Introductory Quantum Chemistry
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Lecture - 14
Finite Well, Continued

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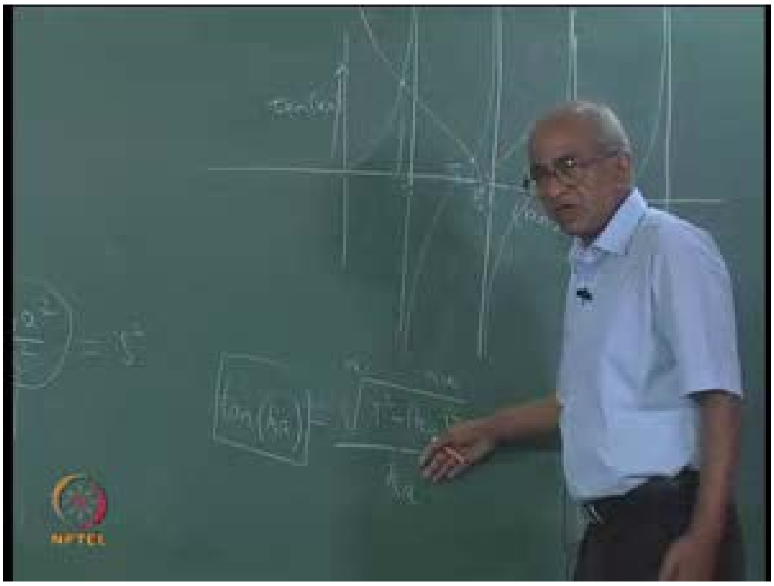

We continue our discussion of last lecture. So, you notice how the curve goes; this ground curve. And you should notice also that you see this is ending this ground curve is ending at the at this point which is k a is equal to zeta; where was my equation k a is equal to zeta. And beyond that if this is imagine this part is imaginary. Now, what will happen if I increase the value of zeta?

How can I increase the value of zeta that is very easy to see; you see we have v 0 which is the depth of your potential value; you also have a which is related to the width 2 a is actually the width of this potential well. So, if you increase the depth of the potential well you are increasing zeta or if you increase the width of the potential well again you are increase the value of zeta. So, by varying either the depth or the width you can vary the value of zeta. In fact, if you increase the depth zeta will increase; if you increase the width again zeta will increase. So, if you increase the value of zeta what will happen actually this curve this point will shift?

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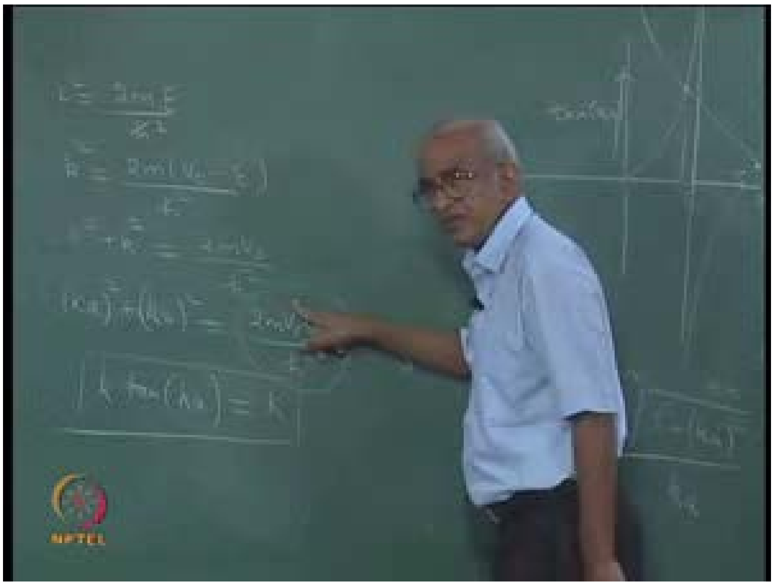

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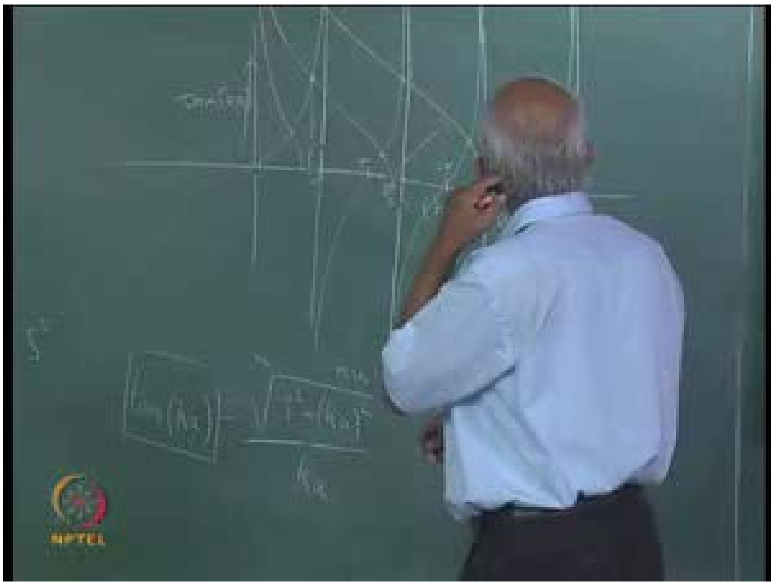

So, you may have a situation where the curve would look like that correct. And then how many solutions do you get? The answer is there are now 3 solutions. That means, actually by increasing the depth or the width; the number of states, number of bound states that exist in your potential well will increase the features. Of course, basically right by increasing the width or by increasing the depth you will cause more bound states for the system. Now, suppose I did the other thing; I decrease the depth or the width what will happen this point is going to shift. So, for example if I decrease it to that value zeta is having this value. Then what will happen is that you will have such an appearance for the curve the because you see at the k is equal to 0 their function is always infinity.

So, the curve will go like that to infinity. Now, you have only 1 bound state correct but can I get rid of that 1 bound state. I do not want any bound state is that possible? Well, whatever you do see the value of zeta will be very small; it may be here still the curve would go like that. And therefore you will find that there is actually 1 solution. So, however weak the potential is it does not matter whether it is very shallow or whether it is very narrow; it does not really matter. You will always have 1 bound state a this is something that happens in 1 dimension. Actually if you are thinking of bound states in 2 dimensions this does not happen this is the specialty of 1 dimensional system. if you have a potential it does not matter how weak it is. If you have an attractive potential well then it will have at least 1 bound state. Now, here I have analyzed the even solutions how would they look like; I mean if I was going to plot them. Let me make a picture showing the plots.

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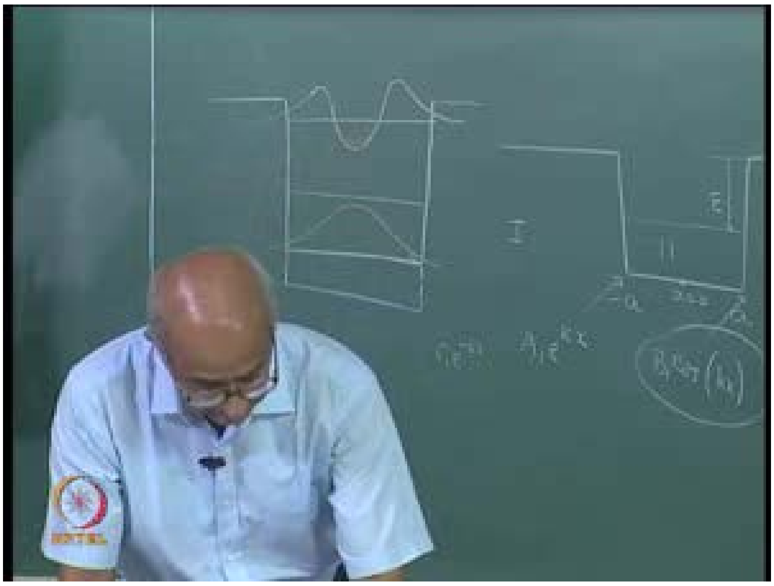

This is my potential well let me say and I have found the values of k the special values of k I have found. And those special values of k can be put in here; and then I can solve for epsilon. Epsilon will give me the allowed arbitrary levels. So, that is the procedure if you I mean you can you say computer program; you know specifically if you like mathematics and get the values of epsilon. And then once you know the values of epsilon you can put those or if you know the values of k you can put those in here. And then of course you will have to determine these constants B 1 and C 1. How will you determine them? Well, the continuity of wave function has to be there; in addition to that you have to ensure that the wave function is normalized.

Therefore, all the constants that you require can be found. And how would they look like the wave function the lowest possible states as we know as we have as I have been repeatedly saying; it would not have any notes. So, the wave function would look something like that. Now, interestingly you see if you look at the wave function in this region how does it appear; the functional form is C 1 e to the power of minus kappa x that is the functional form in this region. So, in that region the wave function is non 0 notices it is non 0 it penetrates into that region. And therefore what is going to happen is that the function would decay in some such fashion; it would penetrate in to this region.

Now, this is against to classical mechanics actually. Because in classical mechanics if the particle has that much energy this line represents the energy of the particle; the potential energy of the particle if it entered in to this region would be so much. So, this is the region where the total energy of the particle is less than the potential energy right. So, here the total energy of the particle is shown by this line. Well, I think I should notify what I said; see this particle classically speaking what it will do is; it will hit this potential wall and will be reflected. So, it does not enter in to that region correct; but the quantum mechanically speaking if you look at the wave function the wave function actually exponentially decays into that.

So, therefore that it is possible for the particle to be found in that region also. But with a very small probability; this is essentially because of the wave nature you see a wave does not terminate abruptly it will only be terminates smoothly. And that is the region why the wave function enters into that region. Similarly, on the other side again the wave function would decay exponentially. So, this is the first possible state; the next state is this one but I am not going to draw it; why because I have not found it. Why because you see the next state has to be anti symmetric rigorously the lowest impossible state is symmetric the next 1 is anti symmetric. And the next one which will be somewhere here will be symmetric and how would it look like? It would look like this. Well, let me very quickly tell you what happens with the odd functions what will happen is quite simple. What will happen is quite simple.

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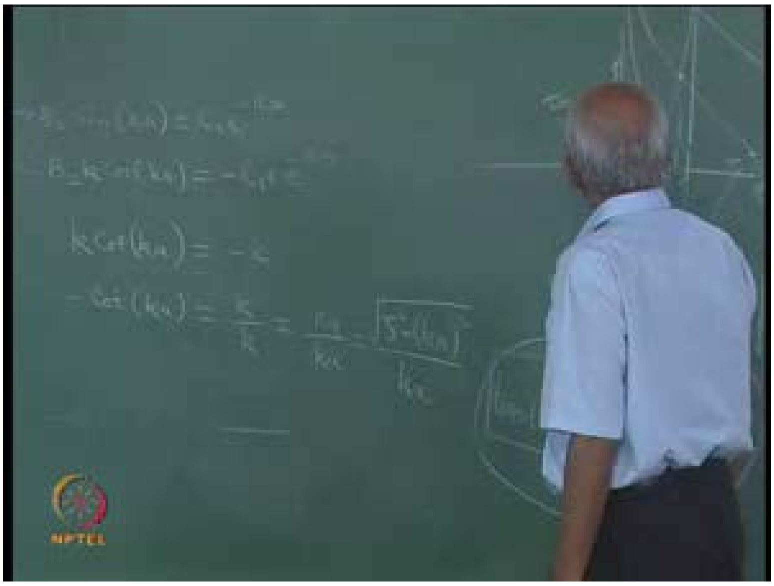

You would not have this B 1 cos k x in this region but instead odd or anti symmetric. You essentially means that if you replace the x with minus x the wave function actually change a sign. So, if that was the way the wave functions where then what will happen is that; right in the middle the function would have the form B 2 sin k x. The other cos k x tan cannot be there because your wave function is anti symmetric; if you replace x with minus x the function has to change sign.

So, then you will have to impose the boundary conditions. What are the boundary conditions at x is equals to a? But you will get a is B 2 sin k a must be equal to C 1 e to the power of minus kappa a right; this is what you are going to get. And the derivative this is actually the wave the continuity of the wave function. The wave function at this point at this boundary, wave function at the point x is equal to a which is the boundary between regions 2 and 3 has to be continuous. Then the derivative of the function also has to be continuous I can easily write it; I will just write it because I would like to finish this part quickly.

If you evaluated the derivative at the boundary using the 2 functions; the function on the right hand side as well as the function on the left hand side. And then put them to be equal this is what you are going to get. And just as before what you will do is you will take this divided by that equation. So, that you will get B 2 and C 1will disappear; answer will be cot k a into k must be equal to minus kappa. That is the result that you will get which I can rearrange as minus cot k a is equal to kappa by k and you remember the manipulations; that we did earlier kappa by k a can be written as kappa a by k a which may be written as zeta square minus k square to the square root divided by k a. So, earlier our transdential equation was this one; all that has happened is instead of having tan k a; the left hand side has been replaced with minus cot k a that is all other than that there is no difference like this function has changed. So, let us I may gave graphical analysis again in a very quick fashion.

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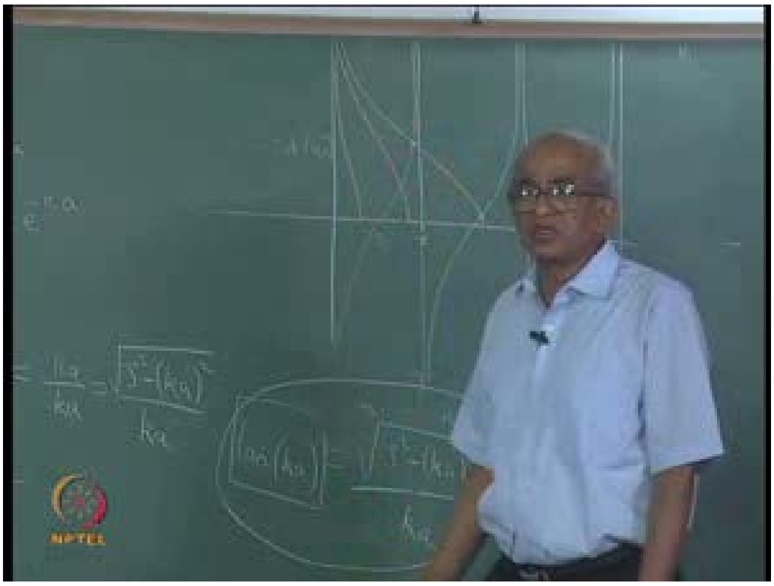

What is this actually this is just that the right hand side. The right hand side is what I have plotted now. And then I the other thing that I should plot is minus cot k a. Well, let me just make a plot of minus k a it looks like this; it becomes 0 at pi by 2 and then goes on to plus infinity at pi. So, that is how it is. So, the way I have dawn this curves how many bound states of anti symmetric nature; 2 of them because you have 2 intersections 1 is here and the other is there. And of course it just as before and if I increase the number of sorry if I increase the width or the depth the number of bound states will increase.

But suppose I decrease I make the potential weaker and weaker and weaker what will happen? If I made it weaker see I can make it weaker and have it in this form that is the possibility. But it is also possible for me to make it fairly weak so that the curve will terminate here. So, that there is no intersection. So, if you made the potential weaker you will find that this is not necessary that there should be a bound state of anti symmetric nature; there will be 1 bound state. But that will have the which nature it will not be anti symmetric but it will be symmetric right. Therefore, what happens is that the lowest possible state will always be there; the lowest possible state or the symmetric state will always be there. But it is not necessary that there should be an anti symmetric state ok.

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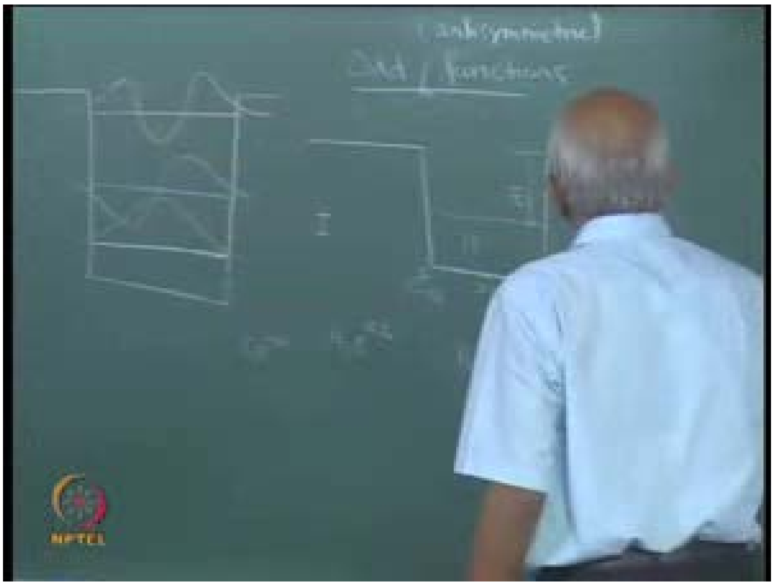

And, having seen let us let me draw this anti symmetric function in the same picture. How would it look like where it is going to be obviously 0 at this point and then it will do that? So, that is the way the wave function will be. Now, we see after having seen the bound states is strictly speaking what I should do is; I should consider the situation where the total energy of the particle is greater than 0 right.

So that means I have a particle which is having that much energy and it is going to move towards this potential that is there. Now, I shall not analyze this in detail because I am going to analyze a related program which essentially tunneling in detail. Therefore, I will not analyze it but it is fairly simple; this particular problem is fairly simple. What happens is that you see here I have a particle; what happens is that the particle is coming from infinity let us say with some energy; it needs the presence of a potential well right.

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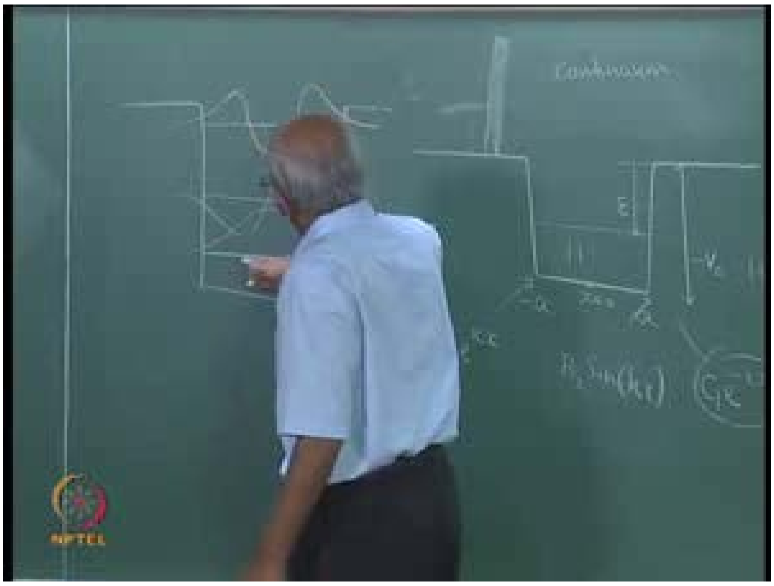

But then what will happen the particle can simply go. It can go it is also possible actually strictly speaking even a potential well can cause the particle to be reflected; this is peculiarly quantum mechanics. We have a even a potential well the particle need not go to the other side these potential well can reflect the particle. We will see these similar things happening when we think of a potential barrier.

Therefore, I am going to describe these but in order to be completed I should tell you what happens. But a particle that is coming from infinity the energy is my choice I can choose whatever energy that I want. And therefore actually I can choose if you have any energy between 0 and infinity right. Therefore, you will find that all energies above 0 are allowed there is no quantization or anything or here I can have the particle can coming with any energy that I choose. Therefore, I will say the allowed energy levels if you like they form a continuum; which essentially means that the allowed energy levels can be anything. So, if you have plot made a plot of the allowed energy levels for the system how would it look like?

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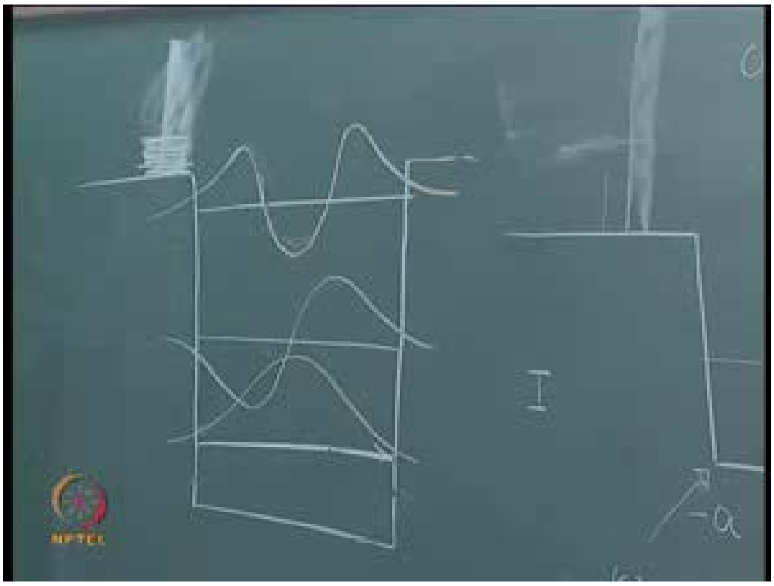

Well, you have 1 2 3; 3 discrete states which are bound. And then starting from 0 when you can say instead of drawing it like this you can say you have energy levels which are extremely close like that. And therefore I say all energies are possible and in the continuum there is no quantization nothing. So, that is how the Eigen values or the allowed energy values of the system are fine.

Thank you for listening.