Introduction to Quantum Mechanics
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Lecture – 02
Solution of Schrodinger equation for a particle in a finite well

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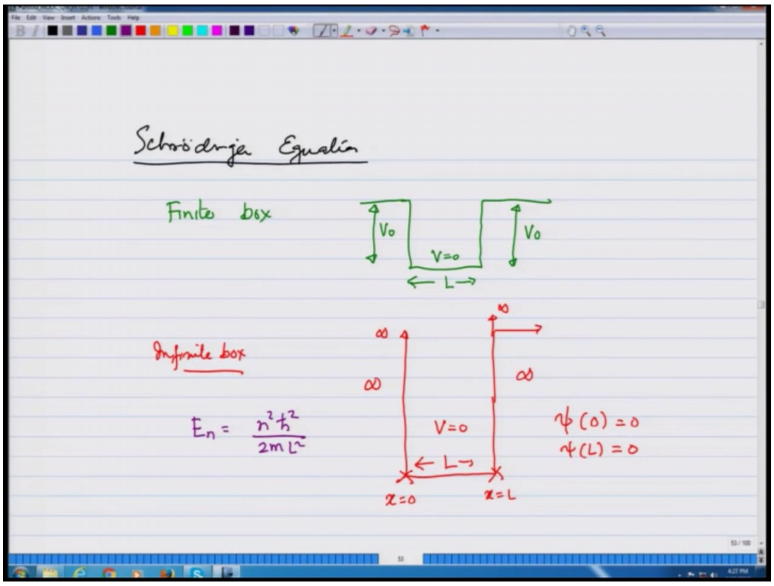

Having solved the Schrodinger equation, for particle moving in a delta function potential, now I will go to different potentials. So, the next potential we consider as a finite box. What you mean by that is this potential is of this shape with a potential being 0 over a length L. So, V equals 0 and being equal to sum V 0 outside. So, this is the finite box and you want to solve the Schrodinger equation for a particle of mass move m moving in this potential.

This is in contrast to the infinite box that we have already solved which was that the potential was going to infinity outside a certain area which is of length L. So, the here V was 0 and outside it was infinity. So, the wave function was taken to be 0 at these edges, when we took this to be x equals 0 and x equals L the wave function satisfied the boundary condition; that psi at 0 0 and psi at L was 0. How about us the energy eigenvalues in this case? The energy eigenvalues I am writing on the left where E n equals n square h cross square over 2 m l square and the wave functions of confined between 0 and L. Compared to this now what we have done is taken the height of the box to be finite and let us see how the solutions change and what happens to the energy.

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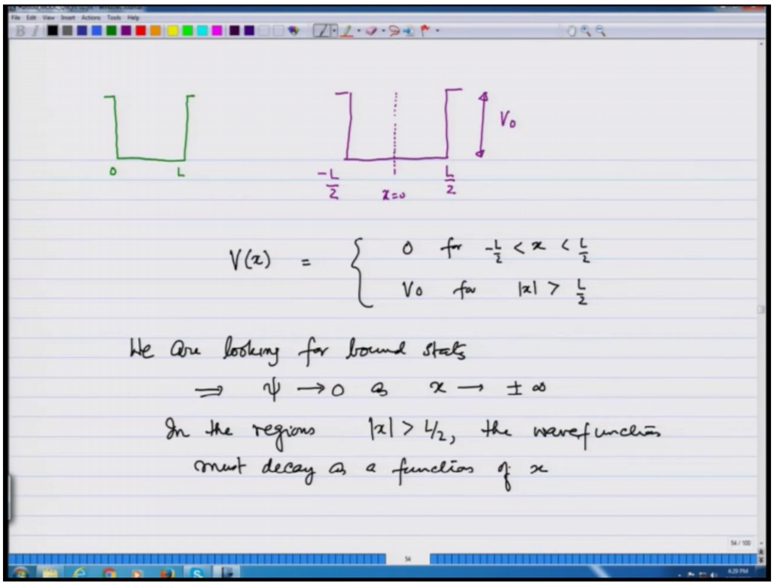

So, when I take this finite size box 0 and L, I can make my life easy if I make it symmetric. The same box I am going to put around x equals 0. So, this is x equals 0 and I will put it is symmetrically about it. I can solve it keeping anywhere but this makes the solution easier; the solution nature remains exactly the same the functions remain exactly the same, energy is remain exactly the same except that makes life easy mathematically.

So, the box extends from minus L by 2 to L by 2 and the height outside this region is V 0. So, let me put this in mathematical form V x equals 0 for x between minus L by 2 L by 2 and V 0 for mod x greater than L by 2 and in between there is a boundary. We are looking for bound states. So, we are looking for bound states; and that means the wave function psi goes to 0 as x goes to plus or minus infinity. So, in the regions mod x greater than L by 2 the wave function must decay as a function of x.

So, let us now solve this where writing the Schrodinger equations.

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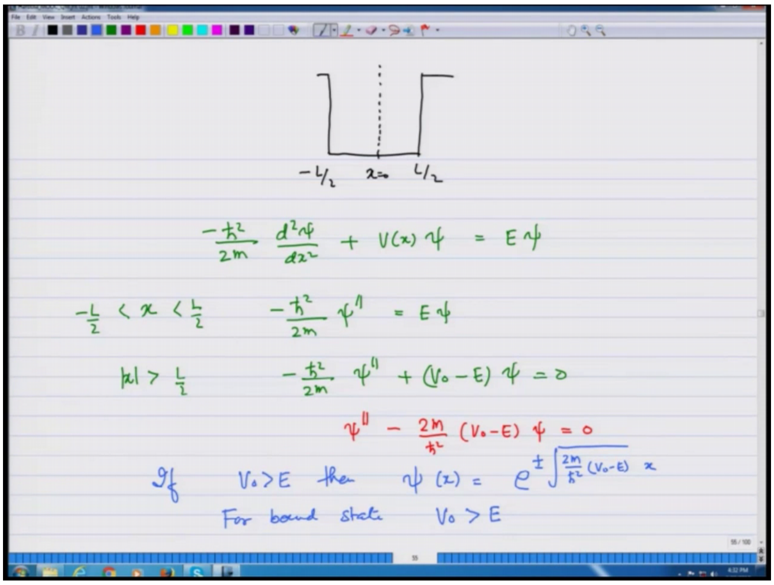

So, here is my potential let me write it again; there is x equals 0 minus L by 2 L by 2 the Schrodinger equation is minus h cross square over 2 m d 2 psi over dx cross plus V x psi equals E psi for x between minus L by 2 to L by 2 the equation becomes minus h square over 2 m psi double prime is equal to E psi. And for mod x greater than L by 2 the equation becomes minus h cross square over 2 m psi double prime plus V 0 minus E psi equals 0.

I can write the second equation by changing the sin as: psi double prime minus 2 m over h cross square V 0 minus E psi equals 0. Now if V 0 is greater than E then psi axis of the form e raise to plus or minus square root of 2 m over h cross square V 0 minus E x. And therefore, this for x greater than 0 by choosing the minus sign I can make the wave function decay. For x less than 0 on the negative sign by choosing the plus sign on the e raise to whatever power 2 m over h cross square V naught by e I can make the wave function decay as I go towards e equals minus infinity.

So, for bound state V 0 must be greater than E otherwise the state would not be bound. If E were greater than V 0 you can see that there will be an I coming in the power of exponential and that will make the solution oscillatory outside the regions of minus L by 2 or L by 2. And that would not be acceptable for a bound state. So, for bound state V naught is greater than E.

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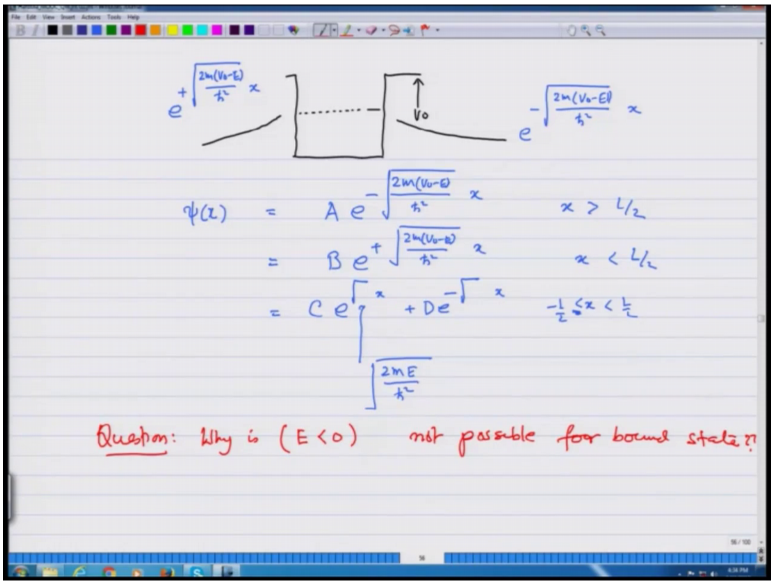

So, what we have now? We have this box of finite height V 0 energy must be somewhere in between for a bound state. And for that the wave function decays on this side and decays on this side. On the right side the wave function goes as e raise to minus square root of 2 m V 0 minus E over h cross square x on the left hand side the wave function goes as e raise to plus square root of 2 m V 0 minus E over h cross square x.

And in between it will be a linear combination. So, psi x we can write as sum A e raise to minus square root of 2 m V 0 minus E over h cross square x for x greater than L by 2 is equal to sum B e raise to plus square root of 2 m V 0 minus E over h square x over x less than L by 2. And a linear combination sum C e raise to plus x plus D e raise to minus the something in under the square root x x between minus L by 2 to L by 2. What is inside in the square root s? Square root of 2 m E over h cross square.

Now you may ask let me ask the question: why is E less than 0 not possible for bound state. After all you could have that, why cannot I have that 'and this question I will let you answer for yourself.

In a simple way if E is less than 0 you would not be able to satisfy certain conditions. So, I leave that for you to think about. So, what I have is.

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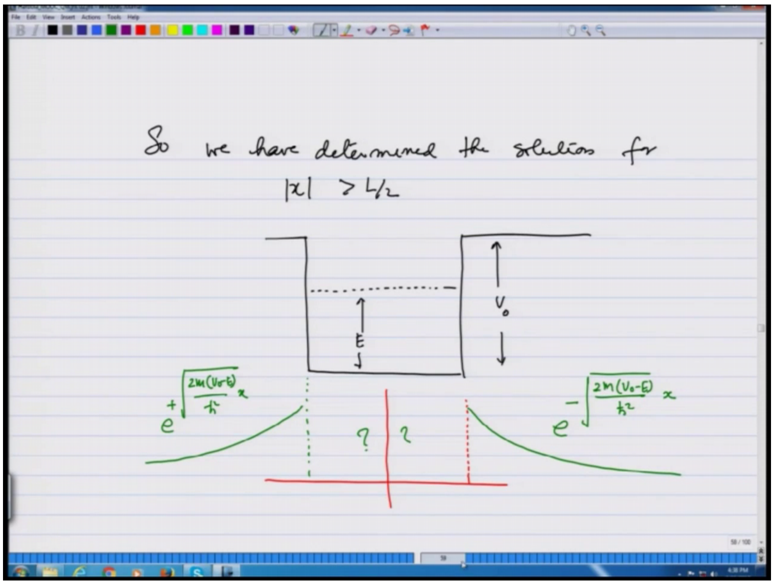

So, we have determined the solution for the region mod x greater than L by 2, and what we have found is that for solution to be a bound state energy E is less than V 0. And on the right hand side the solution should decay let me show it on the over side. On the right hand side greater than L by 2 the solution should decay because go to 0 faraway. On the left hand side the solution should also decay.

Here decays as e raise to minus square root of 2 m V 0 minus E over h cross square x and on the left hand side the solution decays as plus square root of 2 m V 0 minus E over h cross square x. What about in between, what is the solution in between; let us focus on that.

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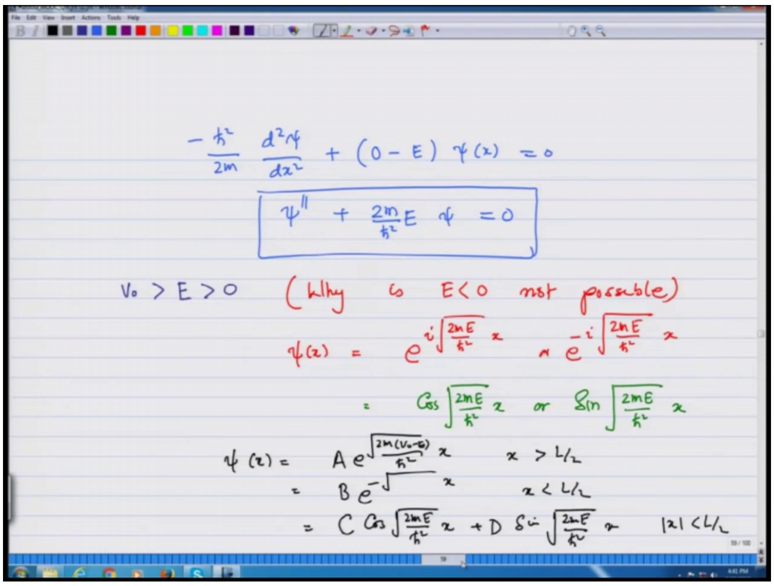

So, in between I had minus h cross square over 2 m d 2 psi over dx square plus the potential is 0 and I have 0 minus E psi x equals 0 or psi double prime plus 2 m over h cross square E psi equal 0. Now I am claiming that E should be greater than 0 and it is less than 0 for bound state. Question I leave you with is why is E less than 0 not possible.

You look through the solution of the equation and tried to satisfy the conditions that has to be satisfied by the wave function and you will fine why E less than 0 is not possible. For the time being we will take that E is greater than 0 and less than V 0 for a bound state.

Immediately the solution is very clear that psi x for this equation is going to be either e raise to I a square root of 2 m E over h cross square x or e raise to minus I square root of 2 m E over h cross square x. I can also write this in real form as: cosine of square root of 2 m E over h cross square x or sign of square root of 2 m E over h cross square x. Cos x is a linear combination of e raise to I square root of 2 m E over h cross square x and e raise to minus I square root of 2 m E over h cross square x and sin x is a linear combination and the minus sign in between. So, I can write it either way.

So this is my psi x, now I have found the solution in all regions so let us write it. That psi x is equal to A e raise to square root of 2 m V 0 minus E over h cross square x for x greater than L by 2 is equal to sum B e raise to minus, the same thing x x less than L by 2. And may be linear combination C cosine of square root of 2 m E over h cross square x plus D sin of square root of 2 m E over h cross square x for mod x less than L by 2. Let me write it again.

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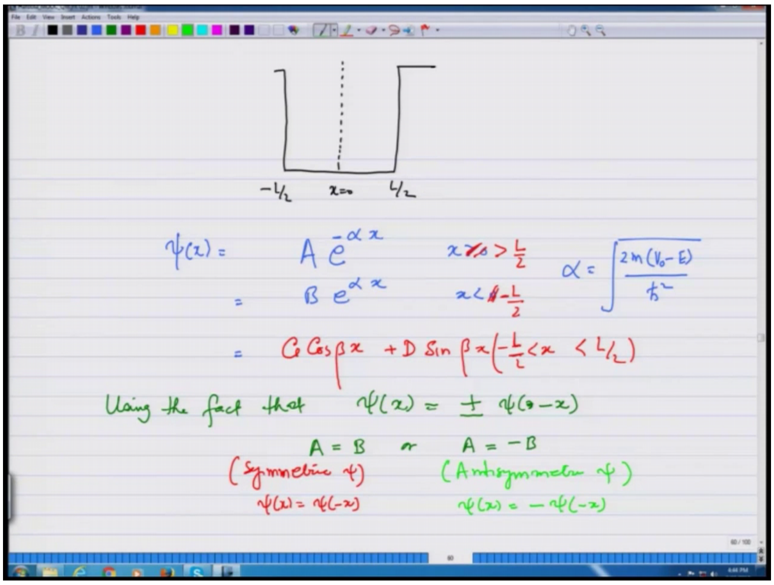

So, now this particle in a box with the centre of the box lying at x equals 0 and the edges lying at L by 2 and plus L by 2 I have psi x equals A e raise to; let me try this is as alpha x minus alpha x for x greater than 0 is equal to B e raise to alpha x for x less than 0, where alpha is equal to square root of 2 m V 0 minus E over h cross square. And is equal to C cosine of beta x plus D sin of beta x for x minus L by 2 this is not 0 this is greater than L by 2, x less than L by 2 and greater than minus L by 2.

These are the solutions. Now by matching the boundaries at different points I can find A B C and D, but I can do better. Now using the fact that psi x is going to be equal to plus or minus psi minus x I can actually find the relationship between a B immediately. I could do it as I said earlier by matching the boundaries I will get the same answer. Now by shifting the potential in such a manner that centralized at x equal 0 and the potential becomes symmetry I can reduce some algebra unnecessary mathematical steps.

So, this immediately tells me that either A equals B or A equals minus B. A equals B would give me symmetric psi that is; psi x equals psi minus x. And the other one would give me anti symmetric psi that is; psi x would be equal to minus psi of minus x. So, let us focus them on at a time.

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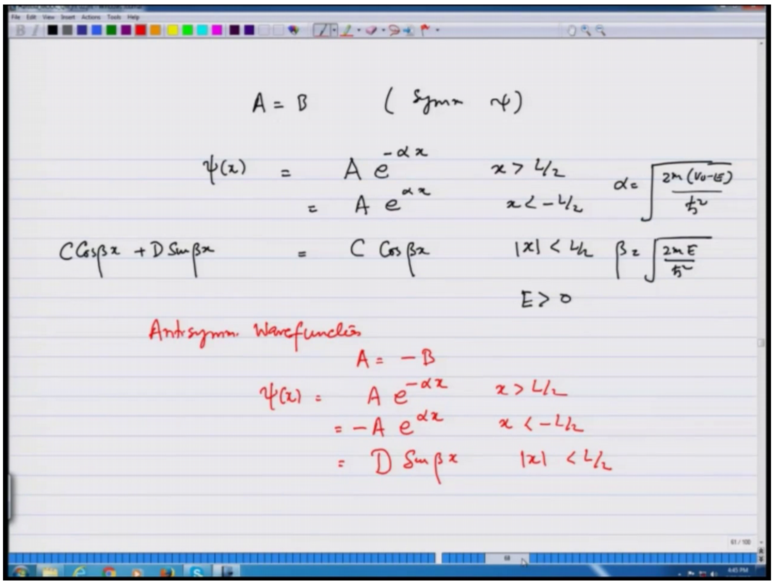

So, let us take A equals B that is I am taking symmetric psi. So, I have psi x equals A e raise to alpha minus alpha x for x greater than L by 2, equals A e raise to alpha x for x less than minus L by 2, alpha equals square root of 2 m V 0 minus E over h cross square and is equal to.

Now, let us look at the combination I have C cosine of beta x plus D sin of beta x for symmetric solution the only function that is symmetric between the two is cosine. So, this is going to be some cosine C times cosine of beta x or mod x less than L by 2 beta equals square root of 2 m E over h cross square. Keep in mind that E is greater than 0.

How about the anti symmetric wave function? So, let us write for anti symmetric wave function. For that I am going to have A equals minus B. So, psi x is going to be A e raise to minus alpha x for x greater than L by 2, is going to be minus A e raise to alpha x for x less than minus L by 2, and is going to be some constant D sin of beta x for mod x less than L by 2 because sin is an anti symmetric wave function around x equal 0.

Now, let us solve the equations and get our answers.

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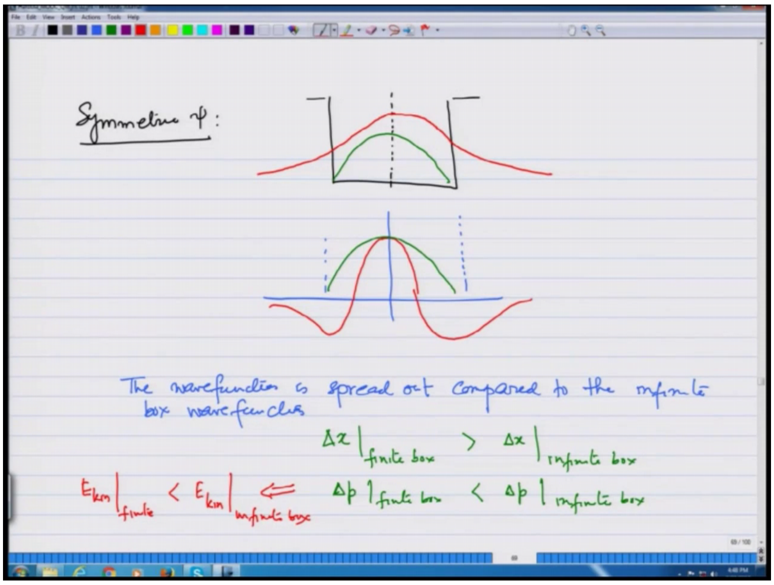

So, I will first consider symmetric psi. Since the wave function is symmetric I need to satisfy conditions only on one side the other side will be automatically satisfied. So, this is the cosine function let me just show it schematically. So, it is going to be nonzero at the center and will decay as you go far away. This is the other way function is going to low. It could also be like this: these are the boundaries. It could also be like this, but symmetric and this is the combination of you know higher cosine on the lower side.

Now, this wave function compared to the infinite box is spread out. So, let me write this: the wave function is spread out compared to the infinite box wave function. Infinite box wave function I show by green most confined here goes confined here, here this is more spread out if this is more spread out; that means, delta x for current problem. So, finite box is greater than delta x for infinite box. This means delta p for finite box is less than delta p for infinite box by uncertain defense box.

And this immediately implies E kinetic for finite box is less than E kinetic; kinetic energy for infinite box. And since the majority of energy is kinetic you will see that now the energy gets lowered a bit. This is the manifestation of the uncertainty principle.

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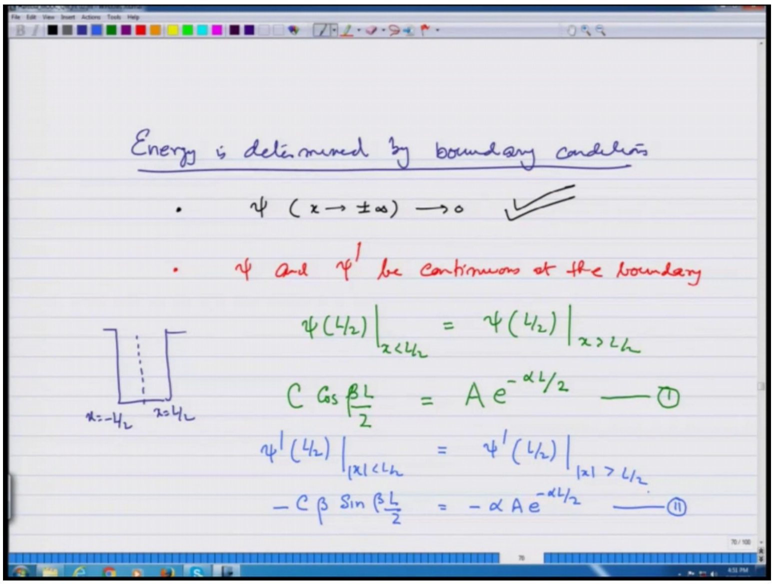

Now, how do we determine the energy? So, the energy is determined by boundary conditions. We have already checked that psi extending to plus or minus infinity goes to 0, this is already done. The only other boundary condition that remains is that the wave function psi and psi prime be continuous at the boundary. So, what is that mean? That means, in this finite box where are the boundaries; boundaries are at x equals L by 2 or x equals minus L by 2. So, if I satisfy dot on one side the other side will automatically be satisfied, because of the symmetric and anti symmetric nature of wave function that we have already taken care of.

So, psi at L by 2 from x less than L by 2 solution be equal to psi at L by 2 for x greater than L by 2 solution. Let us put those functions n. So, I am going to have C cosine of beta L by 2 is equal to A e raise to minus alpha L by 2; that is my equation number 1. And I am also going to have psi prime at L by 2 calculated for function for less than L by 2 is equal to psi prime at L by 2 calculated for function greater than L by 2. And that tells me minus C beta sin of beta L by 2 is equal to minus alpha A e raise to minus alpha L by 2; that is my equation number 2. And these two equations are sufficient to give me the energy.

So, let us see what do we get from this.

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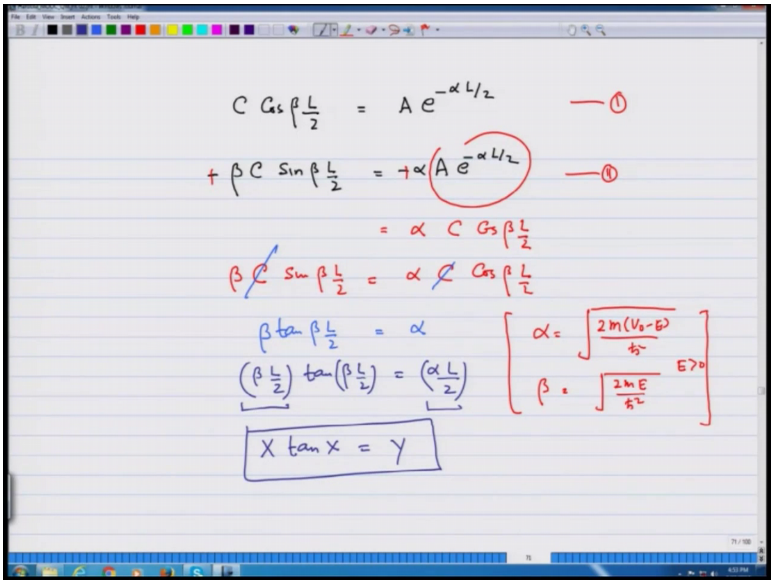

The boundary conditions that we have a C cosine of beta L by 2 is equal to A e raise to minus alpha L by 2 and I have beta minus beta C sin of beta L by 2 is equal to minus alpha A e raise to minus alpha L by 2. I can take care of this minus sign by it here, so this is equation 1 and equation 2. Now if you substitute for A alpha minus alpha L by 2 here so this becomes alpha C cosine of beta L by 2.

So, I have beta C sin beta L by 2 is equal to alpha C cosine of beta L by 2. C cancels from two sides and I have beta tangent of beta L by 2 is equal to alpha. Thus, the condition that arises from the boundary conditions; just to make the whole thing look nice let me multiply it by L by 2 on both sides beta L by 2 tangent of beta L by 2 is equal to alpha L by 2.

At this point let me also remind you what are. Alpha and beta alpha was square root of 2 m V 0 minus E over h cross square and beta was square root of 2 m E over h cross square and E is greater than 0.

Let me call this beta L by 2 sum function x tangent of x equals let me call this y. This is the equation that we have to solve to get the energies.

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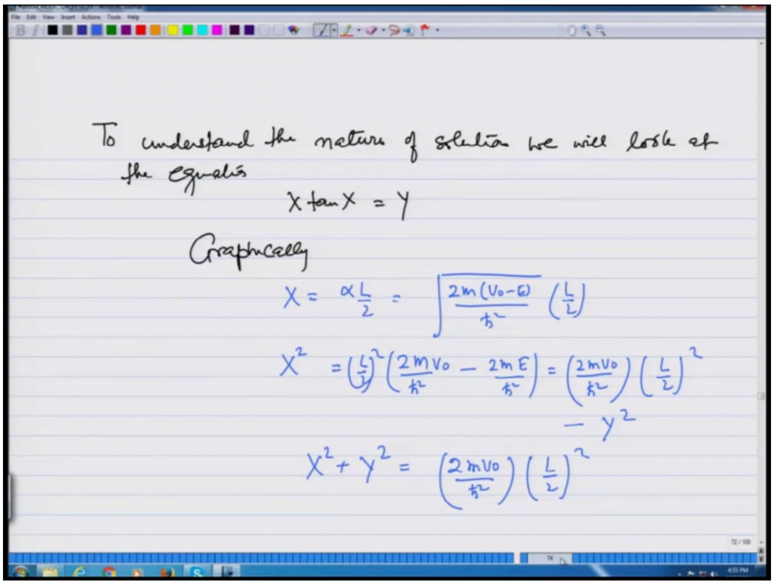

How do we solve this? So, to understand the nature of solution we will look at the equation x tangent of x equals y graphically. Now x is equal to alpha L by 2 which is square root of 2 m V 0 minus E over h cross square. So, x square is nothing but 2 m over h cross square V 0 minus 2 m E over h cross square which is 2 m V 0. There is an L by 2 also; this will be L by 2 square 2 m V 0 over h cross square L by 2 square minus y square.

So, x square plus y square is this constant 2 m V 0 over h cross square L over 2 square.

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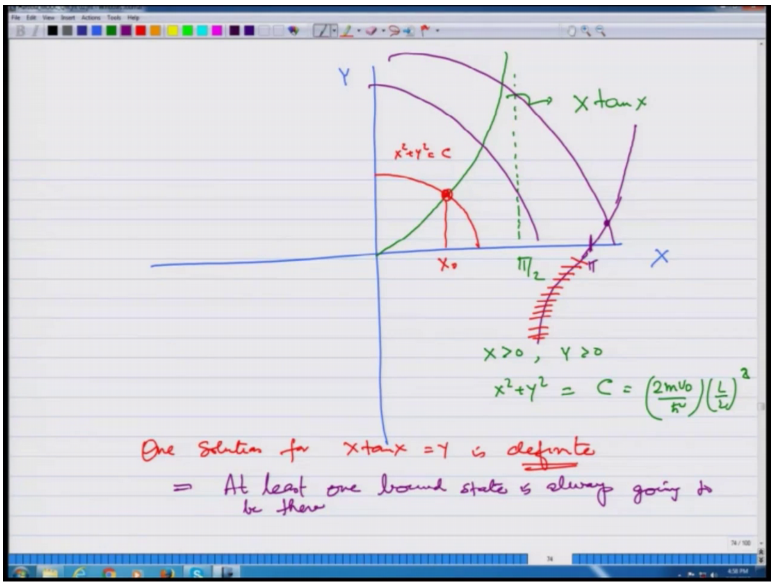

So graphically if I want to plot x versus y that this be pi by 2, then I have this graph as x tangent of x. And I have x greater than 0 y greater than 0, x square plus y square equals some constant which is 2 m V 0 over h cross square L by 2 square. So, x versus y looks like this graph. This is x square plus y square equals the constant. The cross section gives me the solution. So, solution is this particular x let us call it x naught. The next curve is going to look like this is pi. The negative side is not counted, so this is out; this is not counted because x and y are supposed to be greater than 0.

So, you see now one solution is definitely guaranteed. So, one solution for x tangent x equals y is definite. This is always going to be there because the green curve x tangent x passes through 0 and the circle is always going to cut it. So, this means at least one bound state is always going to be there. If you increase V naught and L naught by 2 square I get bigger and bigger circle. So, that if I make V naught times L square by 4 bigger and bigger I may get the second state, but that is not guaranteed for that the V naught has to be larger, L naught by 2 can be larger or a combination V naught L by 2 square has to be larger and larger.

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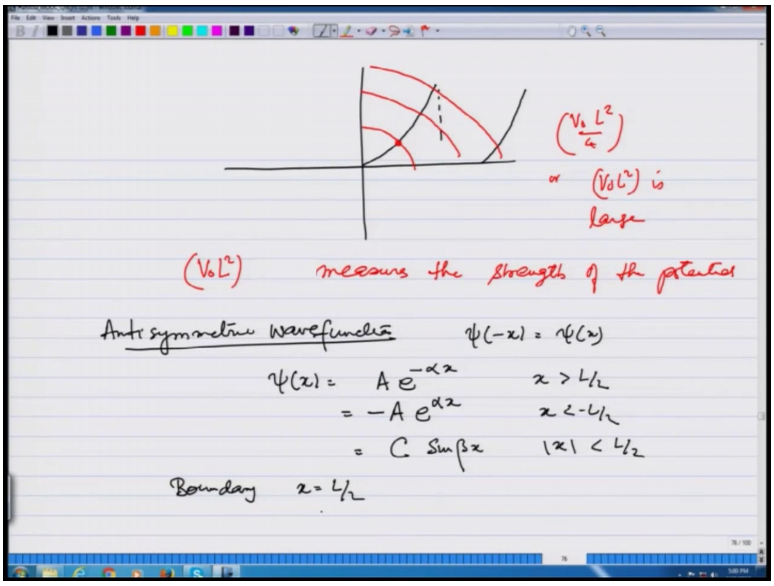

So, what we conclude when I look at the solution this is the first one, the other one starts from pi; and if I look at that y is a function of x this solution is guaranteed the other solution comes only if symmetric solution. If V naught L square by 4 or V naught L square is large. So, sometimes you also say that V naught L square measures the strength of the potential.

So, in quantum mechanics the strength of the potential depends not only is on its height, but also how far it is extended. That make sense because, further away the walls of the potential the delta x is going to become larger and kinetic energy going to become smaller and therefore they will be more bound states, because the same potential can now by in or support more states because they have lower kinetic energy.

Now how about the anti symmetric wave function? Remember in this case psi minus x is equal to psi x. So, in this case I am going to have psi x equals sum A e raise to minus alpha x for x greater than L by 2. And this is going to be minus A e raise to alpha x for x less than L by 2. And is going to be some constant C or d does not matter what I call it sin beta x for x mod x less than L by 2.

So, this is minus L by 2. Now the nature of the solution changes and at the boundary x equals L by 2.

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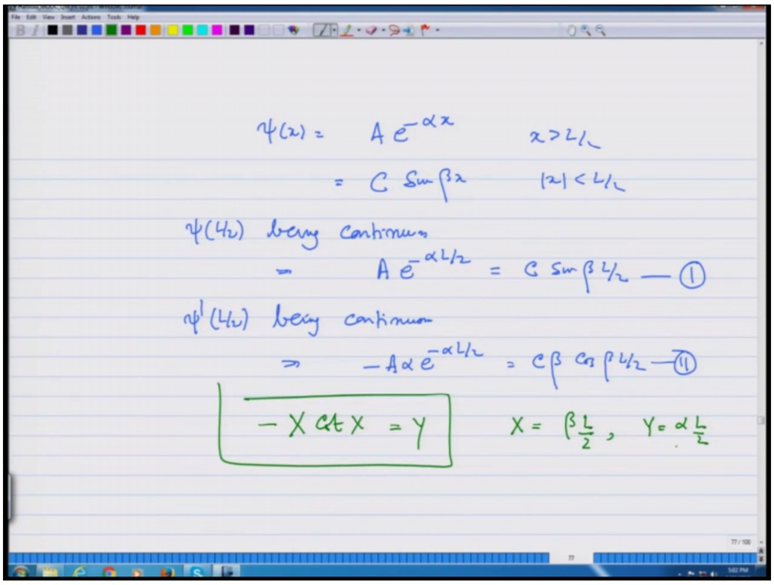

If I match the wave function is derivative again I am going to get the energy. So, I have psi x equals A e raise to minus alpha x x greater than L by 2 and this is equal to sum C sin of beta x for mod x less than L by 2. So, psi at L by 2 being continuous implies A e raise to minus alpha L by 2 is equal to C sin of beta L by 2. And psi prime L by 2 being continuous implies minus A alpha e raise to minus alpha L by 2 is equal to C beta cosine of beta L by 2. This is equation 1 this is equation 2.

This time when you combine the two equations what you get is minus x cotangent of x is equal to y. Where again, x is equal to beta L by 2 and y is equal to alpha L by 2 like earlier.

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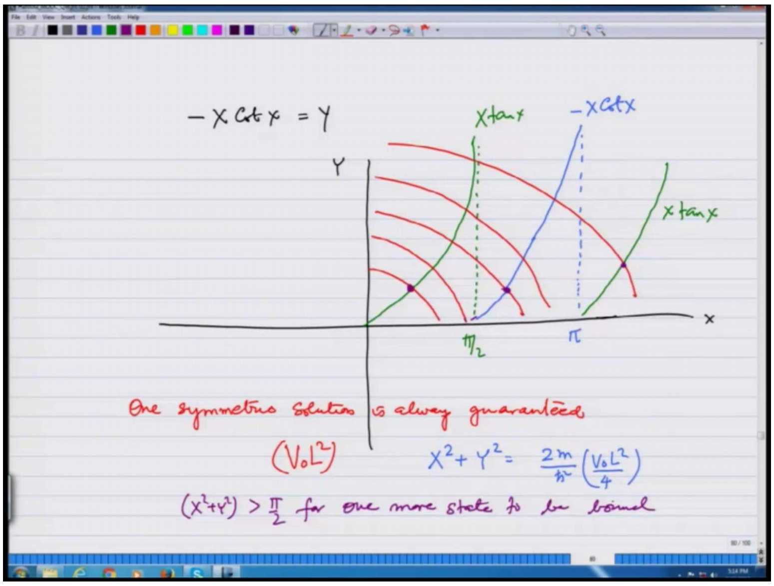

Solution of this equation that is minus x cotangent x equals y can also be obtained graphically as we did earlier for tangent x equals y. And let us see how it is done. So, if I plot x tangent x it was going schematically like this blowing up at x equals pi by 2 this is x. And minus x cotangent x would be 0 at this point. So, this is x tangent x minus cotangent x would go like this and would blow up at x equals pi. And from here again I will get x tangent x. This one is minus x cotangent x.

And remember how y is given as a function of x. So, this is my y, this is x. Y is a function of x is given by the circles. So, intersections give me the solutions. So, one solution is always guaranteed. So, let us conclude one symmetric solution is always guaranteed as we commented earlier. However, the strength of the potential which we earlier defined as V naught L square needs to go up if I want more bound states.

So, remember the equation for x square plus y square is 2 m over h cross square V naught L square by 4. If V naught L square by 4 becomes larger and larger, that means the radius of this red circles becomes larger and larger more states come. Notice that the first state is symmetric, then I get an anti symmetric state, then I get a symmetric state again, next one will be anti symmetric. So, the states flip between symmetric in the lowest energy, next higher is anti symmetric, next higher is again symmetric and so on.

What is the minimum strength that I need for the next two states being there two bounds is being there. So, for that the radius of the circle; let us x square plus y square should be greater than pi by 2 for one more state to be bound.

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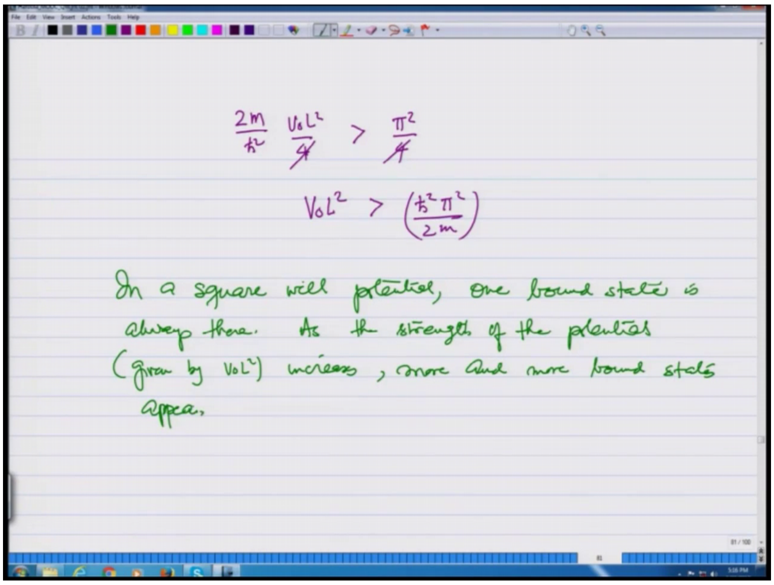

And what that means is: 2 m over h cross square V naught L square by 4 should be greater than pi square by 4 or V naught 1 square should be greater than h cross square pi square over 2 m. If that is the case in that situation I will have two bound states. If I make it larger and larger more and more bound states will come.

So, in this case what we can say is that in a square well potential or finite will potential, one bound state is always there has the strength of the potential. Let us write it given by V naught L square increases more and more bound states appear.

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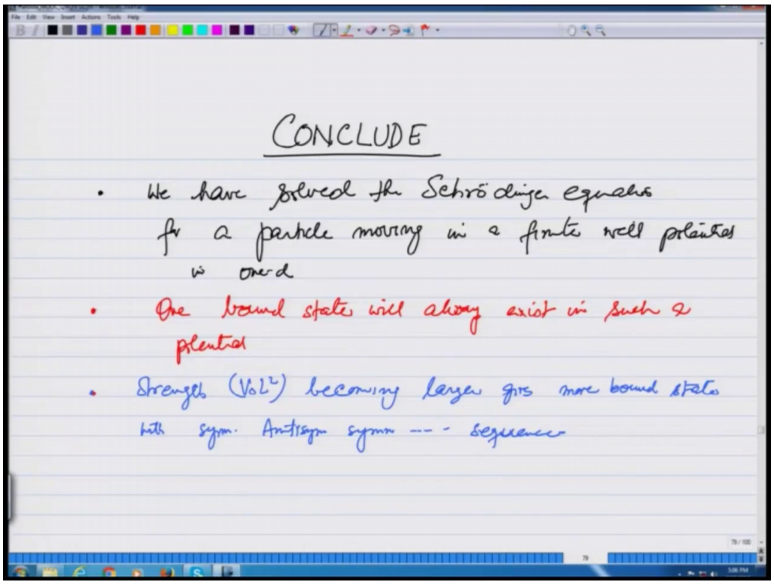

So, to conclude this lecture we have solved the Schrodinger equation for a particle moving in a finite well potential in one d. Second: one bound state always exist in such a potential. And strength V naught L square becoming larger gives more bound state with symmetric, anti symmetric, symmetric-anti symmetric sequence.

So, we stop here on this. And in the next lecture now we are going to do how to solve the one d Schrodinger equation for more complicated potentials using numerical techniques.