Introductory Quantum Chemistry

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Lecture - 15
Tunnelling - Part 1

Today, we are going to discuss the concept of quantum tunnelling. Now, imagine that I have a football in my hand. And I as all of you know if I threw the football on the wall here on this side. Now, obviously the ball will get reflected; the ball is not able to pass through the wall.

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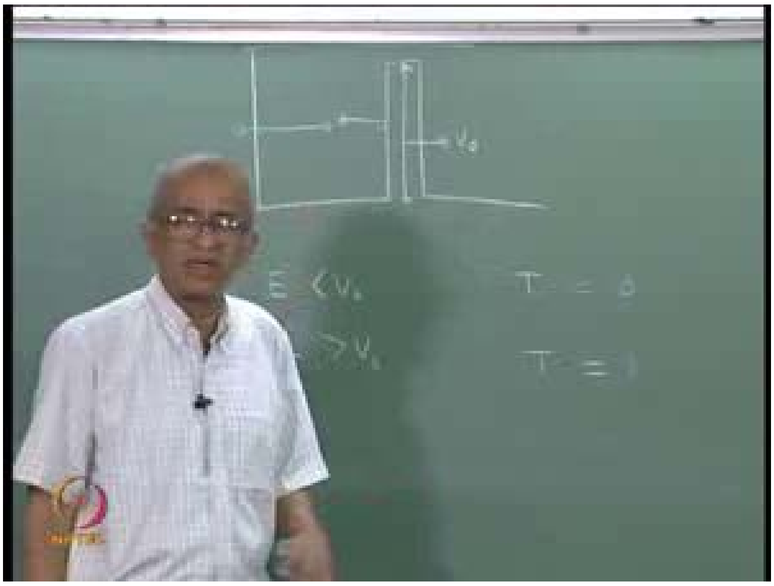

So, let me think of this for a few minutes imagine that I have a particle which obeys the principles of classical mechanics; and imagine that the particle is moving in this direction. And if it encounters an obstacle on the way may be a wall. So, what is meant by a wall; well we can say that a wall is a region where the potential energy felt by the particle in that region is large ok. So, if the particle encounters such a barrier naturally the particle is not able to pass through the barrier; it will get reflected. So, this is what happens in classical mechanics. On the other hand if it had enough energy to go over the barrier that makes oppose the particle at that much energy which is just enough to go over the wall; then it will definitely go to the other side. So, classical mechanically if the energy of the particle which I may say is E; and if you say that the height of the barrier is v 0. Now, if E is less than v 0 the particle is always reflected. And if the energy of the particle is greater than v 0 the particle is always transmitted; it just goes from the from the left hand side of the barrier to the right hand side.

And, therefore if you define something like a transmission factor or transmission probability; if you want if E is less than v 0; t will always be equal to 0 it will not pass through classically. While if E is greater than v 0; t is equal to 1; so this is the classical result. But if you thought of a particle obeying quantum mechanics then things are actually quite different.

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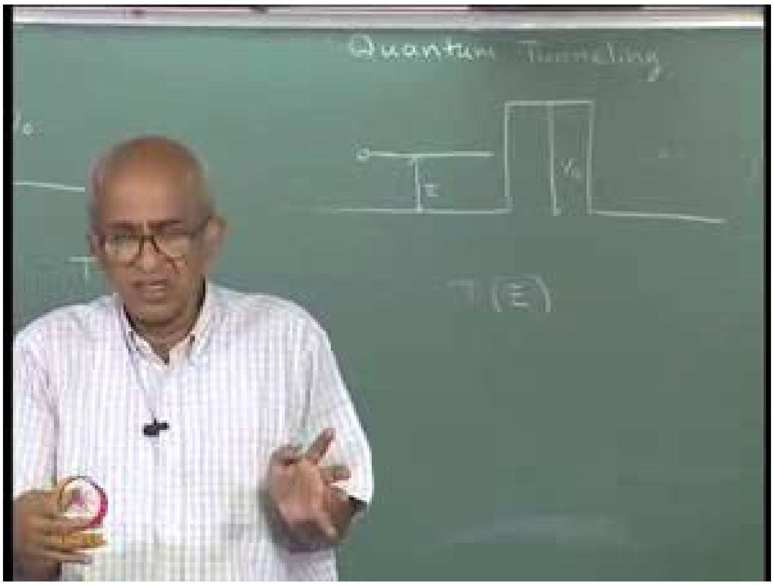

So, for example imagine this is a barrier and I have a quantum mechanical particle the barrier is something like this. And I have a particle which obeys quantum mechanics incident from this side. And it is incident let me say with that much energy which we call E and imagine that this is actually less than the height of the barrier which we denote by v 0. As I told you already if the particle obeys classical mechanics it will not go to the other side. But it so happens that in I mean it is interesting that in quantum mechanics there is a probability that the particle will go to the other side. And there is also a probability that the particle will get reflected.

So, imagine I have 100 particles incident on the barrier; then what might happens is that may be 10 of them will go to wall to the other side; while the remaining 90 will be reflected. Therefore, we want use our knowledge of quantum mechanics to calculate the value of t for a quantum mechanical particle. And in fact the value of t will definitely will depend up on how much energy the particle has. Therefore, I want to calculate the transmission coefficient as a function of energy. And because you see I if I because the particle can pass through the other side even in the case where it does not have enough energy to overcome the barrier; 1 says that the particle have actually tunnelled through the barrier. And this process is referred to as quantum mechanical tunnelling. Now, when you think of it quantum mechanically the this is not very surprising that it happens.

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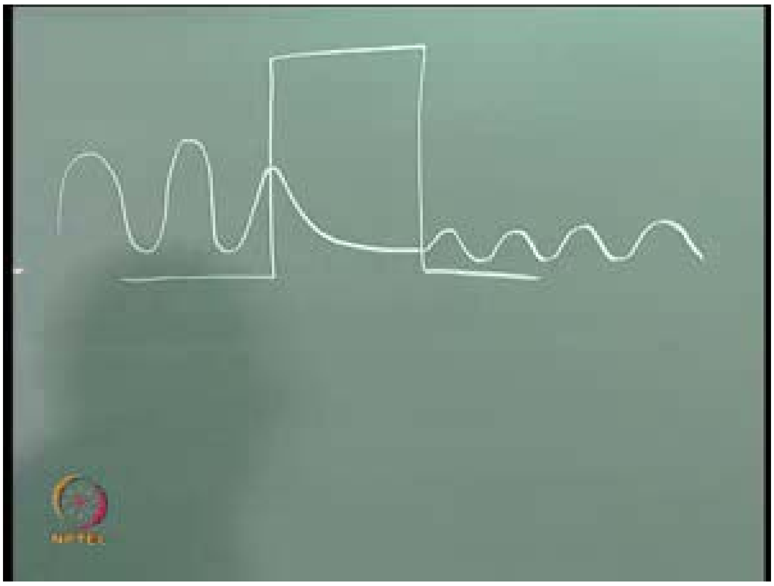

Why is it so well let me draw 1 more picture showing why it happens this is my barrier; remember you see the incident particle it has a wave nature. Therefore, you will have a wave incident from this side. So, I can represent it something like that; and then when it encounters the barrier actually the wave cannot terminate suddenly. So, the wave actually would continue into the barrier; and in fact as we will see the wave decease inside the barrier. And then you see the decay will happen inside the barrier; and eventually on the other side it is possible for it to come out. And of course a part of the wave will be reflected; and the part of the wave will go to the other side ok.

This is the reason why the particle is actually able to go from 1 side to the other side. Essentially because the wave nature of the particle you see the wave actually is able to pass through. So, I want to now treat this problem in a regress mathematical fashion and let us do that. I would rub off all these figures which I do not need except this the 1 in the middle.

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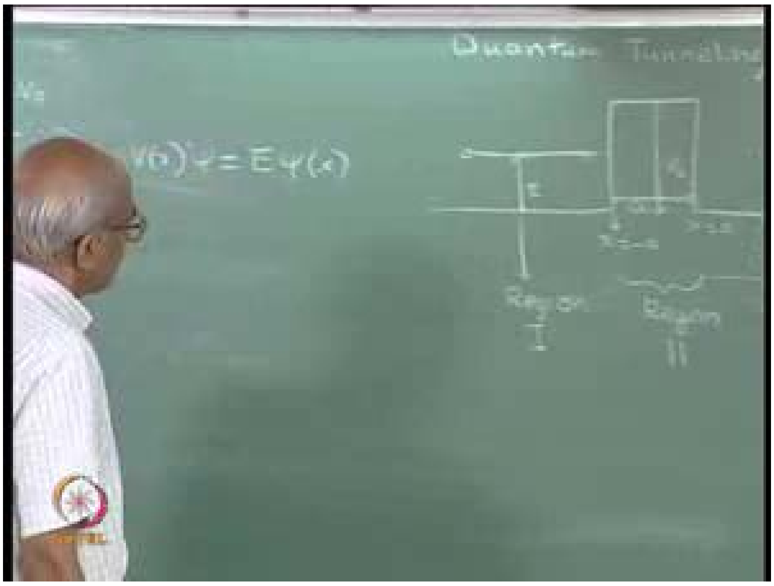

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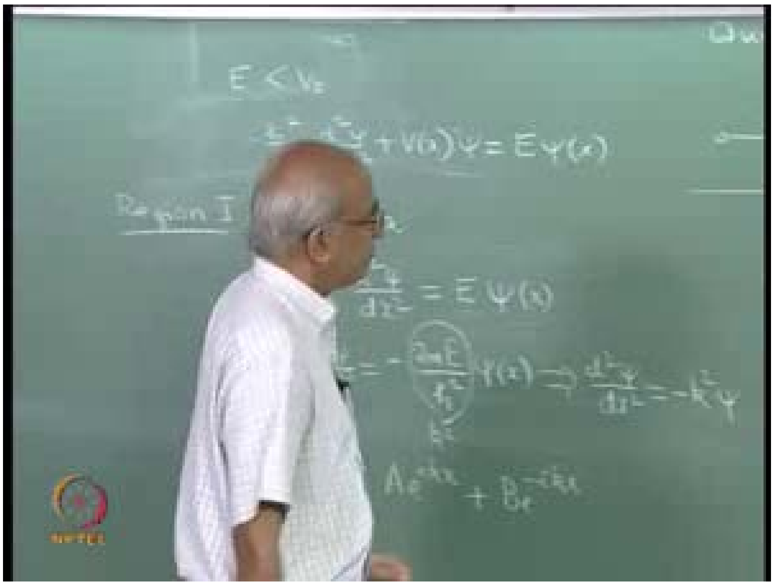

Specifically, we are most interested in the situation where the energy of the particle is less than the height of the barrier. And I shall also say that you see the direction in which the particle is moving is the x direction. And I shall say that the barrier has this nice rectangular shape. And here this point this end of the barrier I shall say is my origin x is equal to 0. And the barrier itself has a width which I shall denote by a; as a result of which at this point x is actually equal to minus a.

And, we want to solve the Schrodinger equation the time independent Schrodinger equation for this problem. So, what is the time independent Schrodinger equation? The time independent Schrodinger equation is that minus h cross square by 2 m d square psi by d x square plus v of x into psi is equal to E psi; this is what the time independent Schrodinger equation says. What we will do now is to solve this equation in all these regions. So, I will have therefore, let us say region 1; that is to the left of the barrier. Then, I have this region which I shall refer to as region 2 that is the region where the barrier x is; and then you have this region which I shall refer to region 3; and that is the region to the right of the barrier.

So, let us first think of region 1. Region 1 is the region which is to the left of the barrier; that means actually x is less than minus a by definition. And in that region what will you say is the potential energy of the particle the potential energy is taken to be 0; and it is flat the potential is 0 everywhere. Therefore, this Schrodinger equation will become minus h cross square divided by 2 m d square psi by d x square; potential energy is 0. Therefore, this is equal to e psi we have already encountered this kind of equation. So, we can simply rearrange this. We are very familiar with this kind of thing you can write this equation as d square psi by d x square is equal to minus 2 m e divided by h cross square into psi (x). And it is quiet convenient if I introduced a constant which I shall define as k square. So, what is my definition of k square I am going to keep it somewhere?

So, let me write it here k square is defined to be equal to 2 m e divided by h cross square. And therefore, this differential equation what happens to it this differential equation becomes d square psi by d x square is equal to minus k square psi. And the solution of this is immediate what the solution is; it says that psi may be written as some constant into e to the power of i into k into x; that is a solution. There is also another possible solution which is b e to the power of minus i k x. And in fact you can easily verify that even if you took a linear combination of this 2; it still satisfies the same equation. And therefore the most general solution to this equation is having this particular form. Now, if you think of region 3.

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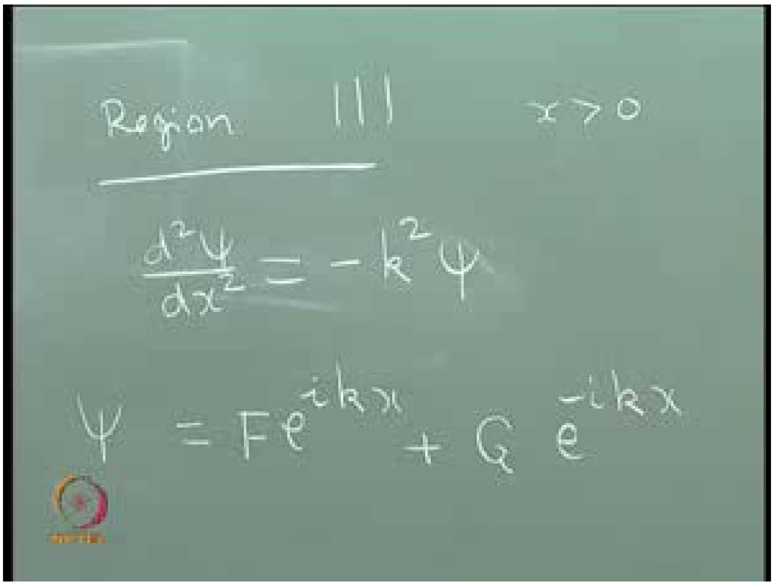

In region 3 again while which is region 3; region 3 is actually the region where x is greater than 0. And in that region also the potential energy of the particle is 0. Therefore, the equations are just the same there is all there is no difference. In fact the differential equation that is to be satisfied is precisely this this differential equations.

So that therefore let me just copy that differential equation. The differential equation would be minus k square psi. And what is the solution the solution is again of the form e to the power of i k x or e to the power of minus i k x or in fact a general linear combination of this 2 which I may write as i equal to may be some F in the e to the power of i k x plus some G into e to the power of minus i k x. So, this is the general solution in that region. Now, let us think of region 2.

Region 2 is this region; in that region what happens to the differential equation? While this is your differential equation in that region there is the barrier. And in that region you know that V (x) actually is equal to v 0 which is a constant; which is the height of this barrier. So, let me write that differential equation it in the region 2 it becomes d square psi by d x square minus h cross square divided by 2 m plus v 0 psi is equal to e psi; this is what happens in that region. And you can do it rewrite this equation in a different form; you can take this v 0 to the other side and to multiply throughout by minus 2 m by h cross square.

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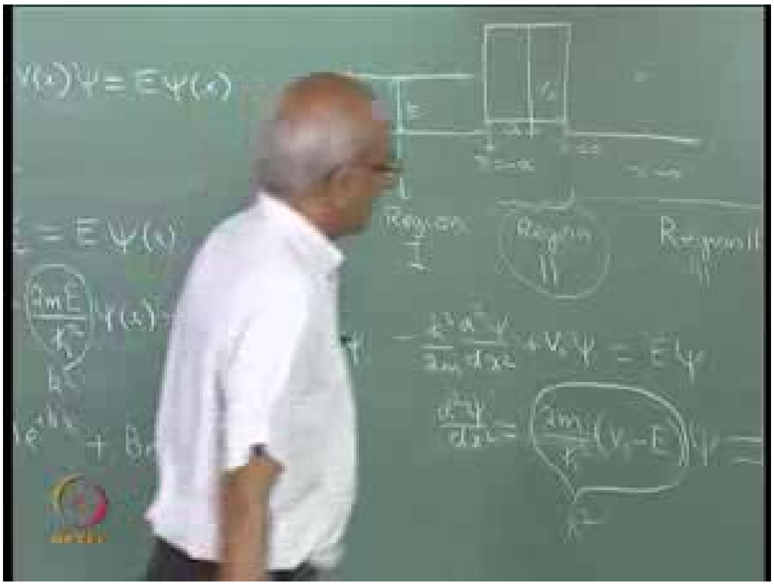

So that you will have only d square psi by d x square on the left hand side, and you will find that that may be written as 2 m divided by h cross square into v 0 minus e into psi; that is just rewriting this differential equation. Why did I write it in this form while you see remember we are thinking of the situation where E where energy of the particle is less than v 0. So, therefore v 0 minus E is a positive number. And therefore this whole thing is actually a constant positive number; and naturally what I will do is I will call that kappa square. And therefore this differential equation becomes d square psi by d x square is equal to kappa square psi. There what is the definition of kappa square?

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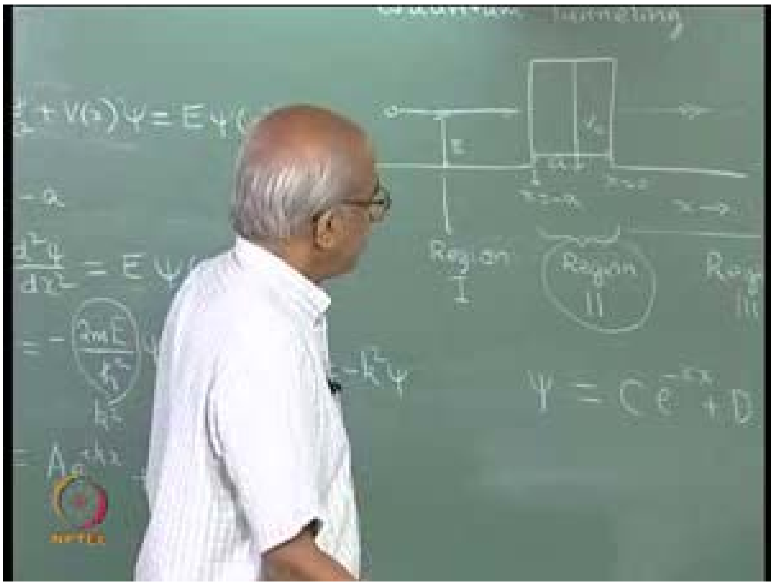

Kappa square is defined by 2 m by h cross square into v 0 minus E; and this again it is symbol differential equation you can easily find the solution. So, of these equations we will write down the most general solution; that will because I want to write it in the same region. Let me remove this equations and just write the value of psi or the expression for psi will you see if you if you have such a differential equation. The solution is immediate you can easily verify that e to the power of minus kappa x is the solution; you can also see that e to the power of plus kappa x is another solution.

And, in fact any combination of the form C e to the power of minus kappa x plus d e to the power of plus kappa x with c and be any 2 constants is a solution of this particular differential equation. And therefore we have the solution now. We have solved the equation in the 3 different regions but then you see we have so many constants. We have the constant A, we have B, then C, D, F and G all these constants have to be determined. And they have to be determined using either physical indusion or using boundary conditions.

So, what do I mean by using physical indusion? Well, we know that the particle is incident from the left hand side. So, the there are particle incident let me say there is a beam of particles; let me say which are incident from the left hand side. Now, what will happen may be some of them will reflected, some of them will pass through the barrier and come out on the other side. But the particles which are coming out on the other side what do you expect? You expect that all of them will be moving in the positive x direction none of them will be moving in the opposite direction. And therefore you see if you look at this wave function this part actually represents particles which are moving in the positive x direction ok.

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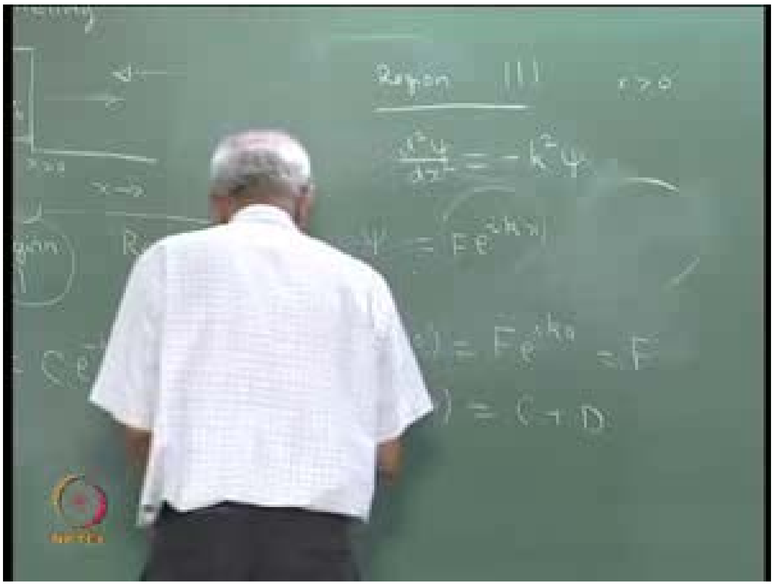

How do I know that while if you took the momentum opera term minus i h cross dou by dou x and allowed it to operate upon that part .You will find that that part allow is an again function of these operator and the again the value that you will get is k h cross. So, this actually this part actually represents particles which are moving in the positive direction with a momentum which is which is k h cross. And therefore this part represents particles which are moving in the positive x direction.

Similar, argument will tell you that this part actually represents particles which are moving in the negative x direction. So that part will represent particles which are moving in the negative x direction. And because of the way I am doing my experiment what is the way in which I am doing my experiment my particles are incident on the barrier from this side. And therefore on the other side I do not expect any particle to be moving in the negative x direction. And that immediately tells me that for this physical situation the value of G must be equal to 0; because I do not expect to have particles moving in the negative x direction. And therefore in this region I realized that the wave function should have only the form F e to the power of i k x and this term is not there. So, is the function is just F e to the power of i k x in this region in the region 3.

Now, coming to the boundary between the 2 regions see I know that the wave function is obeying a second order ordinary differential equation which is of this form the potential has discontinuities. But there are no delta functions is sitting anywhere in here inside the potential. And this actually means that the wave function and its derivative have to be a continuous function of x. What does that mean it means that if I evaluated the function the wave function at this point right; at the x equal to 0 the wave function has to be a continuous function? Therefore, if I evaluated the wave function at this point the x equal to 0 what is special about x is equal to 0 it is the boundary between the regions 2 and 3.

So, if I evaluate the wave function at x is equal to 0 using this functional form which is appropriate for region 3 what would be the answer? The answer will be F e to the power of i k 0 and i e to the power i k 0 obviously is e to the power of 0 which is 1. And therefore you will get the answer F. And exactly at the same point right at x is equal to 0; if I evaluated the wave function using the functional form that is appropriate for region 2. That means, in this function I am going to put x is equal to 0 what will be the answer that I get? I will get the answer C plus D of course I am going to put x is equal to 0 here I am going to put x is equal to 0 there so naturally you will get the answer C plus D. And in order that the wave function is continuous these 2 have to be equal. And therefore using the fact that the wave function is continuous I get this equation.

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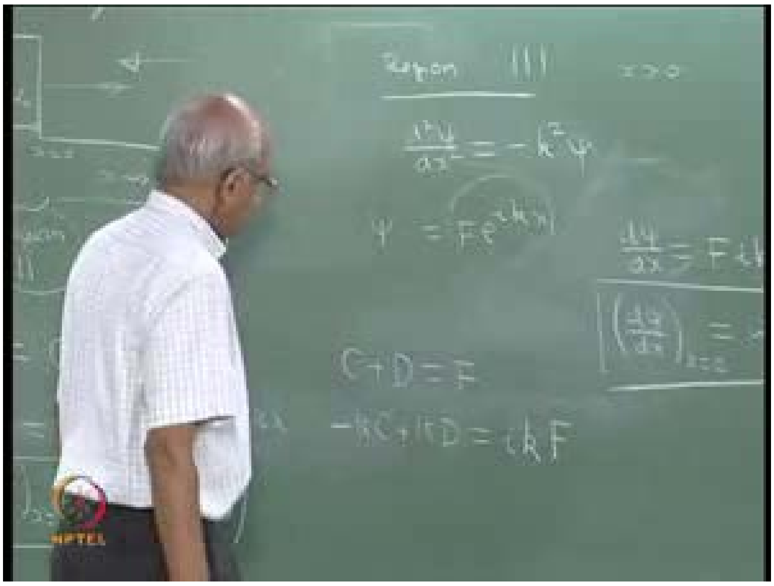

What is the equation the equation is C plus D is equal to F; not only should the wave function it is derivative also be a continuous function. So, what do I do? I take the derivative of this function what is the derivative of this function it is d psi by d x which is equal to F into i k into e to the power of i k x; in particular I evaluate the derivative at x is equal to 0. So, I shall get d psi by d x evaluated at x is equal to 0 and what is the answer? The answer I find is i k times F because if I put a x is equal to 0 near that transfers to be unity.

Similarly, if I evaluated d psi by d x using this function; well let me differentiate this function what is the answer that I will get. The answer that I will get is minus kappa C e to the power of minus kappa x plus kappa D e to the power of kappa x; this is the derivative of that function. But then specifically what I want is I want to evaluate d psi by d x at x is equal to 0. And what is the answer if you put x is equal to 0 this will turn out to be unity this whole thing; that also will turn out to be unity. And therefore you get the result as minus kappa into C plus kappa into D. So, we are have evaluated the derivative of the wave function at the same point using a functional form that is appropriate for region 2. And using a functional form for that is appropriate for region 3 and if the function if the derivative is to be continuous.

Then, what should happen this derivative should be equal to that derivative. And therefore I get another equation. What is the other equation minus kappa into C plus D is equal to sorry minus kappa plus kappa into D should be equal to F into sorry it should be written as i k into F. So, using the condition that the wave function and its derivative are both continuous; I have obtained 2 equations. So, let me rub off these things which I do not need any more.

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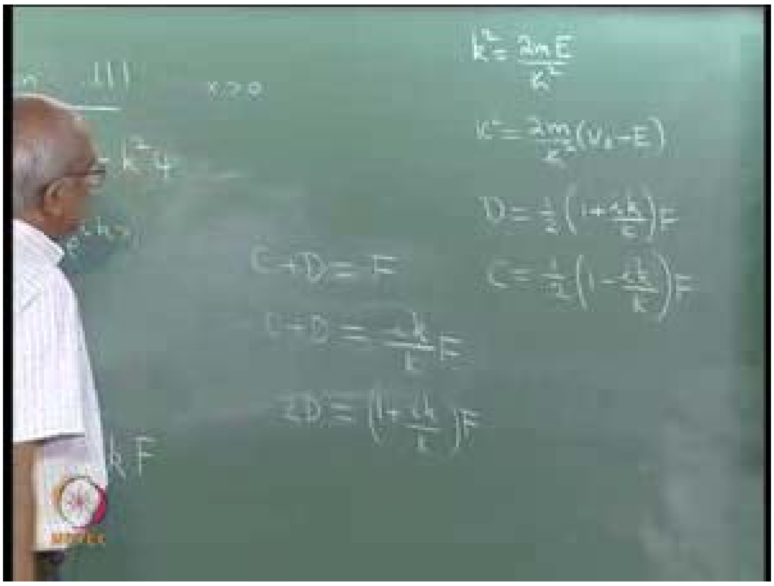

And, let me write this 2 equations once more I will write them here C plus D is equal to F. And this equation I shall divide throughout by kappa. And hence I shall get minus C plus D is equal to i k divided by kappa into F; see what why are we doing this that is the reason we are doing this is simple.

We want to get we want to determine all this constants C, D and so on. Therefore, if I have these 2 equations immediately I can get an expression for C in terms of F; I can also get an expression for D in terms of F. So, what I will do is I will add this 2 equations and if you added this 2 equations I shall get 2 d is equal to 1 plus i k divided by kappa times F. And therefore I can say that D is equal to 1 by 2 into 1 plus i k divided by kappa into F. Similarly, if you subtracted this equation from that equation you will get an expression for 2 C. And you can solve that for C what will be the answer C you will find is 1 by 2 into 1 minus i k divided by kappa into F.

So, having obtained these I will remove the intermediate steps I do not need this steps anymore. And now what I am going to do is I am going to do is similar thing at the other boundary because we have 2 boundaries. At the other boundary what will you do we will you will say; that the wave function evaluated at this point using the functional form. That is appropriate for region 1 should be equal to the wave function evaluated at this point using with the wave function that is appropriate for region 2, so for therefore those 2 have to be equal.

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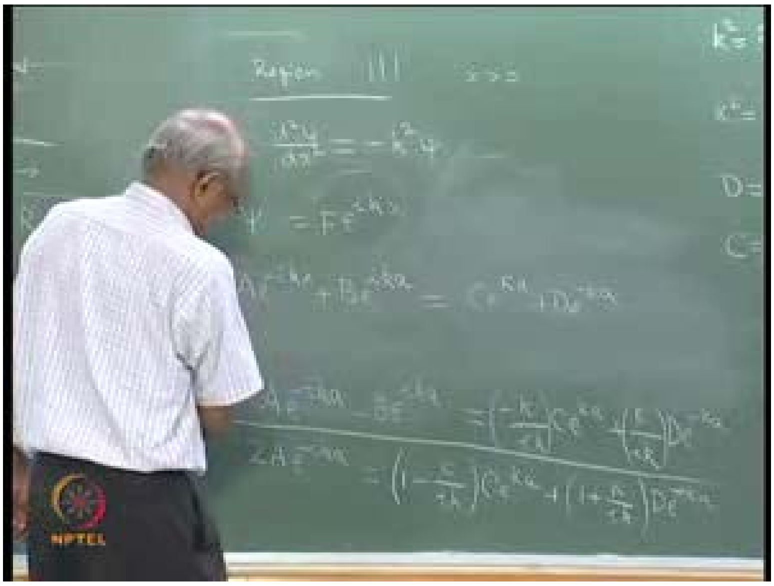

So, the wave function that is appropriate for region 1 is this and if you put x is equal to minus a; what you are going to get is A e to the power of minus i k a plus B e to the power of plus i k a. And it must be equal to this function in which you will put x is equal to minus a. So, let me write the result I have A e to the power of minus i k a plus B e to the power of i k a is equal to this function in which I will substitute x is equal to minus a. So, naturally I shall get C e to the power of kappa a plus D e to the power minus kappa a. And the next step will be to evaluate the derivative of this function there you will put x is equal to minus a. And evaluate the derivative of this function and there again you will put x is equal to minus a; and then say that this 2 have to be equal. So, let take the derivative of this function. The derivative of this function will be equal to i k into A e to the power of i k x minus i k B e to the power of minus i k x.

So that is the derivative and in the derivative I the derivative I am going to actually evaluate at x is equal to minus a. So, if I did that the answer will be i k A e to the power of minus i k a minus i k B e to the power i k a. This is the derivative at x is equal to minus a evaluated to using this functional form. And now I evaluate the derivative of the function at this point again using the other functional form; this is the other functional form that is appropriate for region 2. And in that functional form you see we have already carried out the differentiation the answer is written here. Therefore, all that I need to do is here I shall have to put x is equal to minus a. So, what with answer that I shall get the answer will be minus kappa C e to the power of kappa a plus kappa D e to the power of minus kappa a. And these 2 derivatives have to be equal because they are evaluated at the same point. Therefore, I have now 2 equations and I can actually simplify the second equation if I divided throughout by i k let me do that.

So, after the division this is the equation that results. Now, I have 3 equations but I do not need the equation in the middle. And therefore I shall just be concerned with this 2 equations and it is obvious that if you added this 2 equations. If you added this 2 equations this B; this term that contains B will exactly cancelled with that term containing B. And so let me write the result of that addition. Well, maybe I shall do it here itself if you just added this 2 on the left hand side you are going to get 2 A e to the power of minus i k a. And what will be the result on the right hand side the answer is going to be where this 2 terms I can add what will be the result? The result let me just right down you can easily verify that this is true 1 minus kappa divided by i k into the C e to the power of kappa a; that is obtained by this addition of this 2 plus 1 plus kappa divided by i k into D e to the power of kappa to the power of minus kappa a that is the result.

And, therefore I am having obtained this equation. Let me again get some space by rubbing off the equations that I do not need any more. So, you see the thing that I have an expression for A in terms of C and D; but notice that I have already obtained a expression for C and D earlier they have been obtained in terms of F. So, if I use this 2 equations into this equation; what will I have on the left hand side I will have A; while on the right hand side I will have this object F. And you will find that there is a relation between A and F. And what is it that I want to evaluate the transmission coefficient or the tunnelling factor which is T.

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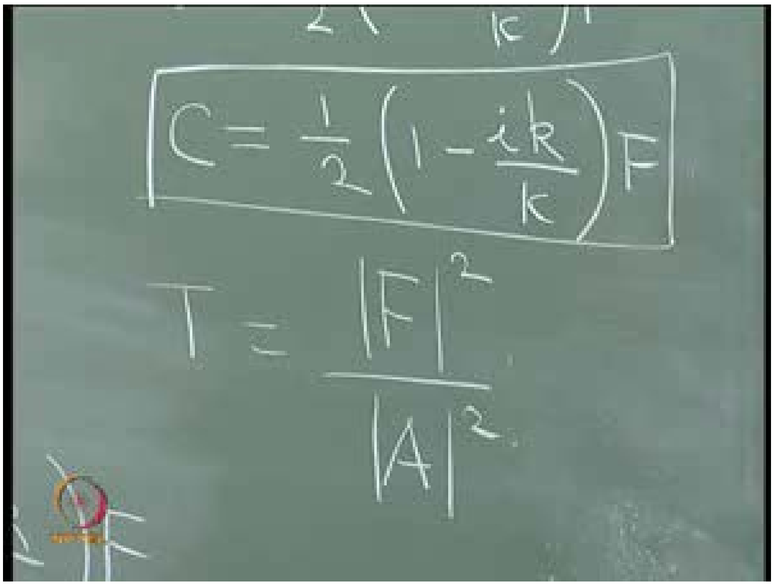

So, how will I determine t we will come to that but before I do that let me get an expression for A in terms of F. So, into here I will substitute for C as well as D that may do that as an equation here 2 A e to the power of minus i k a is equal to 1 minus kappa divided by i k into C e to the power of kappa a. So, I will retain this e to the power of kappa a but for C I will substitute from here. So, I will have a half into 1 minus i k divided by kappa into F plus I am now writing this term. I have 1 plus kappa divided by i k into e to the power of minus kappa a. And now I should substitute for D from here. So, I will get this divided by 2 into 1 plus i k divided by kappa into F. And I hope nothing has gone wrong and in that hope I am going to remove this.

Now, if you look at my look at your wave function in the 3 different regions. What are the wave functions in the 3 different regions? In region 1 you have A e to the power of i k x plus B e to the power of minus i k x; this A e to the power of i k x remember it will represent particles which are moving towards the barrier. And B e to the power of minus i k x will represent particles which are moving away from the barrier; that means particles which are reflected by the barrier. So, the number of particles which is incident on the barrier is actually determined by this A; in fact when as you know psi square is the object that is important in quantum mechanics. Therefore, the number of particles that is that are incident on the barrier from the left hand side is essentially determined by the magnitude of A square. It will be proportional to the number of particles which are incident from the left hand side will be proportional to the magnitude of a square.

Now, if you think at look at region 3 there the wave function is given by this expression. And this has only particles moving in the positive x direction. And the number of particles by the same kind of argument the number of particle which are moving in the positive x direction is determined by this coefficient A sorry coefficient F.

And, the number of particles which are actually moving in the positive direction will be essentially determined by the magnitude of F square. Therefore, if you wanted to calculate the transmission probability or the tunneling probability all that you need to do is you have to ask the question for each incident particle. What is the probability that the particle will come out on the other side? And from the arguments that I have given you it should be obvious that T should be equal to magnitude of F square divided by the magnitude of A square.

And, this is essentially the reason why I have derived this equation. And if you look at this equation you will find that I have a relationship which between A and F. And therefore I can actually evaluate F divided by A. So, let me go ahead and write an expression for F divided by A. So, what would be the expression?

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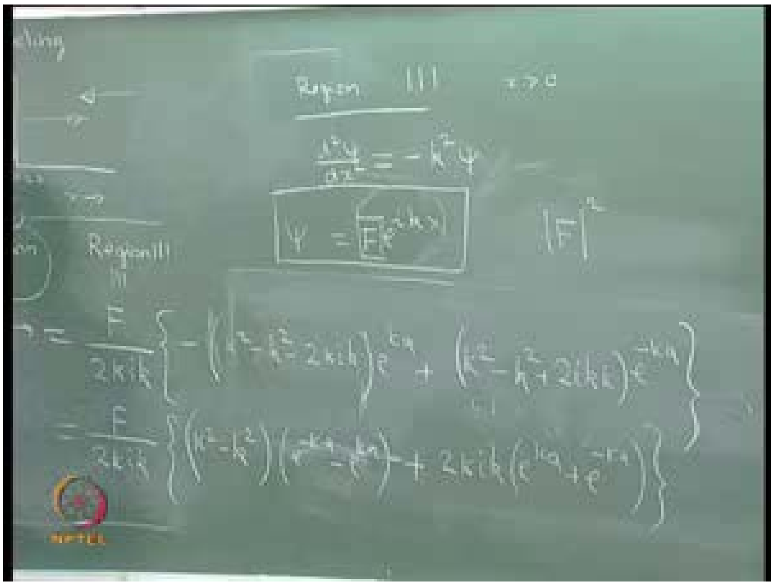

To get that expression what I will do is I will keep the left hand side as it is. And right hand side I shall make some simplifications F is common throughout but you notice that there is an i k here there is a kappa there. So, what I am going to do is I am going to write this as F divided by 2 kappa into i k into something. So, this i k I have taken out, the kappa also I have taken out. So, naturally what I am going to get is i k minus kappa into kappa minus i k e to the power of kappa a that will be 1 term.

And. the other term will be plus i k plus kappa into kappa plus i k e to the power of minus kappa a. And let me continue simplifying this I will get F divided by 2 kappa i k into while you can expand this or maybe I will write 1 more step. This may be written as minus of kappa minus i k into kappa minus i k from here I have just taken out a negative sign e to the power of kappa a plus what is the other thing; the other thing is actually kappa plus i k the whole square e to the power of minus kappa a. Well, let me again do 1 more simplification; well kappa minus i k into kappa i k that is actually kappa minus i k the whole square.

So, therefore you are going to get minus kappa minus i k the whole square e to the power of kappa a plus kappa plus i k the whole square into e to the power of minus kappa a. Well, now I will simply square take the square of both the terms and add them up. What I mean is I shall expand these 2 square and find the answer. So, from here I am going to continue here F divided by 2 kappa i k; when i take this square what is going to happen minus kappa square minus k square minus 2 kappa i k in e to the power of kappa a plus well maybe I should replace this with normal brackets. And if you took the square of the other term I shall get kappa square minus k square plus 2 i k kappa into e to the power of minus kappa a. Let me continue doing this. When you realize that there is kappa square minus k square here that is multiplied by e to the power kappa a there is also kappa square minus k square there.

So, I am going to combine this term with that term let me just write the answer. I am going to get kappa square minus k square into e to the power of minus kappa a minus e to the power of plus kappa a. And you have 2 kappa i k with a negative sign but there is negative sign outside. So that will actually become plus. So, you will get 2 kappa i k e to the power of kappa a. And you will find the similar term from the other side which will contain the e to the power of minus kappa a; and again let me come back here.

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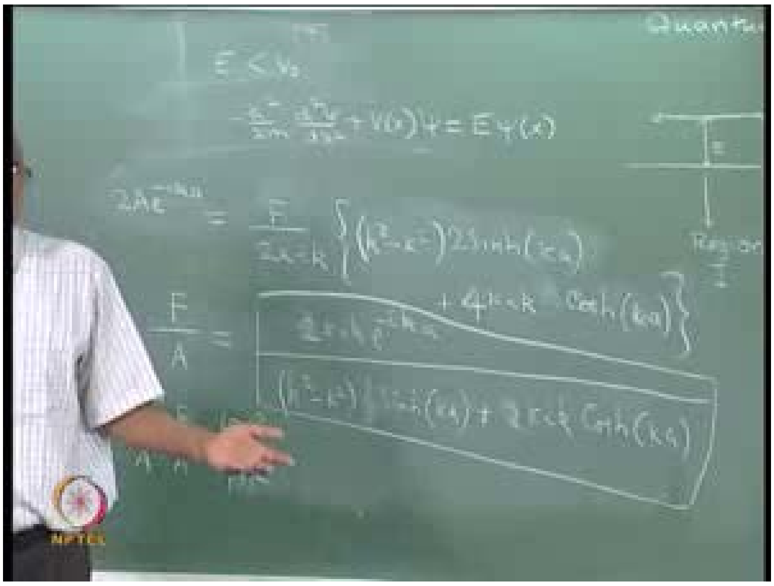

So, this I am going to write as F divided by 2 kappa i k into well I will do a minor modification here. The minor modification is you see I will write this term. So, I shall interchange this 2 terms. So, I shall get k square minus kappa square here that you can obtain by multiplying this by minus 1. So, the only thing is I will have to multiply this term also by minus 1. So, let me just do that. So, I shall get e to the power of this term will come first and the other term will come second.

So, this term can be written like that. Why do I do that the answer is that you see you know the that this object can be written in terms of hyperbolic sin function. So, this makes that I remind you of the 2 equalities e to the power of x minus e to the power of minus x is actually equal to 2 sin h x; and e to the power of x plus e to the power of minus x is equal to 2 cos h x. So, I am going to make use of this 2 equalities which actually means that that this object which is sitting here can be written as 2 sin h kappa a. And this object that is sitting there can be written as 2 cos h kappa a.

So that is what I will do and let me write the result. The result is k square minus kappa square into 2 sin h kappa a plus 2 kappa i k into 2 cos h kappa a right or this 2 and that 2 I can combine them; I can get the answer to the 4 times that. And then if you look at this equation you will also realize that there is A 1 this side, F 1 the other side. So, it is immediately obvious to me that I can write an expression for F divided by A which is what I will do. So, F divided by A is easily you can obtain it is actually going to be 4 kappa into i k into e to the power of minus i k a divided by k square minus kappa square into 2 sin h kappa a plus 4 kappa i k cos h kappa a. And you can see that the I can divide the numerator as well as the denominator by a factor of 2. If you divide it both by a factor of 2 the thing remains unchanged. So, this will become 2, this will become 1 and that will become a 2.

So, this is the expression that we will use in the next lecture to derive an expression for the transmission probability or transmission coefficient T which is equal to F square magnitude of F square divided by magnitude of A square. So, in order to do that what I should do is you see I have an expression for F. I will have to take the magnitude of F and divide sorry I would take the magnitude of F divided by the magnitude of A. Then, take its square or instead of taking magnitudes of F and A. What that I need to do is I multiply this object by complex conjugate of F by A. So, I take complex conjugate of F by A multiply it by F by A. And as you know that will be actually nothing but equal to magnitude of F square divided by magnitude of A square. Therefore, what I have to do is in the next lecture I shall have to take this expression multiply it by its own complex conjugate; and simplify and see what the result is...

Thank you.