Basic Quantum Mechanics

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Module No. # 09

The JWKB Approximation and Applications

Lecture No. # 3

The JWKB Approximation: Use of Connection Formulae to Calculate Tunneling Probability

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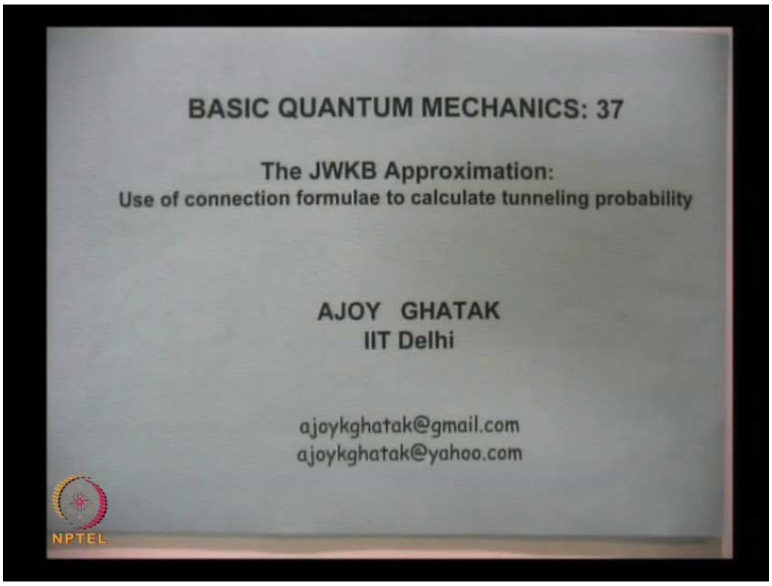

In our last lecture, we had used the JWKB solutions to solve two Eigen value problems. One was corresponding to the linear harmonic oscillator and the second was for the linear potential, linearly varying potential with the potential going to infinity at x equal to 0.

In both cases, we had only one turning point. So, in this lecture, we will eventually calculate tunneling probabilities, but before we do that, we will solve one more problem in which there will be more than two turning points. Actually, there will be four turning points. In fact, one can handle, for that sense, any number of turning points. One just has to hop from one turning point to the other. Look for the approach the other turning points and hop from one to the other. So, we will illustrate this through the calculation of the Eigen value problem for a double well potential.

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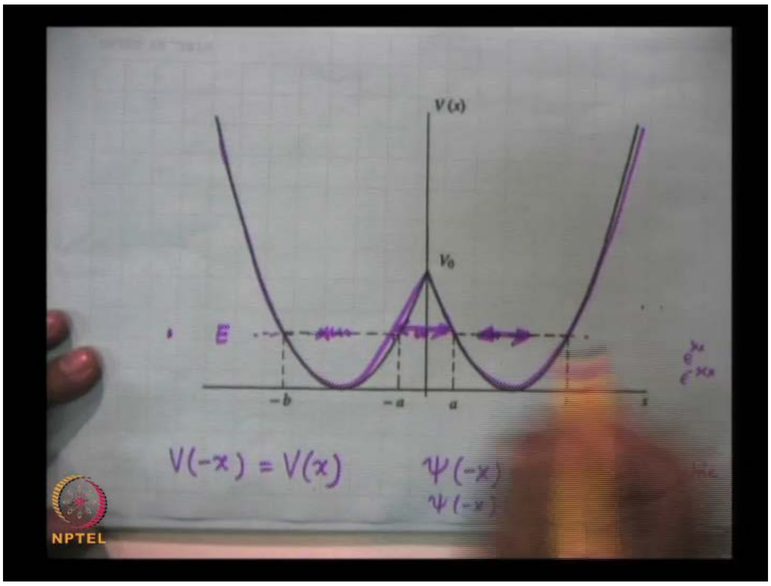

We will choose from the sake of simplicity, a symmetric double well potential, so the V of minus x is equal to V of x, and as we tried to explain, in our last lecture, at the end of our last lecture that the wave functions for such a case are either symmetric functions of x or anti-symmetric functions of x.

Our approach will be that if we have a anti symmetric function of x, we will start with a sine hyperbolic function. If I have a symmetric function of x, we will start with a Cos hyperbolic function. Let us start in the region from minus loop, if I assume this so the potential is given by the double hump, and in fact, in order to, in the double in the ammonia molecule problem one does have a double well like this.

So, I want to find out the energy eigen values for this double well problem. I assume any value of energy here. So, E is equal to V of x at 4 points. So, there are 4 turning points. Actually, technically speaking, we must start with an exponentially decaying solution over here, hop here, obtain the solution here, and then look towards the turning point here, hop from here to here, then from here to here, and then you write in terms of 2 functions; sine and cosine. The coefficient of the cosine term will be 0, because that will lead to an exponentially amplifying solution there. This is the general methodology of using the WKB approximation for solving any eigen value problem.

But this case is particularly simple, so we have either symmetric functions of x or anti symmetric. So, in the region, first we will discuss in this region, and then in this region, and then in this region. So, let me first start with this region.

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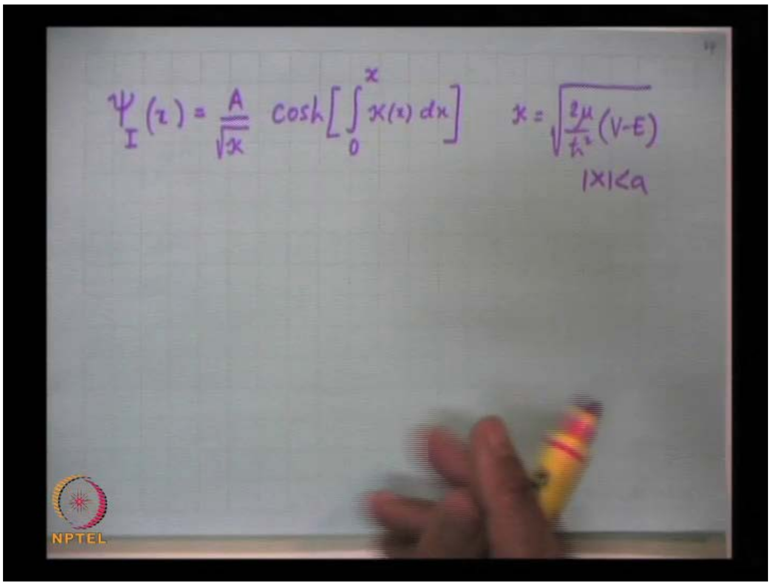

You have psi of x so this is the first region let us suppose first region psi of x is equal to A by root kappa cos hyperbolic or for anti-symmetric function, I can take sine hyperbolic 0 to x kappa of x d x, where kappa of x is equal to under root of 2 mu by h cross square, V minus E, because in this region mod x less than a, V is greater than energy, the assumed energy. Therefore, we must use kappa square of x.

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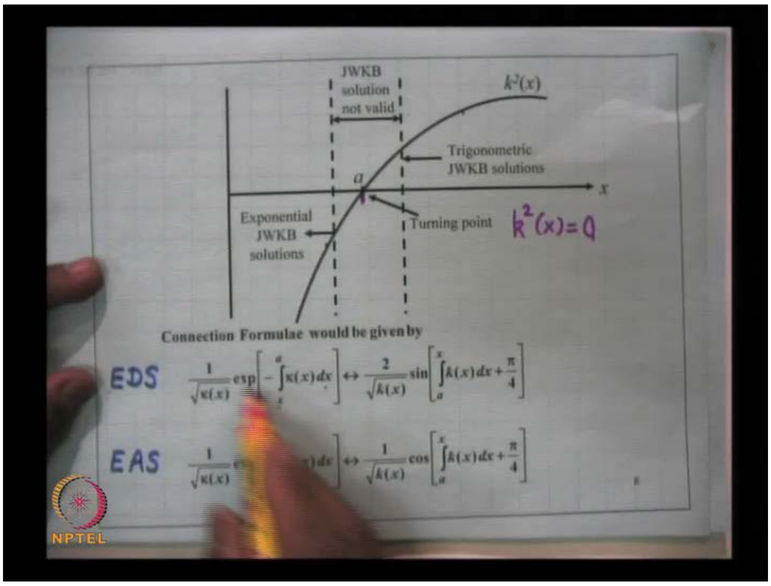

So, in order to use the turning the…, so we will have exponential solutions here and trigonometric solutions to the right. So, you must write it in the form of x 2 A kappa d x exponential minus and exponential plus.

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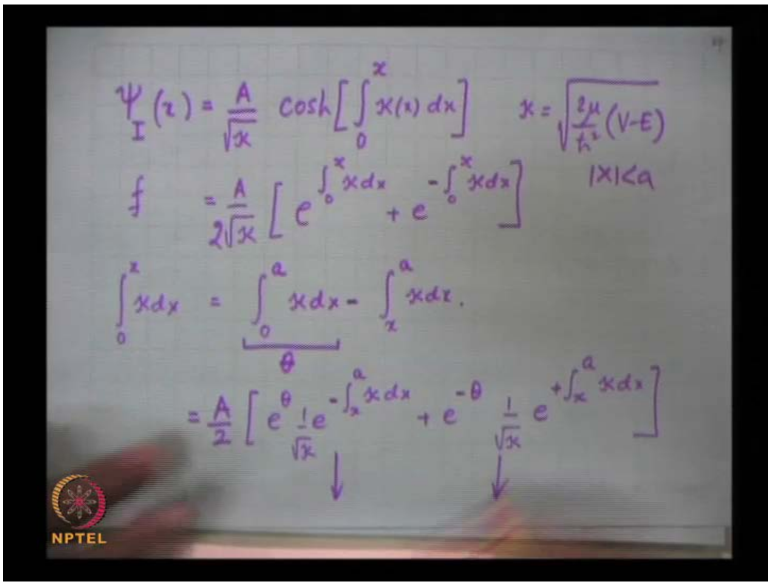

Therefore, first of all, we must write 0, so this is equal to… First, I must write it in terms of the exponentials 0 it by 2 e to the power of integral 0 to x, kappa d x, plus e to the power of minus 0 to x kappa d x, and then the trick is that you write 0 to x kappa d x is equal to 0 to a, kappa d x minus x to a kappa d x. So, we will write that e to the power of… So, let me write this as theta, this as theta, so the first term becomes A by 2 e to the power of theta, e to the power of minus, with 1 over root of k outside, x to a kappa d x plus e to the power of minus theta, 1 over under root of k, because this is the minus sign here. So, this will be minus here and plus here, e to the power of minus theta, e to the power of plus x to a kappa d x.

Now, we have solutions. They are written in terms of x to a kappa d x and x to a kappa d x. So, this will the exponentially decaying solution will go over to sine solution, exponentially amplifying solution will go over to a cosine solution. Then we will have this goes over to this goes over to, let me write it down.

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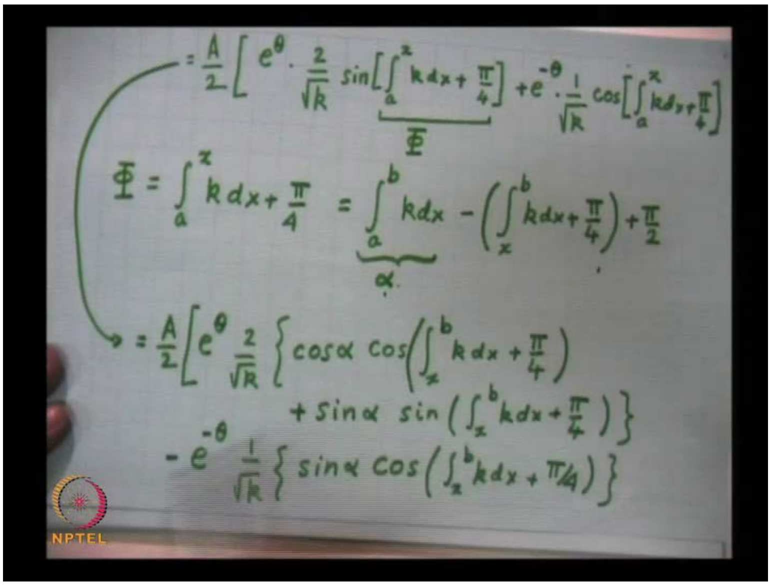

Is equal to A by 2, e to the power of theta, and this will be 2 by root k, that factor 2 you must remember. Sine of a to x, because in that region x is greater than a, k d x plus pi by 4. And this solution will go over to e to the power of minus theta. I thought I will do this example, so that you understand how to use the connection formulae; 1 by root k cos a to x k d x plus pi by 4.

So, you see, if you will have, one is the sine term and the other is this cos term. Now, we have here, so I have obtained the solution in this region. Now, I must write it as integral from x to b, so that I can use the connection formulae connection formulae to hop from here to there (Refer Slide Time: 09:37). Therefore, once again, if this is say phi, so I write phi as integral a to x, k d x plus pi by four.

So, I write it as integral, same trick a to b, k d x, and then minus integral x to b k d x, and I must add pi by 4, because my connection formula has this pi by 4, so it is minus pi by 4, so plus pi by 4, plus pi by 4, so plus pi by 2.

Let me write this down, as this quantity as alpha. So, this becomes sine of alpha plus pi by 2. So, this solution becomes equal to A by 2 e to the power of theta, 2 by root k, sine of alpha plus pi by 2 minus this (Refer Slide Time: 11:12).

And that becomes cos of alpha minus this, so this becomes cos alpha, cos of integral x to b k d x plus pi by 4, plus sine alpha, sine of x to b k d x plus pi by 4, and then we have other term. When there are more than two turning points they are like in general little complicated. Cos of pi by 2 plus the whole thing, so that is minus sine, this becomes minus e to the power of minus theta, 1 over root k. So, sine of alpha minus this thing, this will be sine alpha, cos of the same quantity x to b k d x plus pi by 4 and then this will be minus sine of a minus b, minus cos alpha, sine this thing. I hope all of you understand this.

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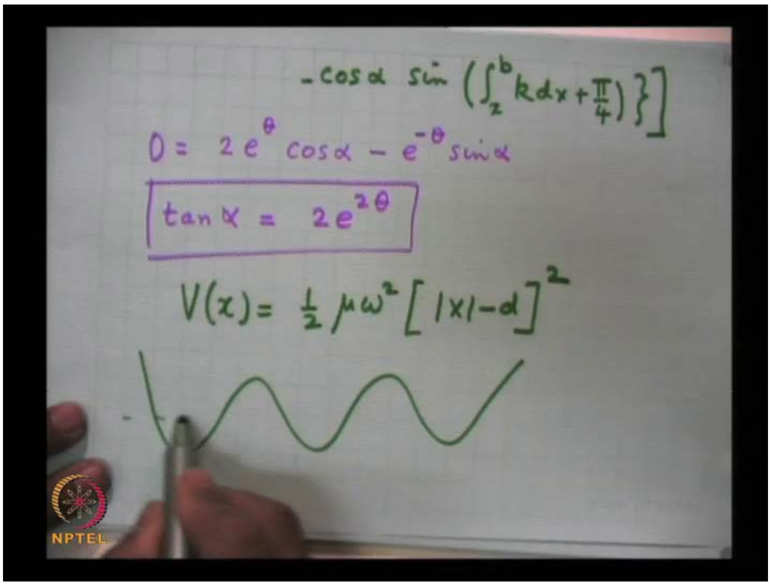

Minus cos alpha, sine of x to b k d x plus pi by 4; I have oscillator solutions here (Refer Slide Time: 13:25) and now I will go over to exponential solutions here. Therefore, I must use this that sine function will go over to an exponentially decaying solution and the cos of x to a will go over to an exponentially amplifying solution.

This term, you see, this term (Refer Slide Time: 13:49) and this term will go over to an exponentially amplifying solution. Therefore, the coefficient of these two terms must add up to 0. Therefore, you see this times this times cos alpha, minus this times this times sine alpha. This is the coefficient of the cosine term and that must be 0.

So, we must have 0 is equal to 2 e to the power of theta cos alpha, minus e to the power of minus theta sine alpha. You will have the final result as say tangent alpha, which is equal to 2 e to the power of 2 theta. This is the eigen value equation that will determine the symmetric eigen values of the problem, and I leave this an exercise for you that if I have the anti-symmetric solution then all that I have to do is I will assume here sine hyperbolic.

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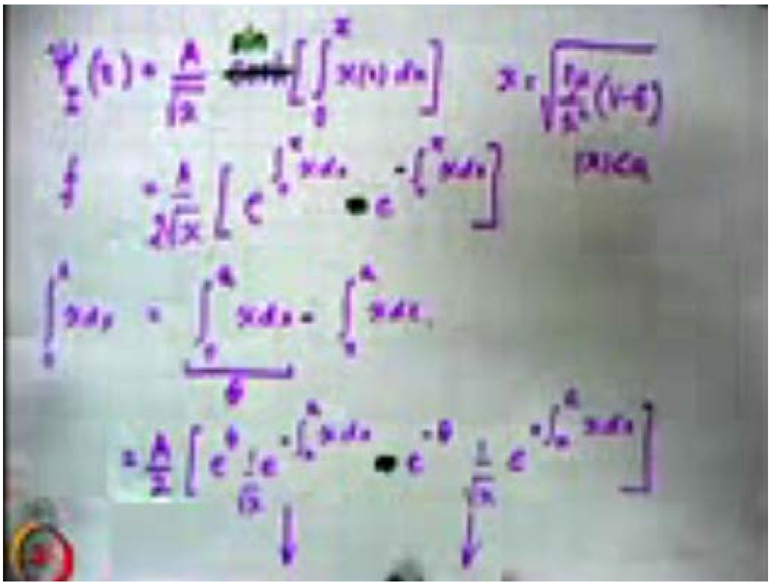

So, as you know the sine hyperbolic term, we will have a minus sign here, and therefore, it will have a minus sign there and so on. The analysis will be almost similar except that there is a minus sign here.

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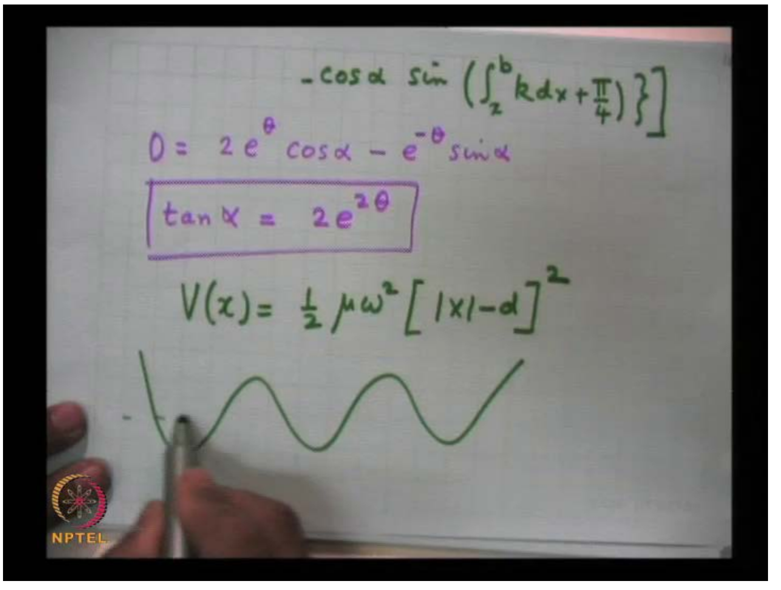

So, you will get similar result, but we have been able to obtain the results of a double well potential and in fact one of the potential that is of great importance, in many areas, is a double well potential, given by half mu omega square, x minus d whole square, and the results that you obtain by using WKB, and the exact results, in terms of confluent hyper geometric functions, they agree quite well with the result, with the exact results.

So, in general, if you have a potential looking like this, let us suppose, and if you assume this as the energy level, in the corresponding k square of x, will look like this (Refer Slide Time: 16:51), so because that will be… These are the turning points, so we have to start with an exponentially decaying solution here, hop over here, hop over here, hop over here, hop over here, hop over here, and so on.

So, this is the methodology, for example, if this was not symmetric (Refer Slide Time: 17:18) then there will be exponential solution here, which will go over to oscillatory solution here, when you look towards this turning point and you go over to the exponential solution here. Then you look towards this turning point then you will get oscillatory solutions here, then you look towards this turning point and then you go over here.

It is a very straight forward procedure, but it does become a bit cumbersome, if you have more than 3 or 4 wells. But, in principle in any potential, you can solve the Schrödinger equation and obtain the eigen values.

Now, what I will do next is what I had promised on the very first like the use of connection formulae to calculate tunneling probability. This is also an extremely important problem not only in quantum mechanics, but in solid state theory, in thermionic emission and things like that.

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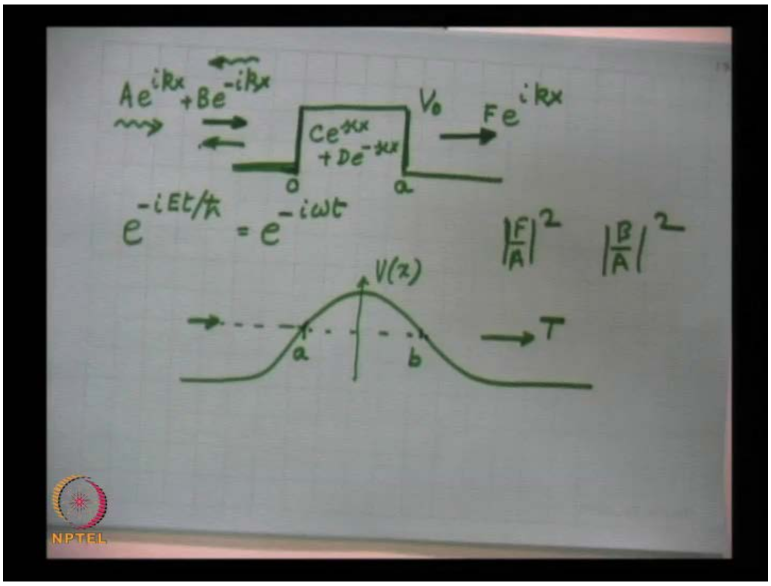

We had discussed one simple potential and we discussed the tunneling, made the tunneling calculation. That we had a potential like this and we assume V to be less than V 0, V can be greater than V 0 also, in general one considers e less than V 0 and then we have an incident wave here, and a reflected wave here, and then we assume only a transmitted wave here. So, here the solutions was A into e to the power of i k x plus B into e to the power of minus i k x.

The first term represents a wave propagating in the plus x direction, the second term represents a wave propagating in the minus x direction. Why, because the time dependence is of the form of minus i E t by h cross, which is equal to e to the power of minus i omega t.

You have an incident wave, incident on this step potential and then there is a reflected wave. But, there is a transmitted wave here and there cannot be any wave propagating in this direction, because there is no reflector here. So, we had assumed a solution, we had assumed a solution, in the form of F into e to the power of i k x, and in this region we have written down the solution as c into e to the power of kappa x plus d into e to the power or of minus kappa x. Then we applied continuity conditions at x is equal to 0 and at x is equal to a, and found out what is F by A whole square. This is the tunneling probability and what was B by A, whole square, this was the reflection probability

But this is a step potential; it is an idealized situation and in general you have a potential variation like this (Refer Slide Time: 20:46) and here the solution of the differential equation becomes extremely difficult. So, if you have a potential like this with a particle like that, if a particle is incident with a certain energy E, then there is a certain probability of it getting tunneling, tunneled through the barrier, and what we would like to do is to calculate the tunneling probability using WKB result.

In the end, this is the V of x variation, and the point at which E is equal to V of x, these are, as I have mentioned earlier, these are the classical turning points, a and b. Why is it a turning point? If for example, if I have a mountain in front of me, and I throw a tennis ball, then the ball will climb up the mountain to a certain height and will come back. To what height will it climb? It will climb to a height so that the ball comes at rest and therefore, that is the point at which the tennis ball turns back. So, those are the turning points and that is why they are known as turning points.

Similarly, we had considered the harmonic oscillator point, the harmonic oscill[ator]- may the linear The pendulum makes an oscillation like this and the extreme point, the displacement is given by x is equal to x 0 cos omega t, 0 is the amplitude and at that point, the total energy is potential and the kinetic energy is 0, and the particle turns back. So, in the case of the linear harmonic oscillator problem, the plus minus x naught or plus minus a, are the turning points and are known as the classical turning points of the problem.

So, here you have the turning points.

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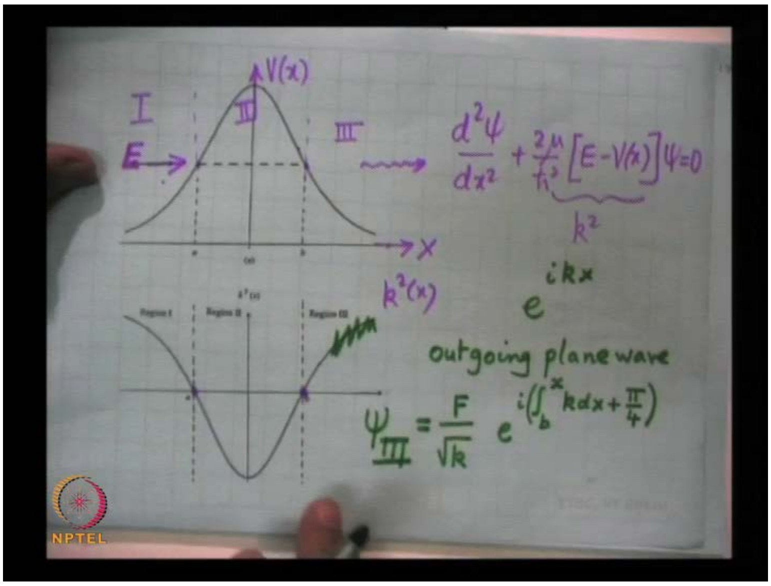

So, what we are planning to do is that this is mine, the potential energy variation, this is the potential energy variation, V of x as a function of x, and here is a particle of energy E, which is incident from the left on the potential. So, I want to solve the Schrödinger equation d 2 psi by d x square plus 2 mu by h cross square, E minus V of x, psi of x. This is my k square of x; is equal to 0.

If I plot k square of x, then it will need to look like this. These are the points at which k square of x is 0 and these are the classical turning points at which the particle will turn. Our approach will be like this.

What we will start out with is there is only an outgoing wave in region 3. So, this is region 1, this is region 2, which is the classically forbidden region. This is the classically forbidden region because the potential energy exceeds the total energy, so classically the particle cannot tunnel through the barrier, and this is the region that there is an outgoing plane wave. So, we will assume in this region, psi of 3, a plain wave. Now, plane wave will be of the form of e to the power of i k x.

We will write an outgoing plane wave. We will write as say F, the WKB solution will be root k, because k is positive here, k square is positive here, root k e to the power of i integral x k d x. I will put the lower limit as b so that it helps us in using the connection formulae and also put the face factor pi by 4, because if you remember that in the connection formula, there is a correction form d, there is a phase factor of pi by 4. So, I will write the solution in the region 3, in this region, as psi 3 is equal to so much.

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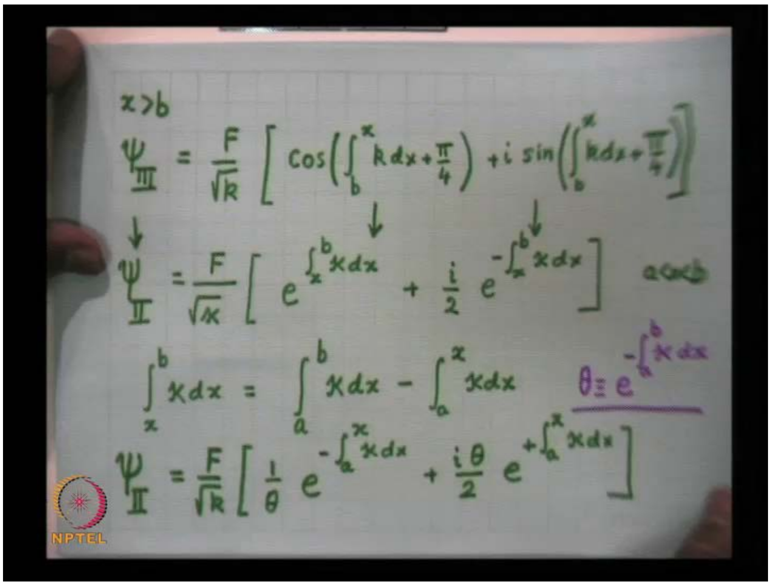

So, in the region x greater than b, therefore, we have the solution F by root k, so we rewrite it. Now, in terms of the third region, we write it as F by root k, in terms of the cos and the sine function. So, you will have cos of b to x k d x plus pi by 4, plus i sine integral b to x k d x plus pi by 4.

Now, this is the solution in this region, for x greater than b. I want to hop over the turning point and come to the region x less than b. So, the sine solution will go to an exponentially decaying solution and the cos solution will go over to an exponentially amplifying solution and we will be using this particular (Refer Slide Time: 27:50). So, the sine solution will, we must remember to put the factor of 2 correctly. So, this 2 will come here and this cos will go over to 1. This will be equal to F over root of kappa. Now, E is less than v of x and so you will have e to the power of x to b kappa d x plus i by 2, there should be a factor of 2, e to the power of minus x to b kappa d x.

So, this is the solution in the second region. In the second region, where x lies between a and b, therefore, it is from x to a (Refer Slide Time: 28:58). So this is x to b, because b is my turning point, b is my turning point here, so the integrals have to be x is less than b, so it is a x to b.

Now, we have the solution in this region. We have to now go over to the first region, so we have look towards the turning point a, and write integrals in terms of a to x. Therefore, let me write it down that x to b kappa d x, we will write as integral a to b kappa d x, minus a to x kappa d x. Since, this is e to the power of this, we define a symbol, which is theta, which is defined to be equal to e to the power of minus integral a to b kappa of x d x. This is the definition of theta, which we must remember.

So, therefore, the wave function in the region second will be F over root k. This is e to the power of a to b kappa d x, so that is 1 over theta, integral e to the power of minus integral a to x kappa d x, plus i theta by 2, because there is a minus sign here, so this will be e to the power of minus a to b kappa d x, and then e to the power of plus a to x kappa d x.

Now, we have here, therefore we have now the third, the oscillatory solutions, the exponential solutions are to the right, oscillatory solutions are to the left. Now, we will use, once again, the connection formulae to go over to region 1.

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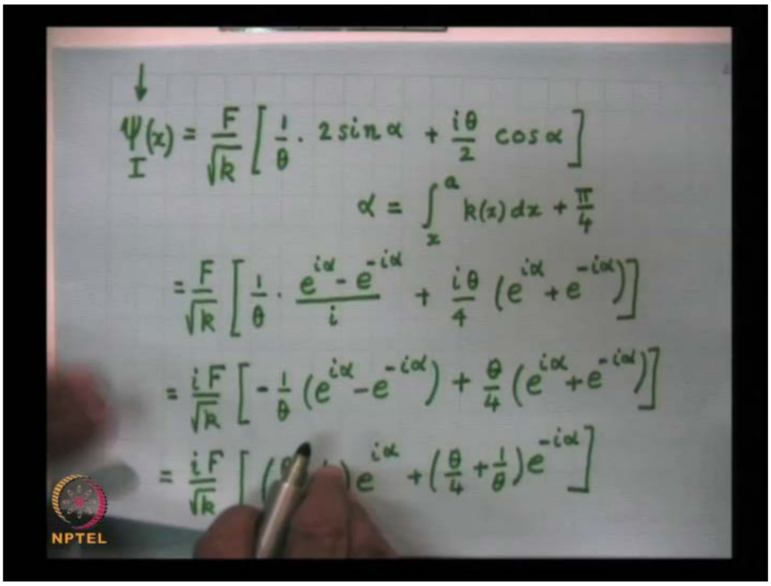

So, this will go over to, you just have to do patiently, psi 1 of x. This is the WKB solution using the connection formulae. I am sorry. This should be kappa, because in this region k square x is negative. So, this will be F by under root of k now, because in region 1, k square of x is positive. So, the exponentially decaying solution will go over to 1 over theta, 2 sin of, let me write it down as alpha. I will write down what is alpha, plus i theta by 2 cos alpha, and what is alpha as we all know; this will be integral x to a, k of x d x plus pi by 4.

So, this I have now obtained the solution in terms of sine and cosine functions. Now, we must express the sine and the cosine functions in terms of the exponentials, so that we know which one represents the wave propagating to the right and which one propagating to the left. So, this becomes equal to F by root k, 1 over theta, sine alpha that is e to the power of i alpha minus, e to the power of minus i alpha, divided by 2 i. So, 2 cancels out with here, so it becomes i, plus i theta by 4 now, because cos alpha will be e to the power of i alpha, plus e to the power of minus i alpha, that is it.

So if I take out i here, so I will get i F; let me do it in 2 steps, i F by root k, although this is trivial. So, this will become minus 1 over theta, e to the power of i alpha minus e to the power of minus i alpha, I have taken i outside, so theta by 4, e to the power of i alpha plus e to the power of minus i alpha. So, this becomes e to the power of (Refer Slide Time: 35:19) i F by root k. So, the e to the power of i alpha will be theta by 4 minus 1 over theta, into e to the power of i alpha, and then theta by 4 plus 1 over theta, that is e to the power of minus i alpha.

I hope this is clear now.

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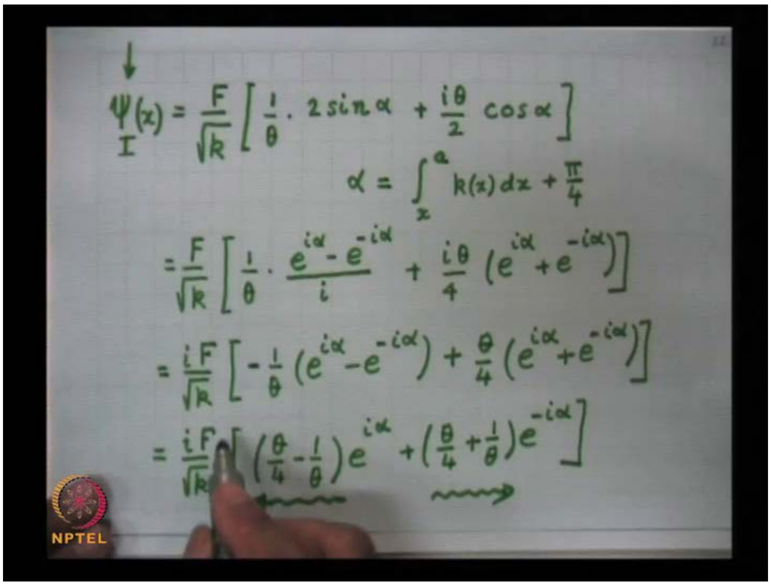

We notice that what is alpha; alpha as we wrote down, alpha was equal to the integral x to a k d x plus pi by 4. So, e to the power of i alpha, of course, there is a phase pack there, e to the power of i pi by four.

This will be x to a k d x plus pi by 4. Of course, there is a pi by 4 here but, that is immaterial. What I want to tell you is that if k was constant then this will be e to the power of minus i k x, so e to the power of alpha represents a wave propagating in the minus x direction, because if k was constant since x appears in the denominate in the lower limit, so this will be minus i k x, of course, there is an a also; so x minus a, actually. But, that is a constant factor, I do not worry about that but, the x dependence is on the form of i k x. So, this represents a wave propagating in the minus x direction similarly, e to the power of minus i alpha is a wave propagating in the plus x direction.

And therefore, this is the coefficient of the wave propagating, this is corresponding to the reflected wave (Refer Slide Time: 37:31) and this is the incident wave and I have the coefficient of the so, the coefficient of the so the co efficient of the so the reflex coefficient of the transmitted wave F. So, this is the coefficient of the transmitted wave. This is the incident wave and this is the reflected wave.

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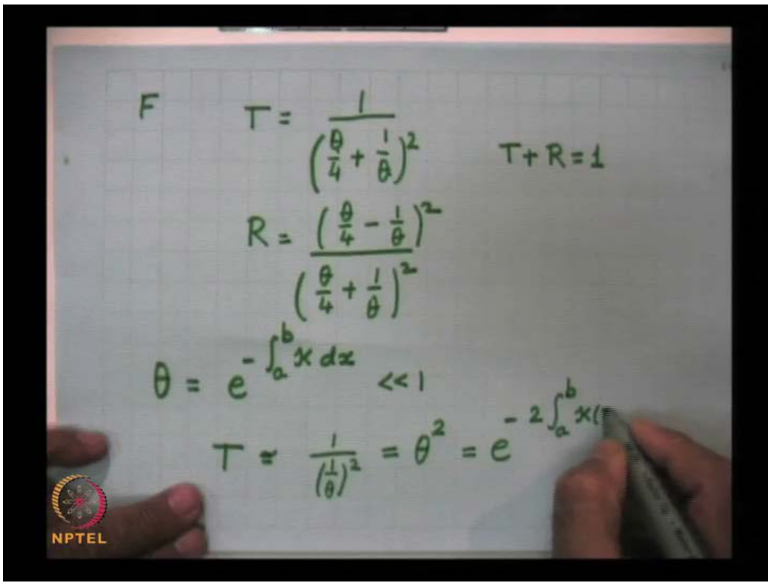

So, that the transmission coefficient will be 1 over theta by 4 plus 1 over theta whole square, and the reflection coefficient will be this reflected amplitude that is theta by 4 minus 1 by theta whole square, divided by the coefficient of the incident wave, so that is theta by 4 plus 1 by theta whole square.

Amazing thing is that in spite of all the approximations that we have made, the sum, the T plus R is equal to 1. Now, we had seen that theta we had defined as equal to e to the power of minus a to b kappa of x d x and therefore, this quantity is usually much less than one. Therefore, in this expression for the transmission coefficient T is equal to…, I left as an exercise for you to show that T plus R is equal to 1. So, T will be, this term (Refer Slide Time: 39:55) will be very small when compared to this term because 1 over theta will be, so I can neglect the theta by 4, this will approximately become 1 by 1 over theta square. So, this is equal to theta square and this is equal to e to the power of minus 2 of a to b kappa of x d x.

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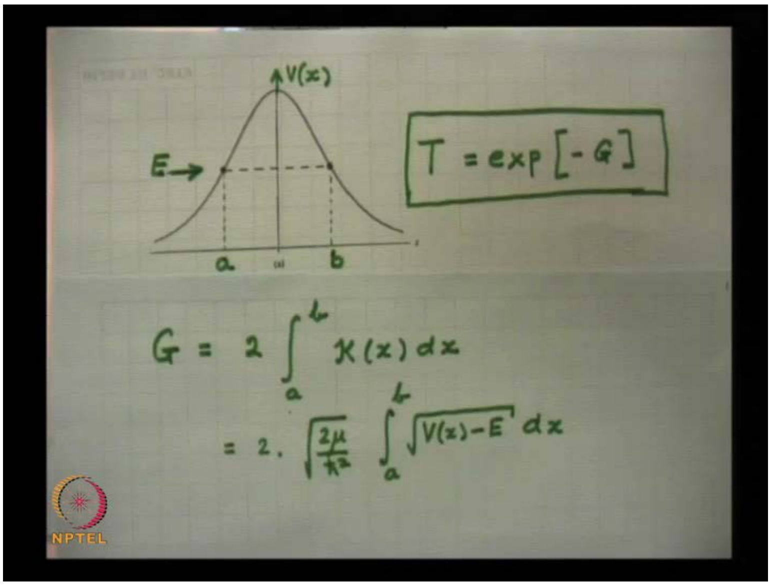

Thus, we have calculated the probability of tunneling as a particle approaches a potential barrier. So, we had started out with a potential barrier, which looked something like this. It is a smoothly bearing potential and a particle of energy E is incident from the left.

E is equal to V of x at these 2 points, so these are the 2 turning points, which we denote by a and b, and we found that the tunneling probability is equal to exponential of minus G, where G is equal to 2 integral a to b kappa of x d x, in the region a to b the potential energy is greater than the total energy, so it is a classically forbidden region and therefore, the expression for kappa is equal to 2 under root of 2 mu by h cross square integral V of x minus E under the root multiplied by d x and the integral is taken from one turning point to the other.

This is a very important result that the tunneling probability in many problems, as we will discuss only two to three applications of this, in our lectures, but this is a formula which is extensively used at many places.

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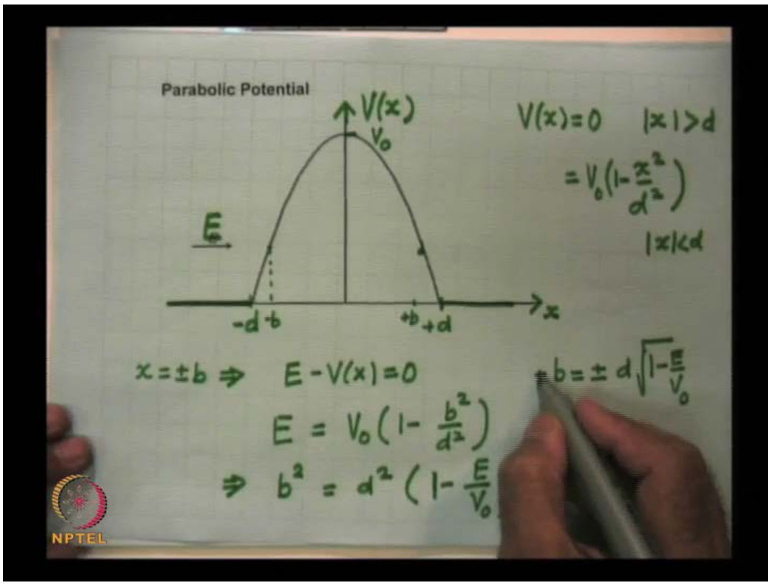

So, let me consider first a parabolic potential. Now, in a parabolic potential, the potential energy variation is 0 in this region and at x is equal to minus d. This is the x-axis and this is my V of x. So, this is a parabola and the particle of incident energy E is incident from the left. So, we write down that V of x is equal to 0, for mod x greater than d. At plus d also, beyond that the potential energy is 0 and beyond this point and between for x less than 0, x less than d, V 0 of 1 minus x square by d square, this is for x less than d. So, at x is equal to 0, the potential energy is V 0. Let me calculate first, the integral. The turning points are for a given value of the energy, let us suppose that the turning points are given by x is equal to plus minus b, because this is a symmetric potential. So, this will be one turning point and this will be one turning point.

Let this distance, let this coordinate be minus b and plus b, so at x is equal to plus minus b, E minus V of x must be 0. That is these are the term, these are the definitions of the turning point, so E is equal to V of x that is V 0 of 1 minus b square by d square. If I take V 0 below, therefore, we will get b square is equal to d square times 1 minus E by V 0. This quantity is less than 1, because E is less than V 0, so this is positive, so the turning points are b is equal to therefore, plus minus d under root 1 minus V 0.

The turning points are actually at plus b or minus b that b is equal to d into under root of 1 minus E by V 0. So, let me calculate the tunneling probability.

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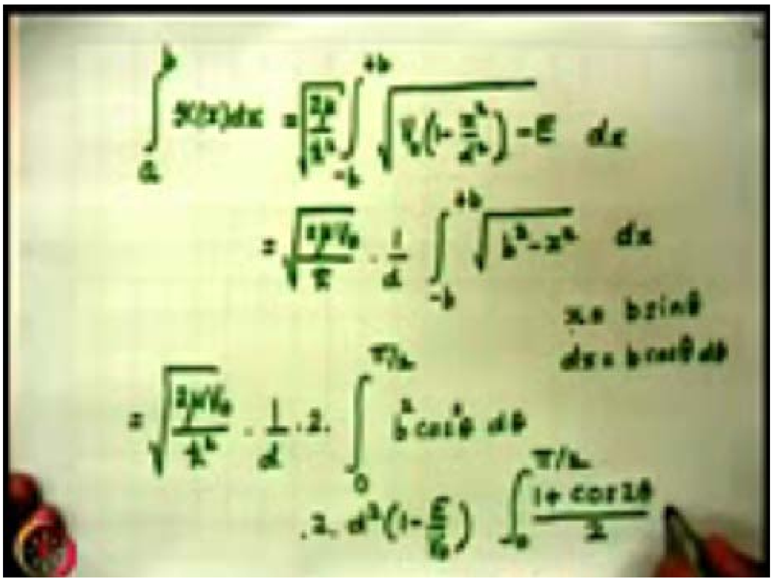

First of all, we will calculate from the integral from one turning point to the other kappa of x. This is the first example that we are considering, so a to b, so this will be from actually a is equal to minus b to plus b 2 mu by h cross square under root V of x that is V 0 times 1 minus x square by d square minus E.

I take V 0 outside. So, I get 2 mu V 0 by h cross square and therefore, I get 1 minus, and I take also square root of d square outside, so 1 over d, so I will get minus b to plus b under root of b square minus x square times d x. So, at the turning point the integral is 0. This is actually two times integral 0 to b. Therefore, let me then do the same kind of algebra as we have done before, x is equal to let us suppose b sin theta, so d x is equal to b cos theta d theta and b square minus, so this becomes….

So, let me write it on the left, under root of 2 mu V 0 by h cross square 1 over d multiplied by 2, because I will put this integral as from 0 to b, when x is 0 then theta is 0 and when x is b the theta is pi by 2. So, b square minus b square sine square theta, under the root is b cos theta and b cos theta, so therefore, this is b square cos square theta d theta. The integral is really trivial.

So, b square as we have already shown before that b square was equal to d square into 1 minus E by V 0. So, we will write down, so b square is equal to, as I take b square outside, so we will get 2 times b square that is d square 1 minus E by V 0, multiplied by

1 plus cos 2 theta by 2, integral from 0 to pi by 2. The second integral will be 0 as we had shown earlier.

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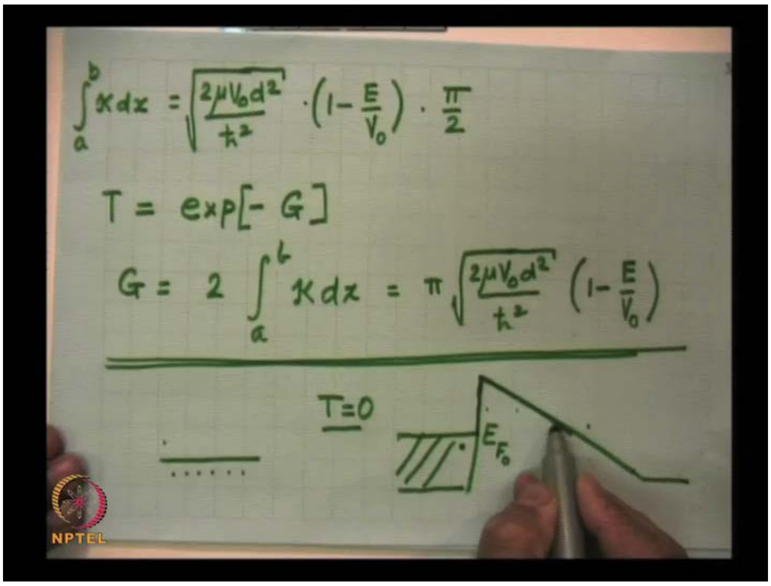

So, the first integral will be half into pi by 2. Therefore, 1 d cancels out with 1 d, I can take d inside, so I will get under root 2 mu V 0 d square by h cross square. This is a dimensionless number, multiplied by 1 minus E by V 0, and so there is a 2 factor. So, this factor 2 cancels out with this factor, and this will become the integral of this, will simply become pi by 2.

This integral as we had just now shown was equal to a to b kappa of d x (Refer Slide Time: 50:57) and the tunneling probability is equal to e to the power of minus G, so G is equal to 2 integral a to b kappa of x d x and this will be 2 into pi by 2, will be pi, under root of 2 mu V 0 d square by h cross square into 1 minus E by V 0.

This is just one example. So, we have just solved the problem, so this we write as example 1 (Refer Slide Time: 51:46) and this is just to give you an idea as to how you use the tunneling probability formula, which we had used by using the JWKB approximation. You first find out the turning points, and then you integrate kappa of x d x from the first turning point to the second turning point, and you will get the expression for the tunneling probability.

Now, then we next consider a very important, a very simple problem but, very important problem in solid state physics, namely cold emission of electrons. That is, that inside the metal, let us suppose you have a metal, and inside the metal there are free electrons, and let us suppose, at T equal to 0, at absolute 0, as all of you know, all the levels up to the Fermi level at T is equal to 0, the Fermi level, say in sodium or potassium, there are few electron boards. We had discussed that when we considered the free electron theory of metals.

Now, then there is a work function that the that the electrons inside the metal experiences a work function that it requires a certain amount of energy to go outside the barrier, to go outside the metal. Now, what we do is we put an electric field here, so that the potential energy variation is something like this. Therefore, the electron here at this energy, see a very high or near the fermi level, see is a very high potential and therefore, it classically, it cannot go to the other side, because in this region the kinetic energy will become negative.

But quantum mechanically, it is possible, for it for the particle to tunnel through, and therefore, if you have a metal surface and you put an electric field then, even at very low temperatures, where all the electrons are below the fermi level, there is a certain probability that the electrons will tunnel out. Let me calculate this probability.

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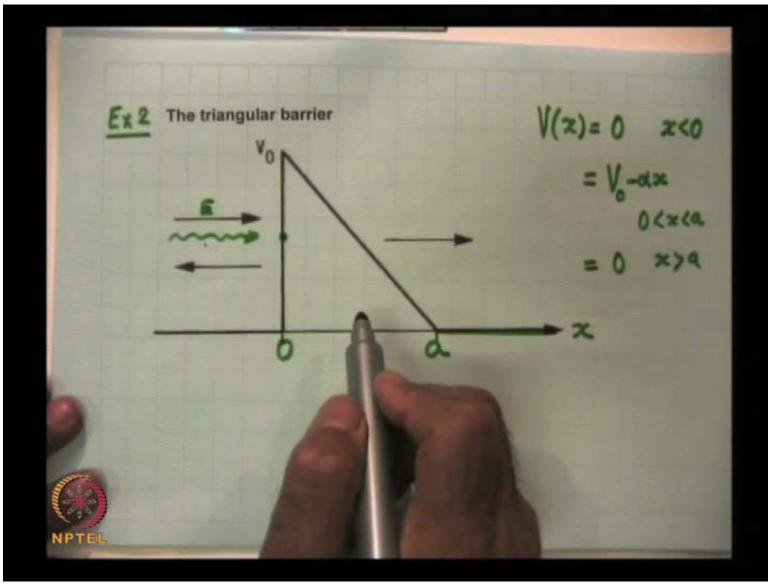

So, we consider this case, where you have what is known as the triangular barrier. So, we consider, just as we consider, the parabolic barrier. So, let me consider example 2 as the triangular barrier. So, this is my x axis and this is the potential energy variation. I have 0 here, and let us suppose this point is a, so the potential energy variation V of x is equal to 0 for x is less than 0. And then this is V 0 minus alpha x, for 0 less than x less than a. This is the potential energy function and then we assume it to be 0 for x greater than a and then it is equal to infinity but, for the sake of simplicity we assumed that this to be.

In this region, it is linear. So, what we will next consider is that in the next lecture, we will assume a particle to be incident of a certain energy E, and for the given energy, we will calculate the first turning point will be at 0, and the second turning point will be here. We will calculate the WKB tunneling, JWKB tunneling probability and from that we will try to derive an expression of thermionic current. That is known as the Fowler Nordheim Cold Emission formula and it is completely a quantum mechanical phenomenon, and it is manifestation of the tunneling of electrons through a potential barrier. So, we leave now here and we will proceed from this point onwards in our next lecture.

Thank you.