Quantum Mechanics- I
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Lecture - 25
One-Dimensional Square Well Potential: The Bound State Problem

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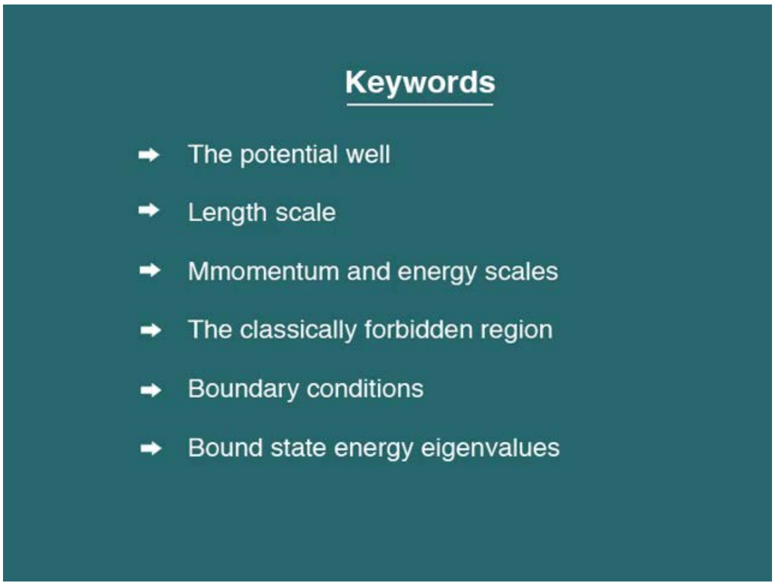

Let me start with a quick recapitulation of what I said about solving for stationery states of the one dimensional harmonic oscillator and their salient features. Before I move on to another topic today, which is a particle of mass m subject to a squared well potential, that is also a one dimensional problem.

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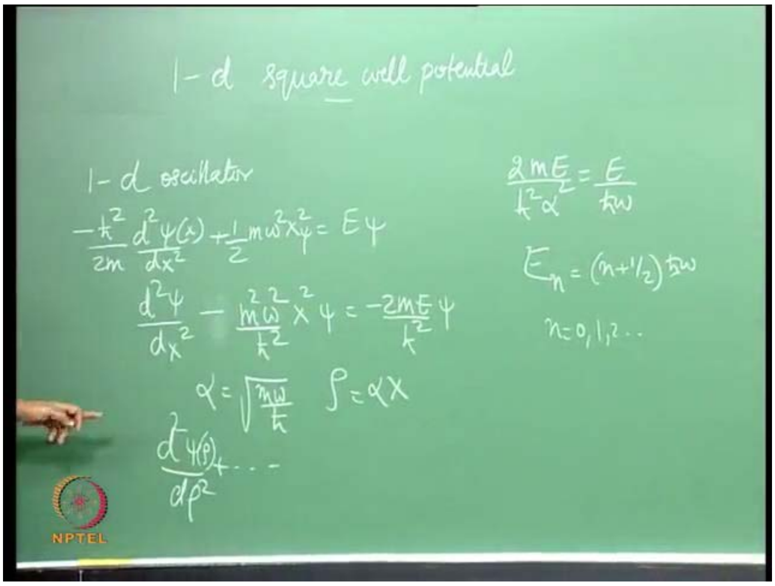

So, really I will be looking at the one dimensional square well potential. But before we go on to that, let me recall for you the essential features of solving a differential equation, the time independent Schrodinger equation, in the case of the harmonic oscillator which we have already done. You will recall that the equation for the oscillator was of this form. This is the potential term half m omega squared x squared there is a psi on which it acts and there is an E psi, psi is a function of x.

Then we defined certain variables. We defined the following. We wrote it in the fashion d 2 psi by d x squared plus m squared omega squared by h cross squared with the minus sign, because of the overall minus in d 2 psi by d x squared is equals to minus 2 m E by h cross squared psi. And, then we said that there is an object of dimensions of inverse length here and in my notation alpha was root of m omega by h cross. Now, that is an object of the dimensions of inverse length, which I have made using the constants that are available here: m, omega and h cross. They are given to me in the problem.

Then we define rho which was alpha x and which was therefore, a dimensionless quantity. Recast this equation in terms of d 2 psi by d rho squared plus so on, where psi was a function of rho. And in the process we also got a quantity 2 m E by h cross squared alpha squared. Now, this can be written as E by h cross omega and therefore, that is a dimensionless variable. In other words, what we are doing is the following. E will be written in terms of h cross omega, 1 h cross omega, 2 h cross omega and in this problem n plus half h cross omega, once E is quantized.

So, we got E sub n where n takes value: 0, 1, 2 etcetera is n plus half h cross omega. So, what is it that we have done? The message that it gives us is the following: identify length scales energy scales in the problem. Find out the energy Eigen-values in the problem in terms of that energy scale in units of h cross omega. The reason why I had a length scale in the problem was in this case to go to dimensionless variable rho is alpha x and that object does not have dimensions.

Now, this is a matter to be remembered in all problems that we will solve and therefore, with this recap I will move on to the one dimensional square well potential. Use some of the tricks that I have learnt here and you will see the similarities in solving problems of this kind.

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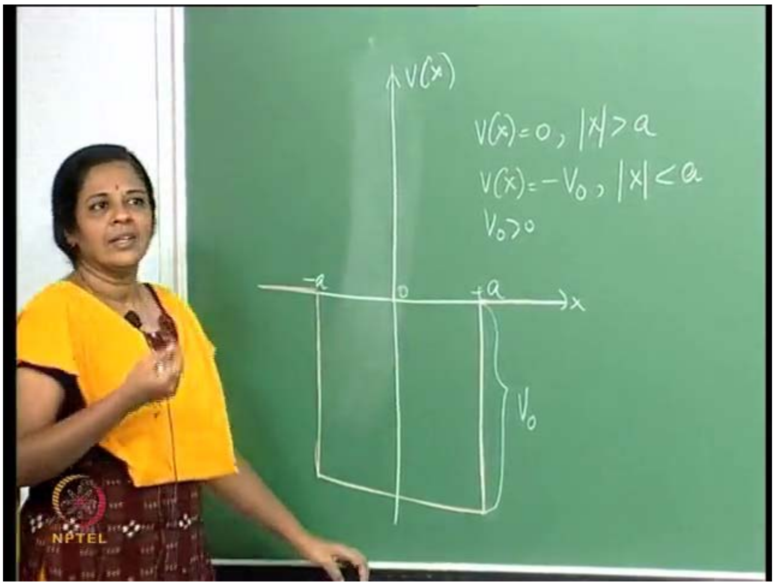

So, here is a schematic sketch of my one dimensional potential. So, this is V of x versus x except that this is the origin and my potential is negative in a certain region. It is a square well, this is x is equal to minus a and that is x equals plus a. Since, this is the origin anything below is negative. Let that height be V naught and let me use another chalk. A potential of this kind so, if you can see the difference between the white and the pink colors that I have used. V of x is 0, if x is greater than a, mod x is greater than a.

So out there and out there all the way to infinity V of x is 0 and V of x is minus V naught, where V naught is positive. So, it is minus v naught for mod x less than a so, this is the square well potential, zero beyond a certain length scale, a non zero within that length scale. This is what I have. Notice that there is a natural length scale in this problem a so, a is the width of the well 2 a if you wish you wish. But a is typically the length scale which determines the width in this problem and therefore, I have a momentum scale in this problem.

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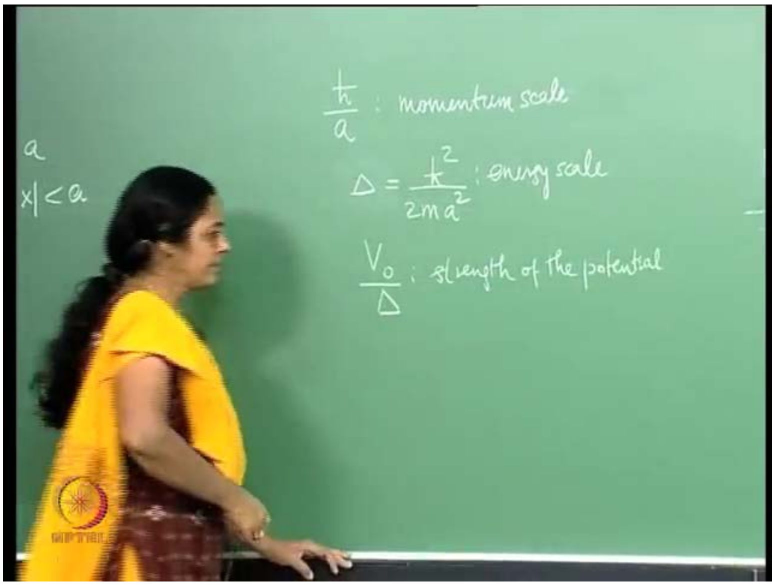

My momentum scale is h cross by a. This is the momentum scale in this problem. There is a nice interpretation. If the particle of mass m were inside this potential well and you do not know where it is. Roughly there is an uncertainty in it is position which is given roughly by a and therefore, there is a corresponding uncertainty in its linear momentum given by h cross by a. Then an energy scale naturally emerges in this problem. So, I have an energy which is given by p square by 2 m which is h cross squared by 2 m a square.

Now, this object has dimensions of energy. This is clearly not going to be the energy of the particle. I am saying that this is an energy scale. In other words, analogous to the harmonic oscillator problem, where h cross omega gave me the energy scale in terms of parameters that are already available in the problem. Then, when I quantized the system I wrote the energy in terms of h cross omega, in units of h cross omega as n plus half h cross omega in the case of the oscillator. Now, I will find energy in units of h cross squared by 2 m a square. To begin with I can talk of the strength of the potential.

So, if I call this object h cross squared by 2 m a squared as delta my potential is V naught. V naught by delta is no dimensions and V naught by delta will tell me the strength of the potential. In other words, we can tell you that V naught is 5 delta, 7 delta, 70 delta, 2.5 delta whatever, but delta sets the energy scale in the problem. So, typically in these problems it is good to identify length scales, energy scales and so on. Shortly I will identify an object of the dimensions of length, but before that I need to pass some comments to understand the classical picture. What happens to a classical particle subject to (Refer Slide Time: 04:31) a potential like this?

Now two things can happen. The total energy of the particle can be greater than 0 although, the potential is negative, the total energy can be greater than 0 because the kinetic energy is overpoweringly positive.

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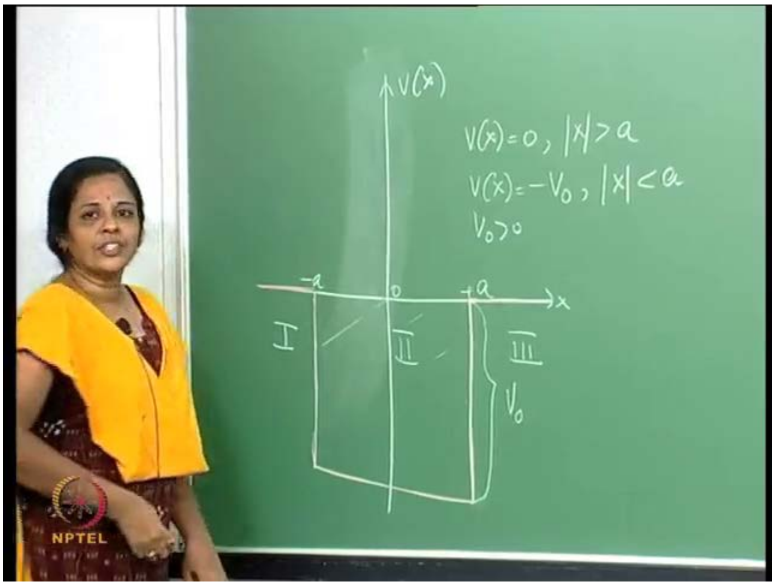

Now, if the total energy is greater than 0 and you have to schematically show where the energy is you would say that, the energy is somewhere out there. You think of this as total energy, and then the energy level is above this axis, because this is the 0 of energy. In that case the particle can move into all these regions. I will refer to this as region 1 whatever, happens inside the potential well this whole thing is region 2 and this is region 3. So, the particle can move any where it wants through region 1, all the way here because the energy is greater than 0. However, you know that kinetic energy cannot be negative. So, if the total energy of the classical particle is less than 0 suppose that happened, because the energy is somewhere out here it is less than 0. Then the particle is classically forbidden from moving into regions 1 or 3 and cannot get from here outside the square well for a very good region.

Because if the total energy is less than 0. Since, the potential is zero here in regions 1 and 3. The kinetic energy will be negative whereas, the kinetic energy is e minus V and since, V is 0 and e is negative, the kinetic energy is negative. And therefore, 1 and 3 are classically forbidden regions, if the total energy is less than 0. So, let me just put down this point. Therefore, there are two cases: the total energy greater than 0 and the total energy is less than 0.

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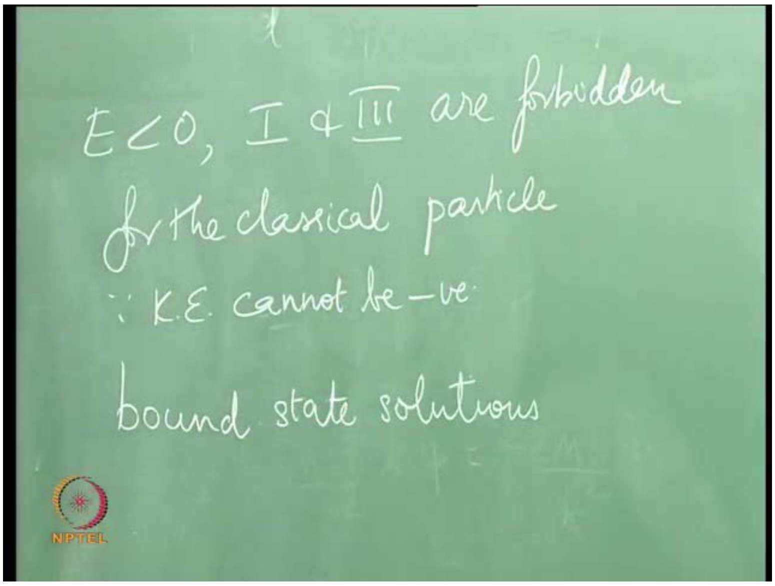

Now if E is less than 0, regions 1 and 3 are forbidden for the classical particle which was initially inside the potential well, classical mass of m. Because kinetic energy cannot be negative, ((Refer Time: 12:40)) V is greater than 0. That is not true, as we have already seen particle can be anywhere. So, there 2 cases to discuss: E less than 0 and E greater than 0. If E is less than 0 since, the particle is confined to within the square well you say that the particle is bound by the potential and therefore, you have bound states solutions. Solutions for the energy Eigen functions with corresponding energy Eigen values.

So, that is what we will look at immediately. We will look at the case energy less than 0, this is the bound sate problem and we will see how exactly the quantum situation differs from the classical situation. So, let us first write down the equations to obtain the stationery state solutions.

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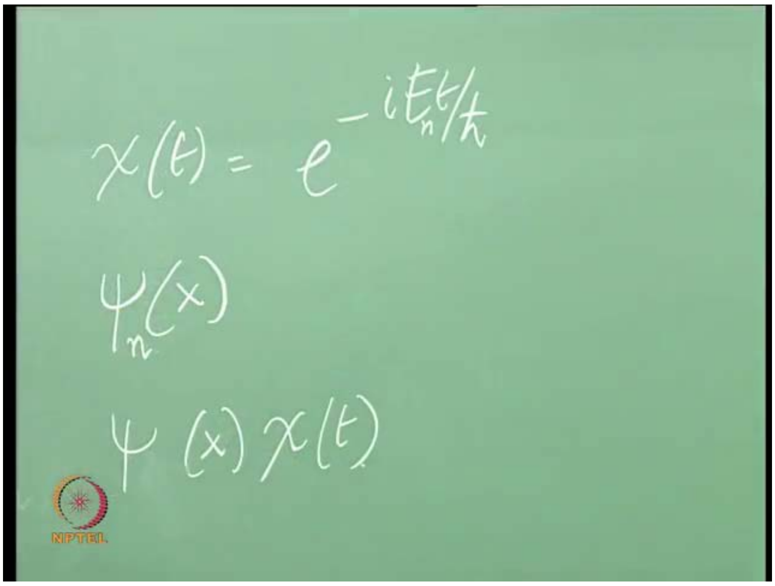

Now, you will recall that the time dependence of a stationery state solution was given by some chi of t which is e to the minus i E t by h cross. And if e were quantized it would be E sub n t by h cross. The total wave function of course, had a contribution from the space part which was psi of x and corresponding to the energy E sub n you would have solution psi sub n of x for the stationery states, the energy Eigen states of the system. The total wave function of course, will be psi of x chi of t in general.

So, we are now suppose to solve for psi of x analogous to what we did in the case of the simple harmonic oscillator where we wrote h psi is equal to e psi. In that case h was given by minus h cross squared by 2 m d 2 psi of x by d x squared plus half m omega square x square h psi and you equated that to e psi.

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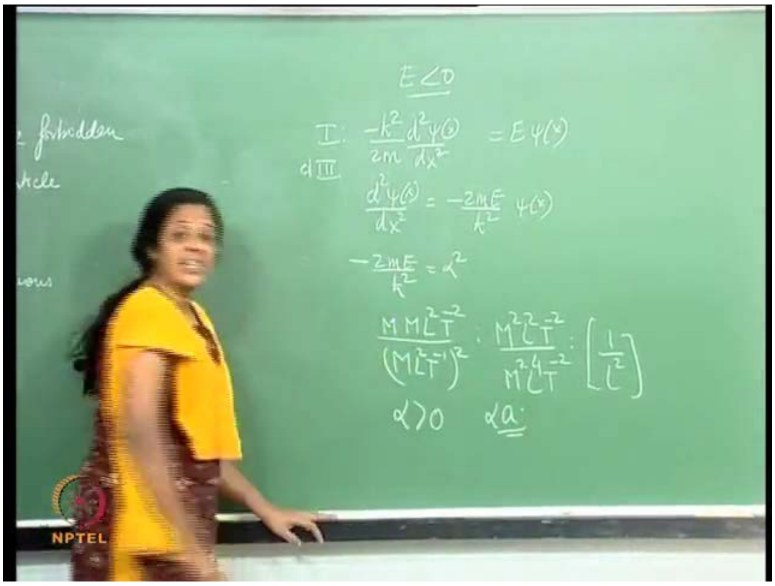

Now, here there are 3 regions two without a potential, the potential was 0 and the square well itself has a non zero potential and therefore, I have the following equations. In region 1, I have minus h cross squared by 2 m d 2 psi of x by d x squared; no potential is E psi of x. The same equation holds in region 3 as well. Of course, it is obvious that it is good to make the equation look less clumsy and therefore, I can write d 2 psi of x by d x squared is minus 2 m E by h cross squared psi of x. Look at this object, minus 2 m e by h cross squared e is less than 0 and there is an overall negative sign. We are looking at bound state problems and therefore, minus 2 m E by h cross squared is a positive quantity. Let me call that alpha squared.

Now, what is the dimension? This object minus 2 m E by h cross squared dimensions that is mass this is M L squared T to the minus 2, h cross itself is M L squared T to the minus 1 the whole squared, because there is an h cross squared. And therefore, that gives me an M squared L squared T to the minus 2 by M squared L to the 4 T to the minus 2 and therefore, the dimensions here is one by L square. Therefore, alpha has the dimensions of 1 by length, like to keep alpha positive.

So, I choose alpha to be greater than 0; no loss of generality and I say that alpha has dimensions 1 by length. That is a good thing to know. If you recall, this would be the analogue of alpha in the case of the harmonic oscillator as well, except that the alpha there had a very different definition it was root of m of omega by h cross and therefore, since this has dimensions of 1 by length, alpha a is a dimensionless quantity.

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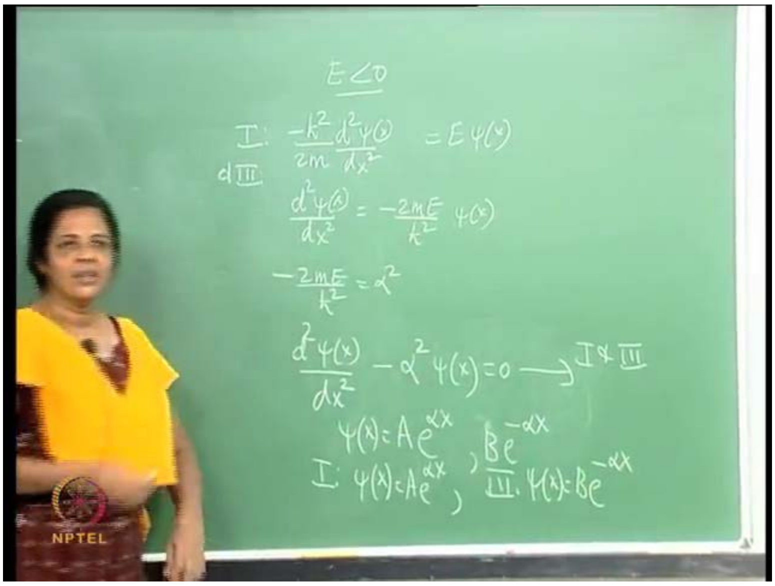

That is a good thing to remember. I can now go back and write my equation very nicely. d two psi of x by d x square is alpha squared psi of x. So, taking into the other side this is my equation for regions 1 and 3. That is what I have. Got to solve for this equation, the solution is simple. The allowed solutions are psi of x is some constant A e to the alpha x. It is also true that there is another solution: e to the minus alpha x, apart from some constant B. But then boundary conditions have to be respected. Certainly at space infinity that is x going to plus infinity or minus infinity, the wave function has to vanish in order to sustain the probabilistic interpretation.

And therefore, since we are looking at the region 1 first. In region 1, x goes to minus infinity and there is no problem here, where as that blows up and therefore, in region 1 psi of x is A e to the alpha x. Now in region 3, psi of x is B e to the minus alpha x, because when x goes to plus infinity this is fine and that is not. So, I have solutions in region 1 and region 3.

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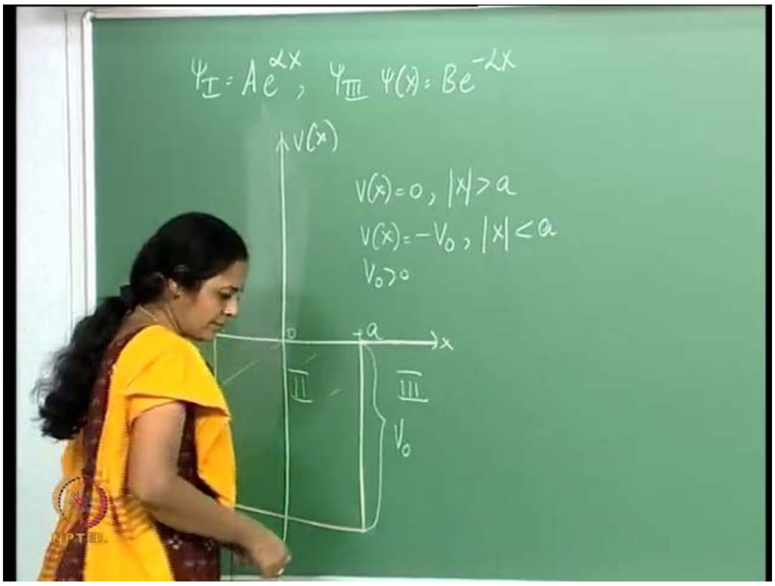

So, let me write that here. Psi in region 1 is A e to the alpha x. Remember that alpha is positive and in region 3 psi of x is B e to the minus alpha x. Now, this is rather interesting of course, we have to check for consistencies we have to solve for A and B, but if we do find solutions which indeed we will. That tells us psi star psi is not 0 in regions 1 and 3. That means there is a non zero probability of saying the particle in regions 1 and 3. But these are classically forbidden regions. So, this is a thing worth checking out. So, the details of the calculation should tell us if indeed classical forbidden regions are accessible to a quantum mechanical particle. So, that is a matter of interest in this problem.

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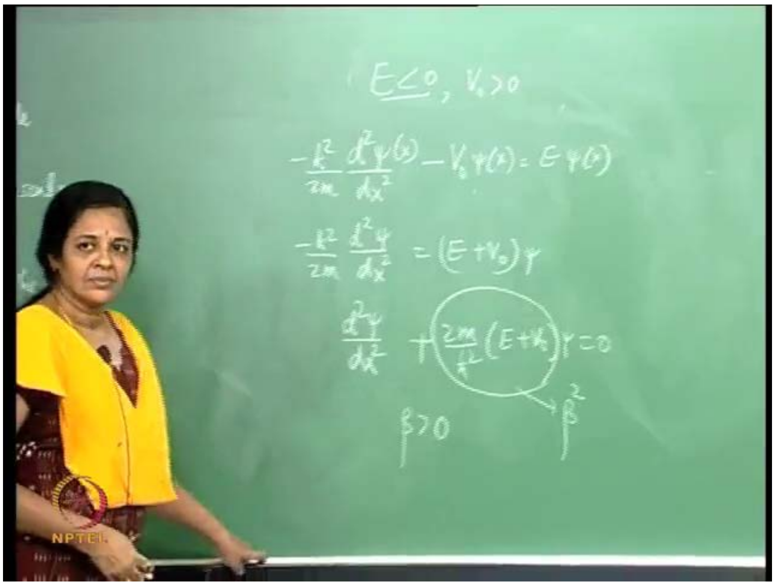

Now, look at region 2. We are looking E less than 0, in region 0 you have the equation: minus h cross squared by 2 m d 2 psi of x by d x squared plus V psi of x is equal to E psi of x. But V is minus V naught, where V naught is greater than 0. And therefore, I have d 2 psi by d x squared by the minus h cross by 2 m outside is E plus V naught psi. So, I write d 2 psi by d x squared is minus 2 m by h cross squared E plus V naught psi. I can always pull it to this side and write that d 2 psi by d x squared plus 2 m E plus V naught by h cross squared psi equals 0. I know that 2 m E by h cross square I have already worked that out is dimensions of 1 by length squared.

So, this also is energy and this two has dimensions 1 by length squared. Here, E is less than 0, V naught is positive and 2 m by h cross squared E plus V naught. If E is less than 0 and V naught is positive so, that is V naught (Refer Slide Time: 04:31) E somewhere, out here so, E plus V naught is any way positive and therefore, this quantity I will call it beta squared, where beta squared like alpha squared, has dimensions of inverse length squared. I defined beta to be greater than zero.

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So, now I have 2 objects: alpha and beta, both positive by my definition, without loss of generality and the natural dimensions is inverse length. I also have a delta, which I have constructed with the constraints that are available in the problem and delta has dimensions of energy. Therefore, the depth of the potential V naught can be written in terms units of delta and lengths are scaled in units of 2 m E by h cross squared or 2 m E plus V naught by h cross squared in terms of alpha and Beta.

So, I have this equation. Let me just rewrite that equation here. I have d 2 psi by d x squared plus beta squared psi equals 0. Again the solution to this equation is obvious. Psi of x since, we have already used A and B let us say C and D is C cos beta x plus D Sin beta x. So, this is the solution in general where C and D are constants. We have to determine A, B, C and D which we will suitably. Now we come to boundary conditions. So, this is the solution in region 2.

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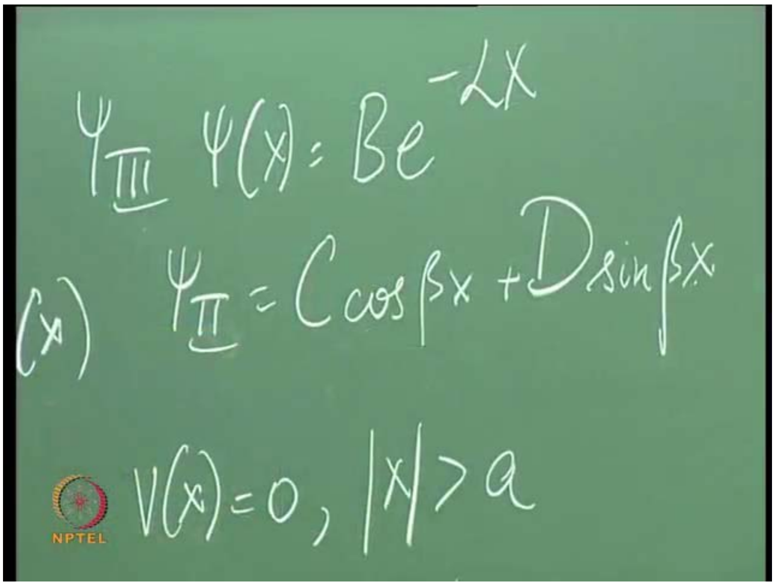

So, let me write that there. Psi in region 2 is C cos beta x plus d sin beta x so, this is what I have by way of solutions. But then you see there are boundary conditions and the boundary conditions are such that the way function is continuous at the boundary and so is the first derivative. Now, how did I get that? So a small digression as to how we get these boundary conditions, at the boundaries. That is in this problem at x is equal to plus a and x is equal to minus a.

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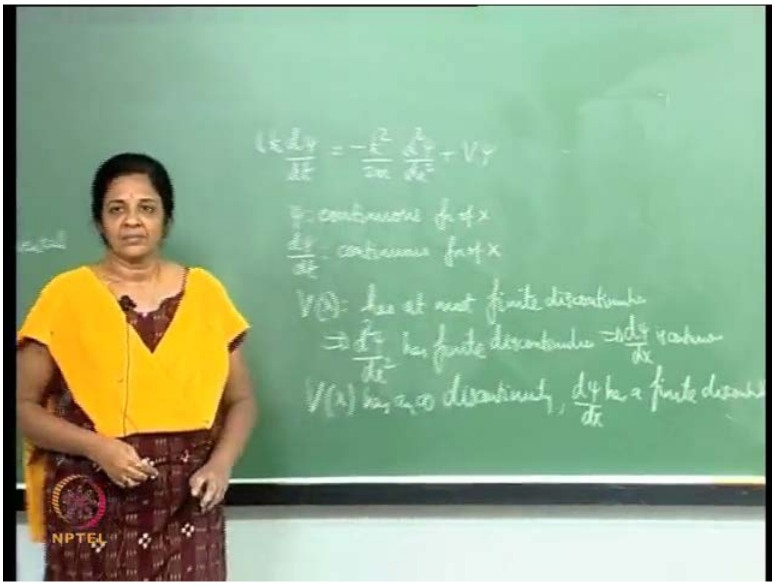

Look at the Schrodinger equation I h cross d psi by d t is minus h cross squared by 2 m d 2 psi by d x squared plus V psi. The wave function is continuous and that is our requirement. You need to take its 1st derivative and its 2nd derivative so, psi is continuous and vanishes at space infinity for the probabilistic interpretation. Therefore, d psi by d t is continuous function of x. So, the left hand side in this equation has a continuous function of x.

Now, look at the right hand side. We assume that the potentials that we are considering has at most it is continuous or finite discontinuities, at some specific values of x. Now, if V of x has finite discontinuities so, does this. But this is a continuous function of x, the left hand side and therefore, between the 2 terms in the right hand side. These discontinuities should cancel out which means d 2 psi by d x squared the 2nd derivative has finite discontinuities in order to cancel out these discontinuities in the potential V of x. That implies the d psi by d x is a continuous function of x.

Now, that is the kind of situation we are facing here. It is obvious that that is not going to be the case in a problem where say V of x has an infinite discontinuities somewhere and suppose this well ((Refer Time:27:37)) (Refer Slide Time: 04:31) infinite well. Suppose, there was an infinite discontinuity in V of x certainly, the left hand side continues to be a continuous function of x and therefore, the infinite discontinuity here must be compensated by an infinite discontinuity there, which means the 2nd derivative of psi has an infinite discontinuity or a set of infinite discontinuities.

Now, that means that the 1st derivative d psi by d x has finite discontinuities. So, if V of x has an infinite discontinuity, d psi by d x was a finite discontinuity at that value of x. Now, in this problem we need to use the fact that d psi by d x is a continuous function of x. There are no discontinuities which mean I need to do the following thing. At x equals minus a (Refer Slide Time: 10:25) I have to match the wave function in region 1 with the wave function in region 2. I also have to match the 1st derivative of the wave function in region 1 with the 1st derivative of the wave function in region 2.

Now, I have to do the same thing here. I have to match the wave functions between 2 and 3 and the corresponding 1st derivatives also at x equals plus a. So, at x equals minus a and plus a, such a matching has to happen. The wave function and the 1st derivative both have to be continuous. So, let me do that first. Now, in this case, I have the following conditions at the boundaries at x equals plus a and minus a.

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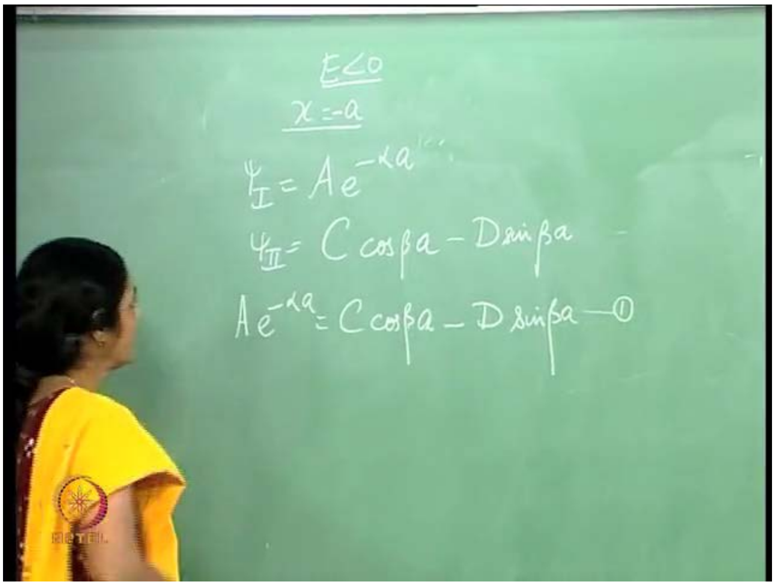

So, let us look at x equals minus a. Remember we are working only with bound state solutions E is less than 0. So, at x equals minus a, psi 1 is A e to the minus alpha a, psi 2 is C cos beta a minus D sign beta a this is what i have at x equals minus a. I have to match both of them so, A e to the minus alpha a is C cos beta a minus D sign beta a. So, this is one equation that I have.

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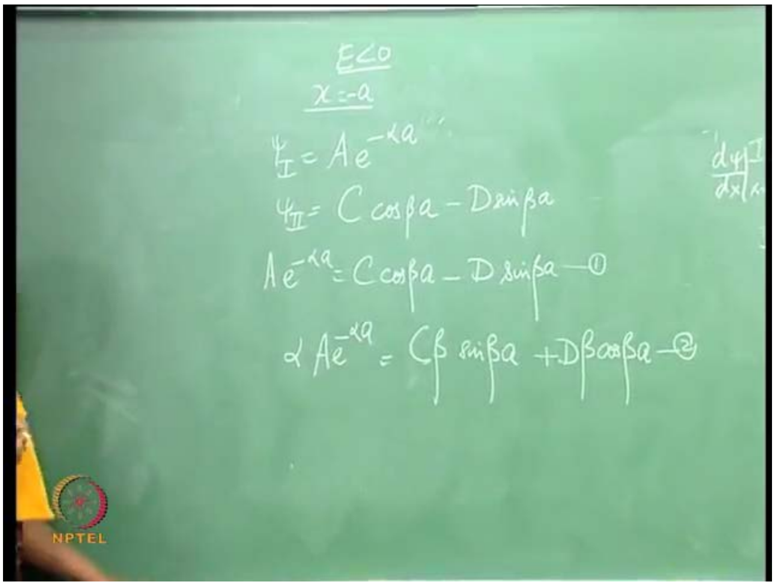

Now, look at the derivatives. At x equals minus a, the derivative there is alpha A e to the alpha x at x equals minus a. So, I have alpha A e to the minus alpha a. This is for region 1 that means d psi by d x at x equals minus a. That is what I have and then, if you look at region 2, d psi by d x is given by minus C beta sin beta x plus D beta cos beta x and you are substituting x equals minus a so, this is what I have. Now, these two should be equated and therefore, I have alpha A e to the minus alpha a is C beta sin beta a plus D beta cos beta a.

So, this is my 2nd equation the 1st came out of matching the wave function, the 2nd equation came out of matching the first derivatives at x equals minus a. I do the same thing for x equals plus a.

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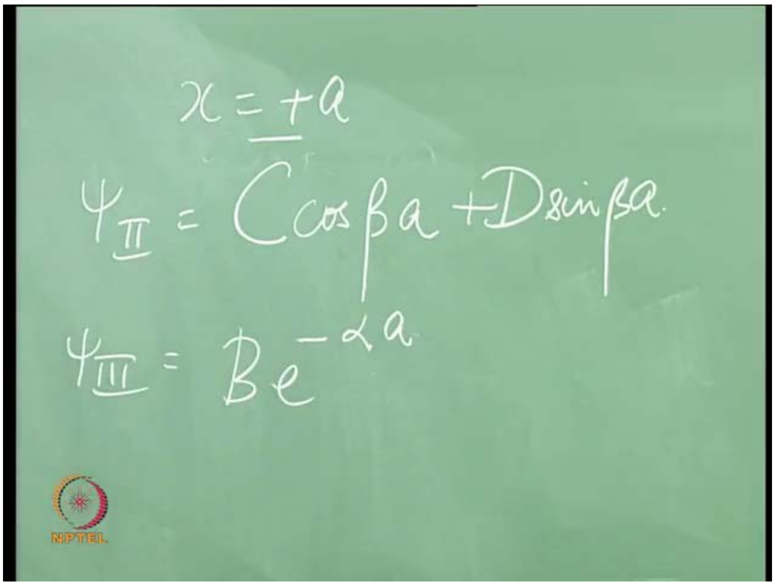

So, let us look at x equals plus a, psi 2 is given by C cos beta a plus D sin beta a and psi 3 is out there so, psi 3 is B e to the minus alpha a.

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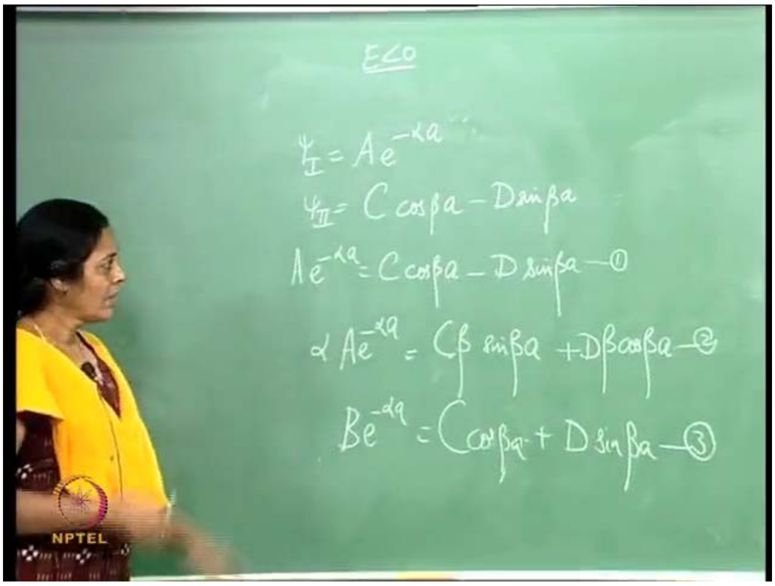

So, this is what I have. I need to match the 2 of them and therefore, my 3rd equation would simply be B e to the minus alpha a is C cos beta a plus D sin beta a. So, that is my 3rd equation, 4th equation comes out of matching the derivatives.

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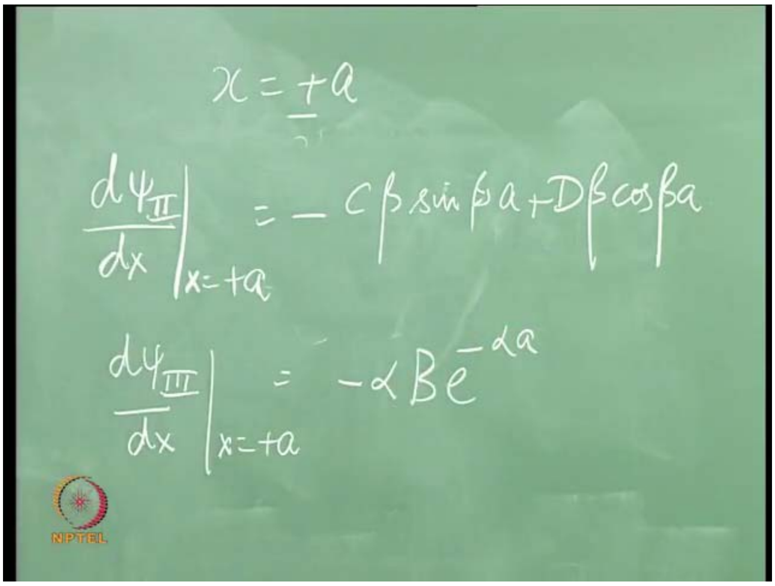

So, the derivative d psi 2 by d x at x equals plus a is what we want. So that is minus C beta sin beta a, that is the 1st term plus D beta cos beta a, whereas D psi 3 by d x at x equals plus a is minus alpha B e to the minus alpha a. So, these have to be matched.

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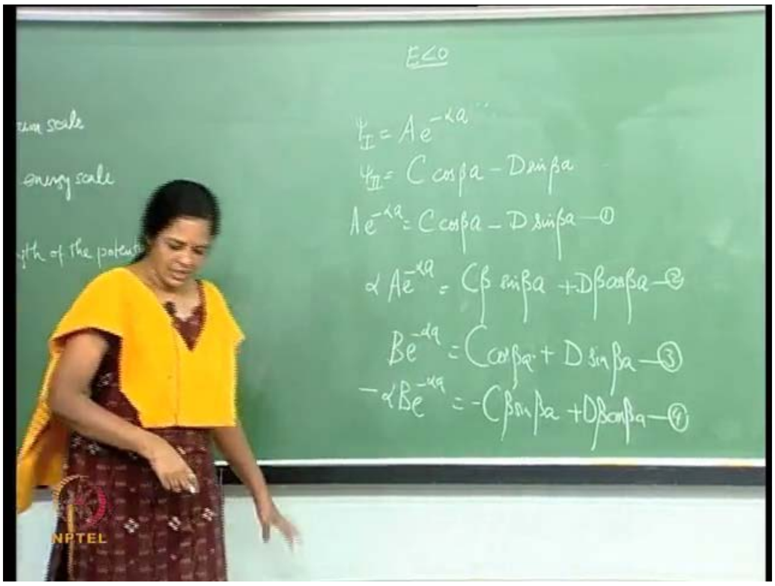

Now 4th equation simply says minus alpha B e to the minus alpha a is minus (Refer Slide Time: 33:47) C beta sin beta a plus D beta cos beta a and that is my 4th equation. So, these are the four equations. The up short of the whole thing is this I will have to work with these 4 equations and fix values for C, D, A and B. Find solutions and see if they are consistent. In fact two types of solutions emerge so, let us look at this.

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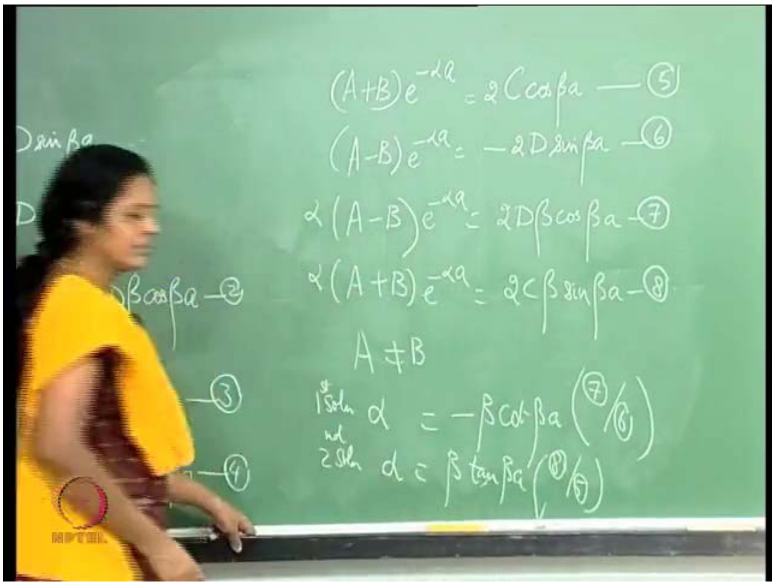

I can add the first 2 equations. So, that gives me a plus b e to the minus alpha a. So, I am adding equation 1 and 3. (Refer Slide Time: 34:36) So, when I add it I get 2 C cos beta a. I will call this equation 5. I can subtract (Refer Slide Time: 34:36) 1 from the other. So, I have A minus B e to the minus alpha a. So, I am subtracting 3 from 1. (Refer Slide Time: 34:36) So, I get minus 2 D sin beta a. So, that is 6. Now, that is not the only thing that I can do I can look at these equations (Refer Slide Time: 34:36) I can look at 2 and 4 and do the same thing so, if I add the two of them. (Refer Slide Time: 34:36) I have alpha times A minus B e to the minus alpha a out here. I am adding the two of them so, the sin terms cancel and I have 2 D beta cos beta a.

So, that is equation 7 then, last equation that I need comes by subtracting (Refer Slide Time: 34:36) 1 from the other and therefore, I have alpha A plus B e to the minus alpha a. So, I subtract 4 from 2 here. (Refer Slide Time: 34:36) When I subtract I have 2 c beta sin beta a and the D term goes. This is what I have. Now, given these four equations, let me start of by saying that a is not equal to b or let me start of by saying that A and B are non zero.

So, which means these terms survive. So, A minus B is not equal to 0. Now, if indeed that is true let me divide 7 by 6. Now, if I did that I get alpha is equal to minus beta Cot beta a. So, that is one thing that I have so, that is possible. I could have used this equation and I could have divided equation 8 by equation 5 and that would have given me alpha is equal to beta tan beta a. So, one solution is alpha is minus beta Cot beta a. I got this by looking at these 2 equations so, equation 7 divided by equation 6 gave me this. The other solution came because I divided equation 8 by equation 5.

So, this is one solution the 2nd solution for alpha is got by dividing equation 8 by equation 5 and that simply tell me that alpha is equals to beta tan beta a. So, this came by dividing 8 by 5 both solutions are there. We need to proceed and see what these solutions give us. So, let me first consider the 2nd solution alpha is equal to beta tan beta a. Right away one thing is clear that only certain values of beta a are allowed in this problem because alpha is positive and beta is positive so, the tan function only some values, some regions are allowed and that I can easily check out now.

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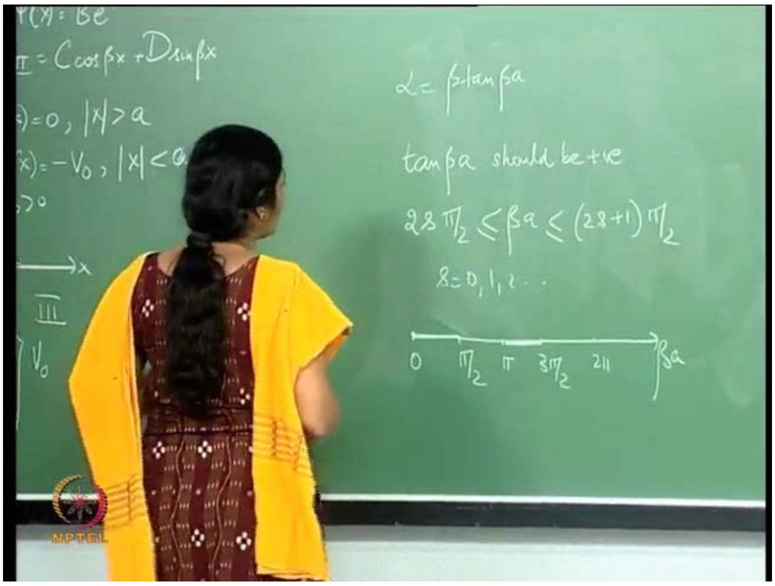

So, tan beta a should be positive. I am considering the 2nd solution. Since, tan beta a should be positive, it is clear that 2 s pi by 2 less than or equal to beta a less than or equal to 2 s plus 1 pi by 2, where s can take value 0, 1, 2, 3 etcetera. So, if you now, have beta a on this axis and this is the origin and you have pi by 2, pi, 3 pi by 2, 2 pi etcetera on this axis. 0 to pi by 2 is an allowed region for tan beta a in this problem, but pi by 2 pi is not. Then when s is 1 pi by 2 3 pi by 2 is allowed and so on. So, there are only some regions which are allowed for beta a in this problem. So, that aspect has to be looked at.

Now, let us go back and use the fact (Refer Slide Time: 35:38) that alpha a is dimensionless and beta a is dimensionless .

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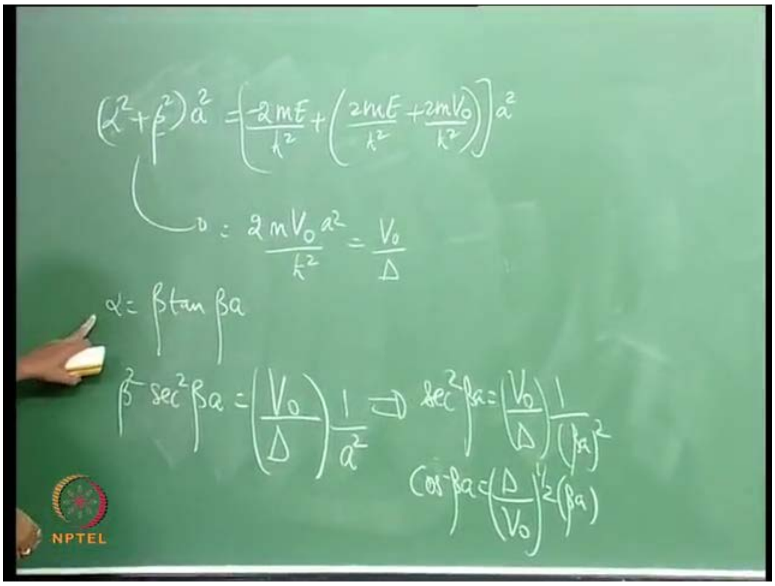

Therefore, I can do the following thing. I can find out alpha squared plus beta squared a squared. Now alpha square plus beta square a square you will recall is minus 2 m E by h cross square plus 2 m E by h cross squared plus 2 m V naught by h cross squared times a square. So, this object is simply equal to 2 m V naught a squared by h cross square but that is the same as V naught by delta, where delta was h cross squared by 2 m E squared. So, here is a dimensionless quantity that is equal to another dimensionless quantity V naught by delta, which is the strength of the potential. So, that is the significance of alpha squared plus beta squared times a squared.

So, let me substitute in this equation alpha is beta tan beta a. Now, if I did that I have beta squared times secant squared beta a is equal to V naught by delta, 1 by a squared and therefore, this implies that secant square beta a is V naught by delta 1 by beta a the whole square. In other words, cos beta a is delta by V naught to the power of half times beta a. That is what I have for my equation.

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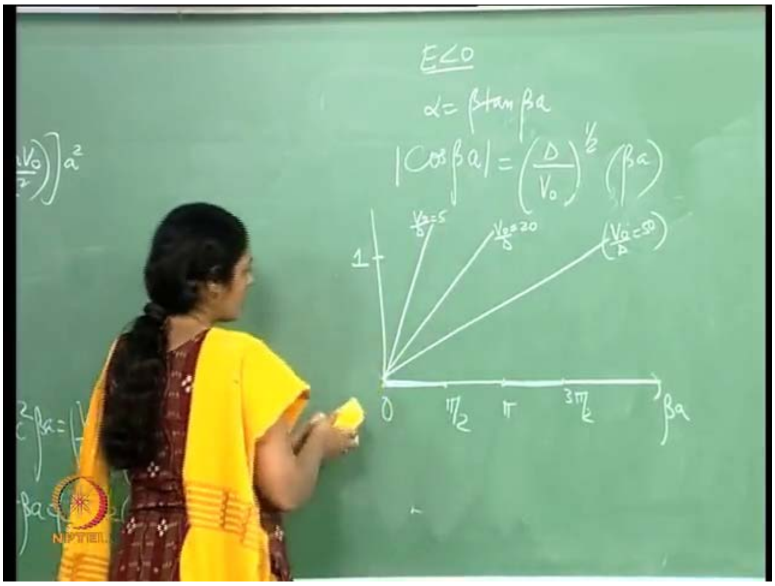

Let us look at this equation. This equation simply tells me the following: cos beta a I chose alpha to be beta tan beta a. I chose that solution and then I have cos beta a is delta by V naught to the half times beta a. You see this equation can be solved for beta, beta is what has the energy in it. Beta is 2 m E by h cross squared plus 2 m V naught by h cross squared and therefore, to solve for beta and see if the energy is quantized. The only way I can do it is by using some sort of graphical plot. So, I have beta a here and as I have already argued 0 to pi by 2 is an allowed region in this problem for beta a, pi to 3 pi by 2 is an allowed region in this problem.

So, these are the values that are allowed for beta a in this problem. I also know that this quantity is positive, delta is positive, V naught is positive and beta and a are positive. So, indeed I should be writing modulus of cos beta a is delta by V naught to the power of half beta a. So, I can plot the right hand side separately here. So, I plot delta by V naught to the power of half beta a versus beta a, not going to be a straight line. So, basically I can choose various values of V naught by delta so, I get straight lines depending on the value of V naught by delta. For instance, if V naught by delta we shall say is 50 remember this is dimensionless. This could be the straight line and V naught by delta is less than that. Let us say 20 this would be the line, V naught by delta is 5 this could be the line and so on.

So, I get various straight lines with different slopes. It is clear that the line passes though the origin and that is an important point which I will talk about a little later. So, you have various straight lines depending upon the numerical value of V naught. In other words, depending upon the strength of the potential, how much bigger V naught is compared to delta. So, what are the allowed solutions? Where cos beta a, let us take that to be 1 where cos beta a cuts these lines.

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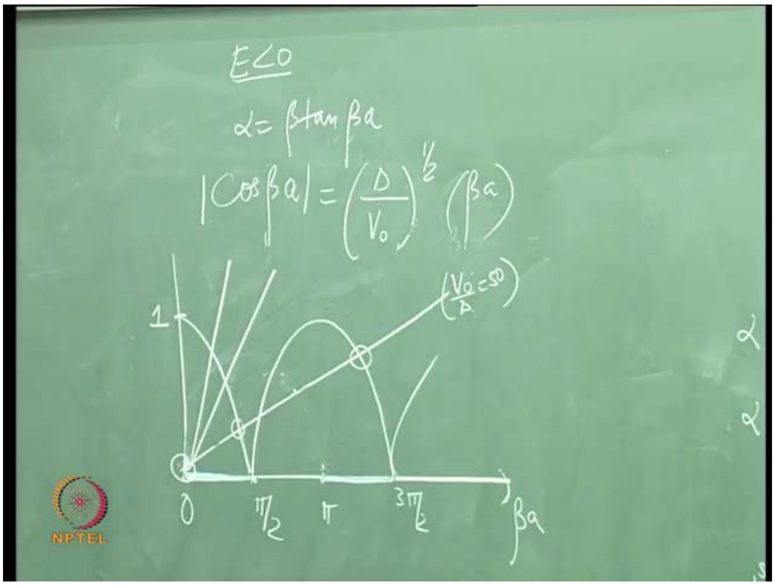

So, let me for reference keep just one line and draw cos beta a. So, this modulus of cos beta is what we want. So it starts from one like that and so on. So, I am not drawing that part. The question is: where does this modulus of cos beta a cut that straight line? Certainly, the origin is not a point and that is an important matter, because certainly one solution for beta is there, there is certainly 1 cut right. Now this is within the allowed region. This is a forbidden region so, this is not an allowed point, but this is an allowed region so, that is an allowed point.

So, you already see that beta is quantized and since beta is quantized, the energy is quantized. So, if you fix V naught by delta so, given the strength of the potential it is clear that there are only some values of beta which are allowed and since those are the values of beta that are allowed, the energy also is allowed only discrete values. Now, I could have done the same thing using the first solution alpha equals minus beta cot beta a.

So, you can repeat the argument it is clear that one bound state is definitely allowed. So, see one bound state is definitely allowed. This is an important point because however, shallow the well may be in other words, even if the well were not deep enough to hold several bound states you are guaranteed that there is one bound state available in the square well problem. Now, this is an important aspect because you see whenever, I study bound state problems, I have to choose a model potential.

Certainly, sometime in the near feature I will talk about the deuteron on problem as an application of the square well potential. The deuteron is a bound sate of the neutron and the proton. It is a very loosely bound state there is exactly one state of energy which keeps it bound for which energy is negative, and then even a small perturbation, a small kick, a small amount of energy given to the deuteron will separate the neutron from the proton and the energy will no longer be negative, it would not be a bound state.

So, the square well is a very good potential to choose for the deuteron because it allows for at least one bound state. I know the deuteron exists in nature and I know it is a loosely bound state. So, depending upon the shallowness of the well you can arrange for a certain number of bound states to be there in the problem.

Returning to the 1st solution, (Refer Slide Time: 35:38) I will urge you to put that in alpha is minus Cot beta a. If you did that (Refer Slide Time: 41:40) you would find that things do not change too much. You will have modulus of sin beta a is this quantity. It should be easy for you to see that and once more instead of modulus of cos beta a, which I have plotted here you would plot modulus of sin beta a you will discover that whatever, I have said till now, about at least one bound state being guaranteed holds good. So, that is the story of the energy Eigen values in this problem, given beta I can always so back and write out my energy.

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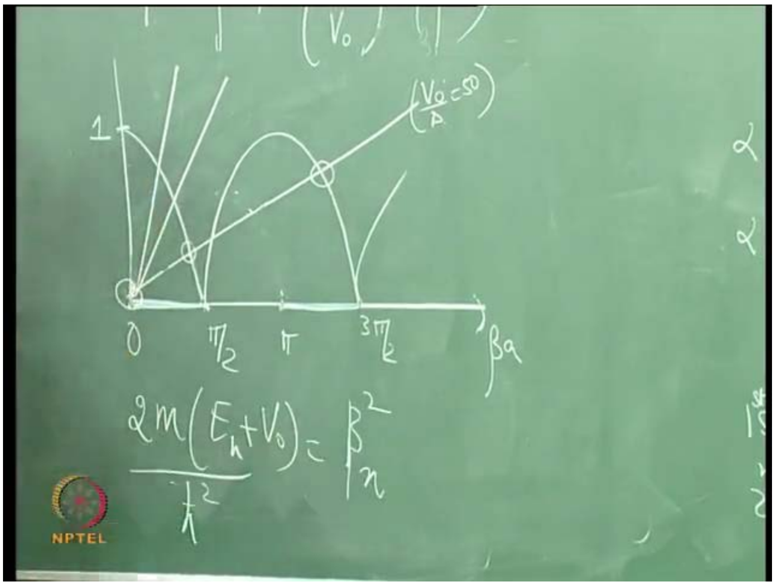

So, E sub n can be written, because I know that 2 m E sub n plus V naught by h cross squared is beta n now squared. So given this, given the values of beta I can find out E sub n discrete energy values corresponding to which we have to find the energy Eigen functions which is what I will take up in my next lecture.