solutions, what is the regime of energies where the solution will be a bound state or it will be the regime where the solutions will be a scattered state, okay. So let us get to the bound system. So I kind of convinced you that it is confined to a region, particle in a box is a bound system.

Harmonic oscillator is also a bound system because the energy of the particle is always going to be less than the potential at ∞, + or -∞ in a 1D problems, okay, right. So they are all bound systems. Formally, you can write 1-dimensional harmonic oscillator where the force is proportional to the displacement and from there for conservative systems, you can find what is the potential energy and you get V(x), okay.

You can fix the boundary condition and fix the constant to be 0. So far we did potential energies which are even thought it is x dependent, it was constant in certain regions. It was 0 in certain region. But we never did problems where V(x) is different at different x, okay. So this is the x dependence which is the simplest problem we always see in any system. Even if you take any system with potential, you can try to expand that potential energy in a Taylor series.

The first non-trivial term will have an $(x - x_0)^2$ *some function p double prime. So in some sense, very close to certain regions you can see it to be like a harmonic oscillator. And harmonic oscillator potential that plays very important to know how to solve, okay.

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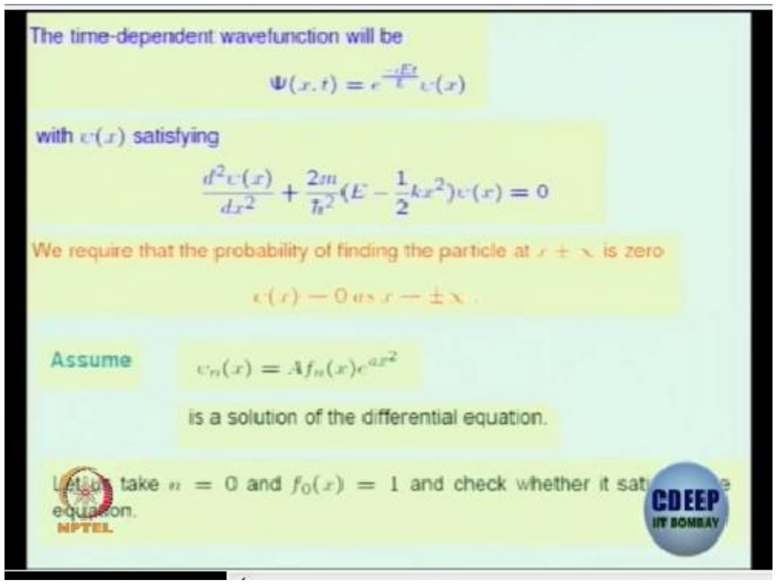

And potential energies independent of time. So you can write your wavefunction as the time-dependent piece as a phase factor*$\psi(x)$ and you can try and solve the Schrodinger equation. So what are the requirements? The wavefunction should be well-defined, should not blow up. So as x tends to 0 or x tends to + or -∞, the wavefunction has to go to 0. This is what you did in your last year course.

You took a functional form and this functional form has this property that as x tends to + or - infinity, it goes to 0. You all agree? Provided A should be negative, okay. So for n=0, take f_0 to be 1 and check whether it satisfies the equation.

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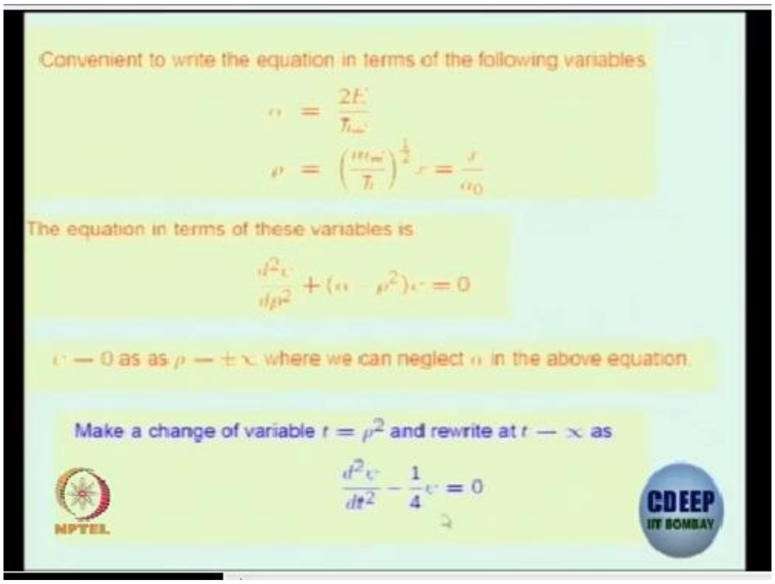

And then we can figure it out. You can do a convenient change of variables and solve this and put in this condition that. I just made a change of variable for just the equation to look more better. Nothing else, okay. Alpha and rho makes the change of variable look better and you can neglect alpha in the above equation. Further replace, make a change of variables so that it becomes a familiar equation whose solution can be found. What is the solution to this equation? Is the power of -1/2T, + or -1/2T, okay? So I will stop here.