Basic Quantum Mechanics
Prof. Ajoy Ghatak
Department of Physics
Indian Institute of Technology, Delhi

Module No. # 09
The JWKB approximation and Applications
Lecture No. # 01
The JWKB approximation

At the end of the pervious lecture, we had started discussing on one of the very powerful methods in quantum mechanics in solving a second order differential equation. Since, second order differential equations appear in many diverse areas of physics and engineering.

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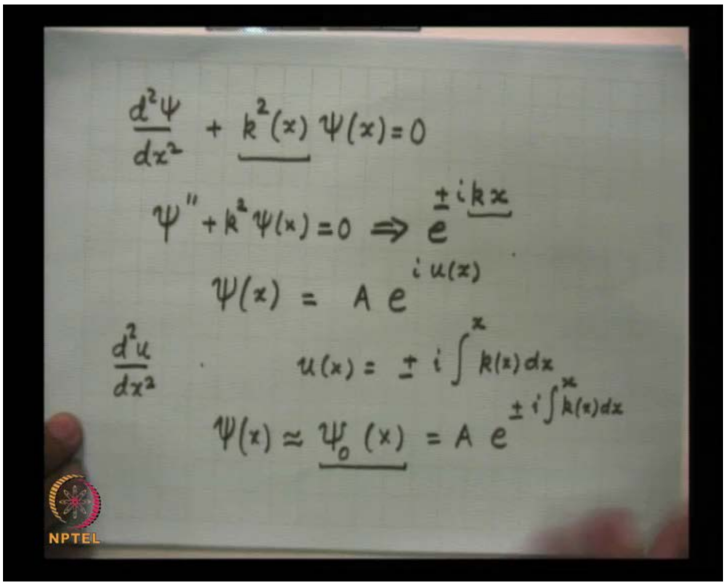

This is a very powerful method for solving the second order differential equation. Of the type d 2 psi by d x square plus k square of x psi of x is equal to 0, where k square of x is an arbitrary function of x. However, we assume it to be a smoothly varying function of x. It does not change too much. How much is too much? We will quantify that statement as we go along the lecture.

In my last lecture, I had said that when k square of x is independent of x, that is let us suppose k square of x is just k square, then the solutions of this equation are simple exponentials e to the power of plus minus i k times x. This suggested that for psi of x, we try out a solution of the form of e to the power of i u of x and we obtain a differential equation satisfied by u. If we neglected terms which are proportional to d 2 u by d x square and this is justified because when k square of x is constant u of x is just k x, so u double prime is 0.

Then, we found that if we neglect this term, then we found that u of x would be plus minus i integral k of x d x. Therefore, the zeroeth order WKB solution which is psi of x, the zeroeth order WKB solution is given by a exponential e to the power of plus minus i integral k of x d x. Then, we tried to find out the equation that is rigorously satisfied by psi 0 of x.

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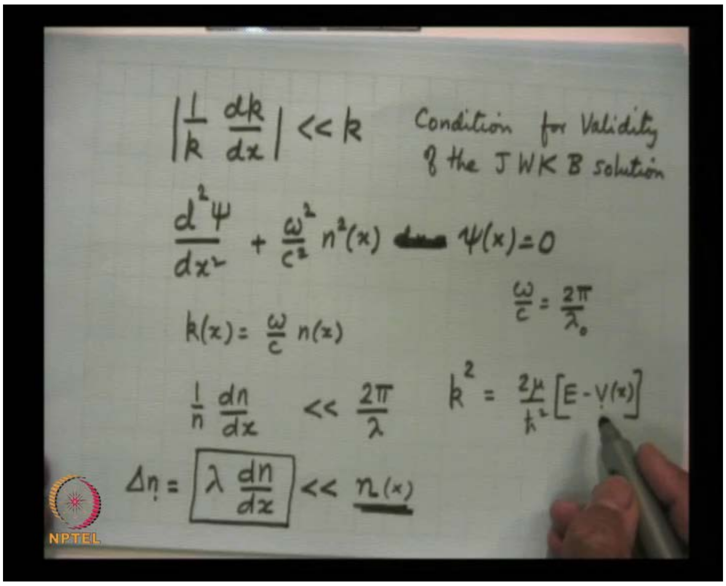

We found that this solution will be an accurate solution if 1 over k d k by d x modulus of that is less than k, this is the condition for validity of the JWKB solution.

Now, we also mention that in an inhomogeneous media, when we consider wave propagation in inhomogeneous medium, the field associated with an electromagnetic wave satisfies this equation omega square by c square n square of x d x multiplied by psi of x d x, where n is the refractive index and omega by c is the free space wavelength, omega by c is 2 pi by lambda naught.

Now, therefore, k of x as you can see is just omega by c n of x and therefore, 1 over k d k by d x is just 1 over n d n by d x should be less than the magnitude of this k is 2 pi by lambda, the local refractive index. Therefore, if I multiply both sides with lambda, I will get lambda d n by d x neglecting the factor of 2 pi is less than n d n by d x is the rate of change of the refractive index multiplied by wavelength. That means, this quantity on the left hand side is the change in the refractive index in a distance of the order of the wavelength.

So, therefore, this condition tells us that if the refractive index changes slowly, then my WKB solution is valid. The question is how slowly? The answer is that the change in the refractive index should be small in a distance of the order of this is delta n of x change in the refractive index in a distance of the order of the wavelength that should be small compared to the refractive index itself and of course, in quantum mechanics problem k square is equal to 2 mu by h cross square e minus v of x.

Obviously, even if v of x is slowly varying function, but let us suppose I am in a region where the potential energy is close to the total energy than k square becomes 0. So, the left hand side becomes infinity points at which v of x becomes e. Those are known as the turning points or rather classical turning points. We will discuss this little later as to why they are called turning points, but near the turning points, the k square itself becomes very small. So, therefore, this inequality does not remain valid and the WKB solutions fail. So, this also we will discuss little later.

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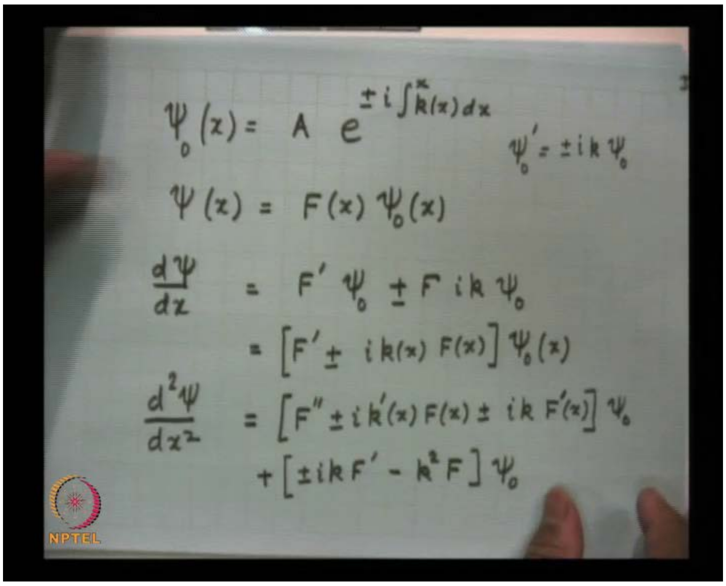

Now, therefore, the first order the zeroeth order WKB solution is psi 0 of x is equal to a e to the power of plus minus i integral k of x d x. Now, we want to do better than this. So, let me assume that psi of x is some function times psi 0 of x, where psi 0 of x is given by this and let me find out the differential equation that is satisfied by psi. So, you have psi d psi by d x or psi prime. This is equal to f prime psi 0 plus f psi 0 prime. So, if you differentiate psi 0 prime, so this will be plus minus i. The differential of integral of k of x d x is just k times psi 0, so psi 0 prime is equal to plus minus i k psi 0. So, this will be plus minus i k i k of x psi 0. So, I can write this down as f prime plus minus i k of x f of x psi 0 psi 0 of x i. Differentiate this again. So, I get d 2 psi by d x square. This is equal to if I differentiate this, I get f double prime d 2 f by d x square plus minus i k prime of x of x plus minus plus minus i k times f of x psi 0 of x plus this quantity multiplied by psi 0 prime. So, that is plus minus i k times this.

So, if I take the plus minus i k inside, so you get plus minus i k f prime. I am here. There should be an f prime because when I differentiate this, I will get first k prime f plus k f prime. So, this is plus minus i k f prime and plus minus times. Plus minus is just plus i square is minus k square f psi 0. So, let me write down the, let me combine these two terms and I will obtain, so this term adds up with this term and this term if I take on this side.

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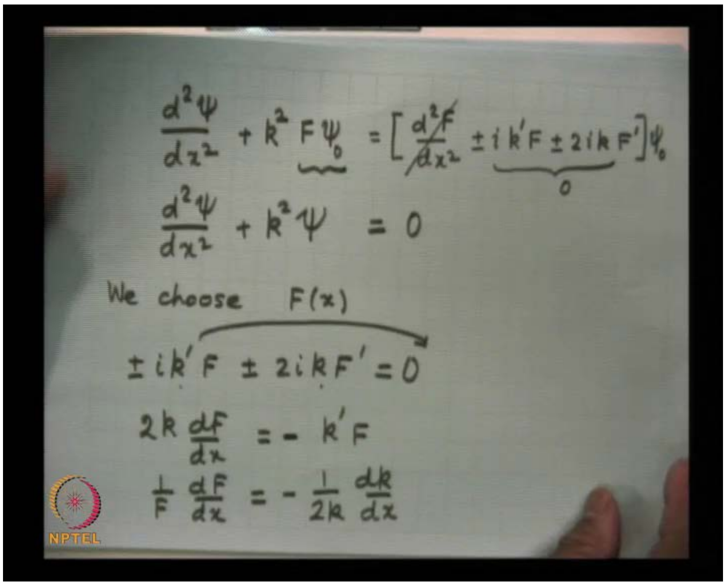

So, all right let me do it step by step, d 2 psi by d x square and if I take this side this here, so it will be plus k square f times psi 0. Then, this is equal to d 2 f by d x square and then, plus minus i k prime f plus minus 2 i k f prime psi 0.

Now, as we had assumed that psi of x is equal to f times psi 0, so this is psi. So, we obtain d 2 psi by d x square plus k square of psi and what I do is that in the first order look at the approximation, I make this, I neglect this term and I still have not chosen the f of x function and I take this equal to 0. So, the right hand side becomes 0. So, therefore, we choose f of x, such that plus minus i k prime f plus minus 2 i k f prime is equal to 0. So, therefore, plus minus, this cancels out. So, if I take this term on the right hand side, so I will get k 2 k d f by d x. This term is equal to minus 2 k d f by d x will become minus k prime times f.

So, I rewrite this. If I divide this, so I get 1 over f d f by d x is equal to minus 1 over 2 k times k prime, that is d k by d x. So, if I integrate this, I will obtain a very straightforward integration.

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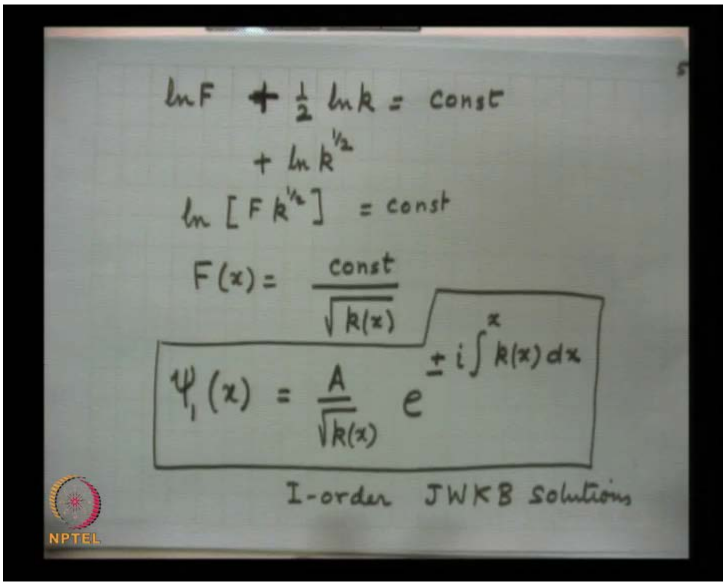

So, you will get log of f is equal to if I take it on this side. So, plus half log of k is a constant. Half log k means log of k to the power of half. So, log a plus log b is log a b. So, log of f k to the power of half is a constant and therefore, we obtain that f of x will be equal to constant times under root of k of x.

Therefore, the first order WKB solution is psi. First order will be of x will be equal to a by under root of k x e to the power of plus minus i integral x k of x d x. Let me recapitulate that as to what we did. When k of x is slowly varying, we found that this is the zeroeth order WKB solution. Now, we said that we want to do better than this. So, this is the zeroeth order WKB solution. So, we assume for psi of x a solution of this type f of x plus psi 0 of x and remember that psi of x satisfies this equation d 2 psi by d x square plus k square psi is equal to 0.

So, we substitute this solution in this equation. So, we first calculated at this stage. We do not know what f of x is. We will in fact find out what f of x is. So, we calculated the first differential, we calculated the second differential and we found that at this f times psi naught is psi. So, we obtained that this equation that d 2 psi by d x square plus k square f psi naught is equal to so much, but this is 0. The left hand side is 0. So, therefore, if once again if we are able to solve this equation d 2 f by d x square plus minus i k prime f plus minus 2 i k f prime is equal to 0, if we are able to solve this equation and then, if we substitute it here, we will obtain a rigorously correct solution of the second order differential equation.

Once again if I am able to solve this equation exactly and obtain an f of x substitute, then this will be a rigorously correct solution of the Schrödinger equation. We assume that f of x is a very slowly varying function, so that we neglect the term d 2 f by d x square and we choose f of x, so that this term is equal to 0. So, you have plus minus i k prime f plus minus 2 i k f prime is equal to 0. We solve this equation and we find that f of x comes out to be constant times under root of k of x. So, we finally obtain this as the first order JWKB solutions. These are the first order JWKB solutions.

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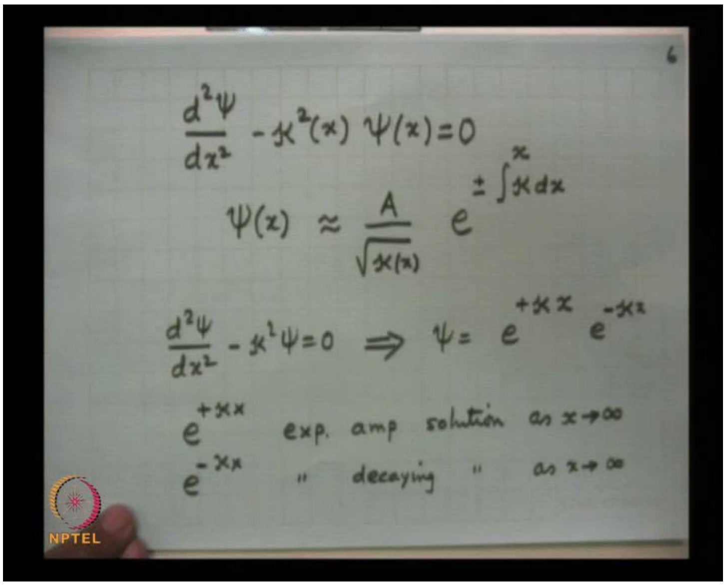

In fact, in all everywhere, the second order is so difficult that everywhere one uses only this type of solutions. These are known as therefore the JWKB solutions. Now, we had assumed k square of x to be positive. Let us suppose if k square of x is negative, we have an equation like this minus kappa square of x psi of x equal to 0. If we have an equation like this, we can again solve it in a exactly similar manner and we will obtain the WKB solution as constant. So, say a by square root of kappa x, but since there is a minus sign here instead of i k x, it is the plus or minus integral kappa d x. Either it will be an exponentially amplifying solution or it will be an exponentially decaying solution.

These solutions are oscillatory solutions in terms of sin. Sin as you all know that if d 2 psi by d x square if the constant is positive, then the solutions are either I can write it as sin k x or cos k x or I can write it in terms of plus minus i k x. So, these are the oscillatory JWKB solutions. On the other hand, if I have an equation of this type d 2 psi by d x square minus kappa square psi of x is equal to 0, then it has two solutions. One is e to the power of plus kappa times x if kappa is a constant which is an exponentially amplifying solution as x goes to infinity and e to the power of minus kappa x which is an exponentially decaying solution.

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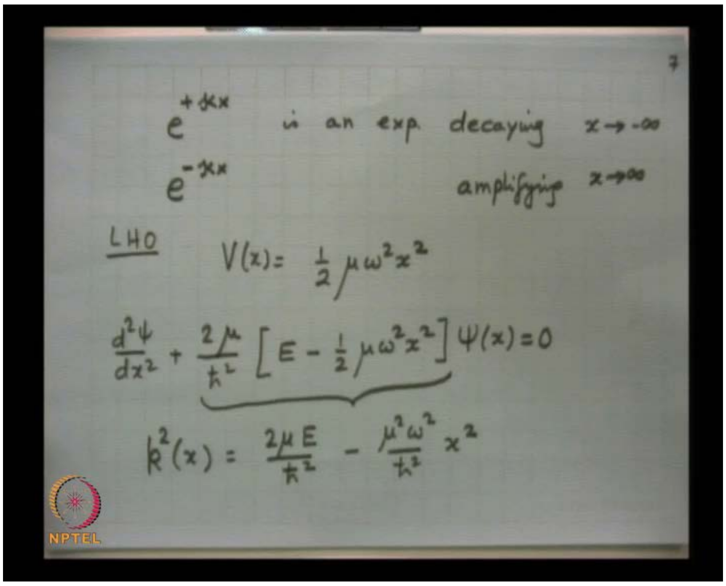

So, you must remember that e to the power of plus kappa x is exponentially amplifying solution as x goes to infinity and e to the power of minus kappa x is an exponentially decaying solution as x goes to infinity. However, if x goes to minus infinity, then exponential plus kappa x is an exponentially decaying solution as x goes to minus infinity. Similarly, e to the power of minus kappa x is an exponentially amplifying solution as x goes to minus infinity. Both are exponential solutions whereas, when k square x is positive, you have what are known as oscillatory solutions. So, these are the complete JWKB solutions. The question is how do we use them?

Now, let me consider a simple problem that the linear harmonic oscillator problem and you have for the linear harmonic oscillator v of x is equal to half mu omega square x square . Now, therefore, Schrödinger equation is d 2 psi by d x square plus 2 mu by h cross square e minus v of x. So, in this particular case, it is so much. So, half mu omega square x square psi of x is equal to 0. So, my k square of x is given by this k square of x is equal to 2 mu e by h cross square minus mu square omega square by h cross square x square.

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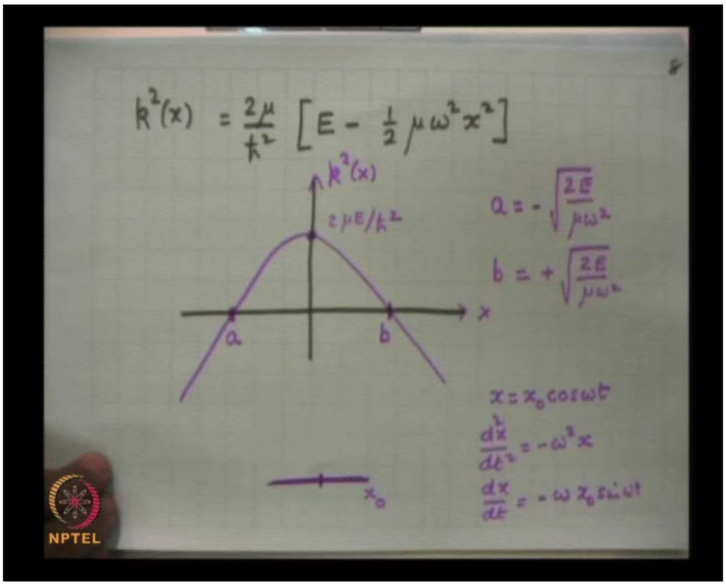

So, therefore, if I plot this, so my k square of x, let me rewrite. It is equal to 2 mu by h cross square e minus half mu omega square x square. Now, let us suppose e is positive, then how will this function look like. If you plot this, then it will be an inverted parabola. So, at x is equal to 0 k square, I am plotting k square of x as a function of x. So, at x is equal to 0, it has a positive value equal to 2 mu e by h cross square. So, this is 2 mu e by h cross square.

Then, at two points, then it starts decreasing with x and these are known as the turning points, where k square of x is 0. So, let us suppose this point is a, this is x is equal to b as you can immediately find out that a is equal to minus of under root of 2 e by mu omega square and b is equal to plus under root of 2 e by mu omega square. These are known as the turning points because in a classical oscillator, let us suppose I have a classical simple pendulum which is oscillating like this. Now, let us suppose that the maximum amplitude of the classical oscillator is x naught. So, at this point the kinetic energy is so let us suppose x. The vibrations are x is equal to x naught cos omega t. So, my d 2 x by d t square. This d 2 x by d t square is equal to minus omega square of x and d x by d t d x by d t is equal to if I differentiate, that is minus omega omega. I am sorry minus omega x naught sin omega t.

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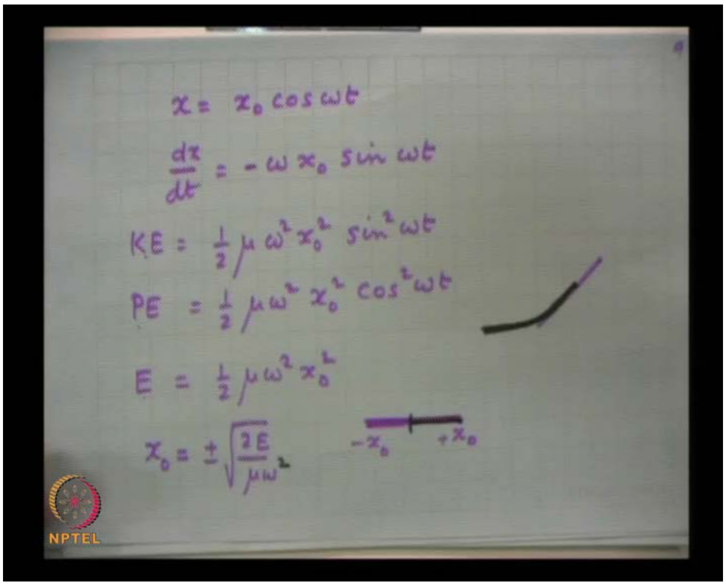

So, the kinetic energy, let me write this again that x is equal to x naught cos omega t and therefore, the velocity d x by d t is equal to minus omega x naught sin omega t. So, therefore, its kinetic energy is equal to half mu velocity square omega square x naught square sin square omega t and the potential energy is half mu omega square x square. So, that is x naught square cos square omega t.

So, the total energy is equal to half mu omega square x naught square. So, as we all know that if a particle of mass m of mass mu is making a simple harmonic motion, then at the point x naught, the kinetic energy is 0 and it turns back. So, this point x naught which is equal to plus minus under root of 2e by mu omega square, where e is the total energy of the oscillator which is independent of time e is kinetic energy plus potential energy and that is half mu omega square x naught square.

So, x naught is the point where the kinetic energy is 0, the total energy is potential and therefore, it turns back. So, therefore, the point plus x naught and minus x naught are known as the turning points of the oscillator, where the kinetic energy becomes 0 and therefore, the particle turns back. Let us suppose, I have a particle, I have a tennis ball which is climbing up the hill. Now, what will happen is that if you roll the tennis ball, it goes up and then, it turns back. At this point the kinetic energy becomes 0. So, here also the classical oscillator when it reaches the maximum displacement point, the kinetic energy is 0 and the particle turns back.

So, this x naught is equal to plus minus 2 u by mu, sorry mu omega square 2e by mu omega square are known as the classical turning points. So, in this figure, in this diagram you can see that at the point at x is equal to a and at x is equal to b k square of x is 0 and the turning points at x is equal to a and at x is equal to b. Now, I have the condition for the validity of the JWKB solution is 1 over k d k by d x. The modulus of that is should be less than k. So, around this regions, where k is 0, this condition is not satisfied. So, we have the WKB solutions in this region, we can have WKB solutions in this region and we can have WKB solutions in this region, but not near the turning points and therefore, how do we use these solutions.

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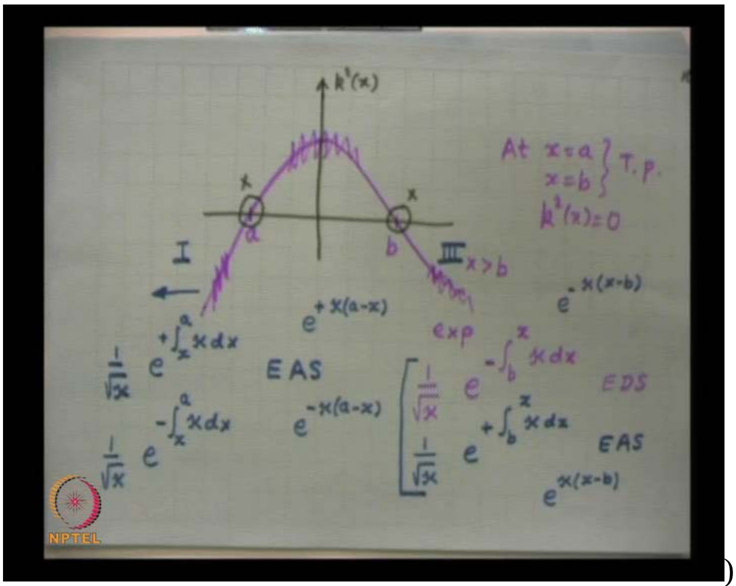

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So, let me discuss this point once again that let me draw this potential energy distribution and let us suppose, it is something like this. So, I plot k square of x and you have like this. These are the two turning points. At the turning points at x is equal to a and at x is equal to b, k square of x is 0. These are known as the turning points.

So, my WKB solution is valid here, WKB solution is valid here, WKB solution is valid here, but not in this region. In this region, WKB solutions are not valid. So, if I know the solution in this region, how do I go here or if I know the solution in this region, how do I go here or if I know the solution here, how do I go here. These are done through what are known as the connection formulae and we will discuss the, first of all we will state what are the connection formulae, use them in solving problems and may be at the end of this lecture, the next lecture may be when we finish JWKB approximation, we will give the theory behind the connection formulae.

First of all, let us suppose that let me write down the solution in this region here, x is greater than d, but k square of x is negative. So, my solutions are exponential solutions and we can write the exponential solutions as 1 over root k e to the power of minus b 2 x kappa d x. This is an exponentially decaying solution because if kappa were constant, then the upper limit is x. So, this will be e to the power of minus kappa x minus b and as x tends to infinity, this will be an exponentially decaying solution.

So, similarly 1 over root kappa e to the power of plus integral b to x kappa d x is an exponentially amplifying solution because if kappa was a constant, if I take it out of the integral, so this becomes kappa x minus b. Now, these are the JWKB solutions in region 3, far away from this turning point. Let us consider region 1. The solutions are 1 over root k. Now, here x is less than a. So, I write these down solutions as e to the power of x to a say, plus kappa d x. Now, you see that if kappa was a constant, then this will be e to the power of plus kappa a minus x and as x goes to minus infinity. This becomes exponentially amplifying solution.

Similarly, 1 over root kappa exponential minus here x is less than a kappa d x here if I take kappa to be a constant. So, you will have e to the power of minus kappa a minus x. So, this will be e to the power of plus kappa x. So, this is a as x goes to minus infinity, this becomes an exponentially decaying solution.

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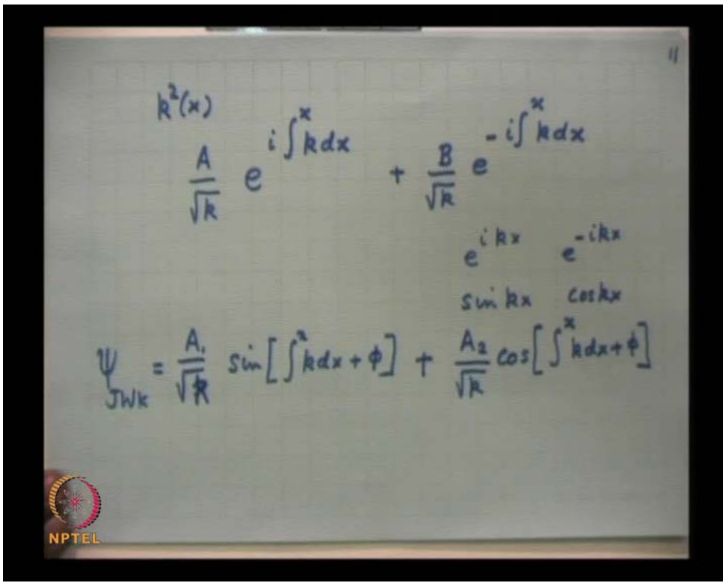

Now, let me first mention that you have here when k square of x is positive, the two independent solutions are a by root k e to the power of i integral k d x plus and minus. The two independent solutions are under root of k e to the power of minus i x k d x. I can take any linear combination also. For example, when k square is constant, I can write the solution as e to the power of i k x and e to the power of minus i k x or I can write down this as sin k x and cos k x. That is also well behaved, that is also a legitimate solution.

So, I can write this down as a by root kappa, say a 1 by root kappa k root k, sorry sin of integral say a x plus a phi. Some face factor and the other independent solution I can take as a 2 by root k cos of integral x. X can be at the top or at the bottom. It does not really matter. We will see k d x plus phi. So, the general solution is the sum of this. So, this is the general JWKB solution.

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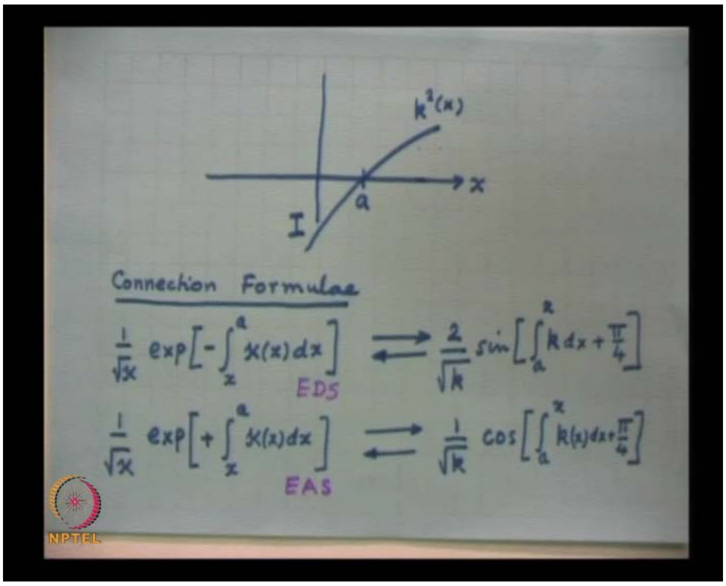

So, let us consider the connection formula when the exponential solutions are to the left and oscillatory solutions are to the right.

So, let us suppose there is a turning point at a, there is a turning point at x is equal to a. This is my x and this is k square of x. K square of x passes through 0. It is positive on right side. So, here you have oscillatory solutions, here there is exponential solution. So, the connection formulae are 1 over root k exponential minus x to a because in this region, this is the first region. Let us suppose for x less than a, so kappa of x d x. This goes over to there is a factor of 2, there 2 by root k sin of integral a to x k of x d x. Let me just write it down as k d x plus pi by 4.

So, this is the exponentially decaying solution in region 1 far away from the turning point. This is the oscillatory solution to the right far away to the right of the turning point x is equal to a. Similarly, an exponentially amplifying solution. So, this is under root of k. This you must remember, I remember them, so you must also remember them x to a kappa of x d x. Once you remember the correction formulae, then the use of the WKB approximation is really extremely simple and very elegant and this goes over to 1 over root k. It is a cos function cos a to x k of x d x k of x d x plus pi by 4.

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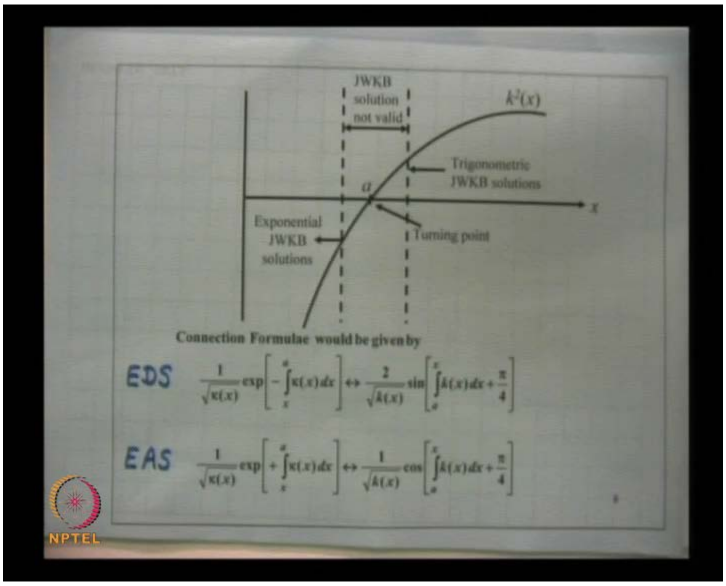

So, this is the exponentially decaying solution and this is the exponentially amplifying solution. To the left of the turning point, I have drawn a picture. Let me show that to you. So, you have a turning point at x is equal to a. Now, near the turning point, the JWKB solutions are not valid. So, beyond little on the right of the turning point, where k square of x is positive, you have trigonometric of sinusoidal JWKB solutions. Beyond a certain distance to the left of the turning point, you have exponential JWKB solutions. This is the variation that I have assumed. It is a smoothly varying function, but it passes through 0 at x is equal to a and these are the two connection formula.

If you have an exponentially decaying solution here, it will go over to the sin function plus pi by 4. This phase is important. On the other hand, if there is an exponentially amplifying solution here because if kappa was constant, then this would be e to the power of minus kappa x and as x extends to minus infinity, this will be an exponentially amplifying solution. So, the solution on the left is exponentially decaying solution and the solution to the left is an exponentially amplifying solution and that is equal to 1 over root k. That goes over. I have not given you the proof of the connection formulae and I hope to give you the proof at the end of the next lecture, but right now, you take it for granted. So, once again you do not know the solution near this part, you do not know the solution near this part. You only know the solution far to the left of the turning point.

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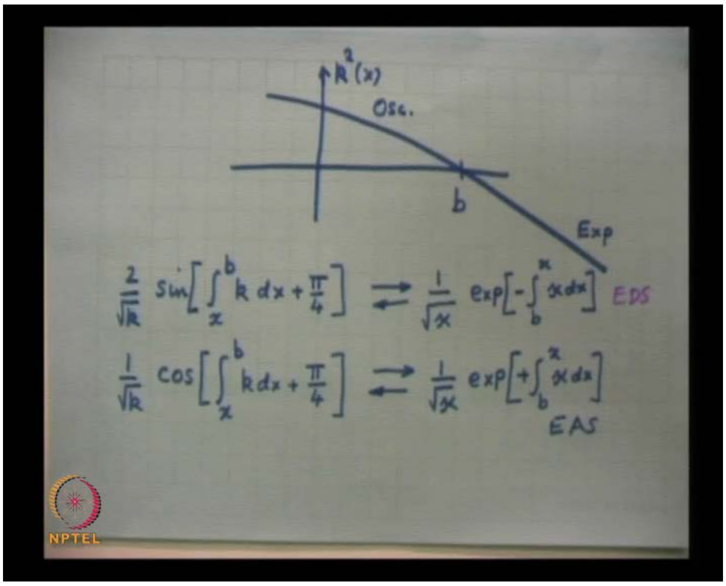

So, these are the solution and so these are the solutions far to the right of the turning. What happens if I have a k square of x variation in which there are variations like this. So, let us suppose this is a turning point and you have oscillatory solutions here because k square of x is positive here, k square of x is positive here and k square of x is negative here. So, here, these are exponential solutions and here, they are oscillatory solutions. So, here we will write like this. In this region, we will write 2 by root k 2 by root k sin of please see the limits now x is now less than d. So, it is x to b k d x k of x d x plus pi by 4. This goes over to the exponentially decaying solution.

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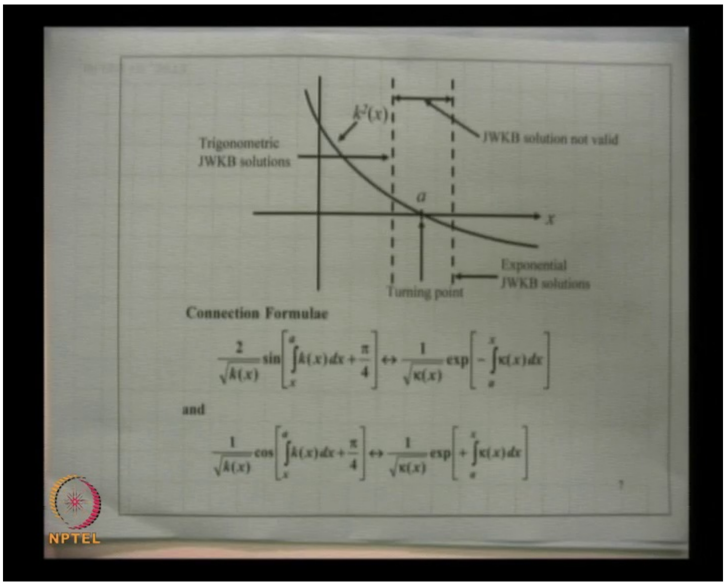

So, this is 1 over root k exponential minus integral b to x kappa d x. This is the exponentially decaying solution and the cos term 1 over root k cos integral x to b k d x plus pi by 4, this goes over to 1 over root k exponential plus b to x kappa d x. This is an exponentially amplifying solution. So, here I have shown this again the turning point. Here I have shown as a does not matter. So, what I have tried to show here is that in this region near the point x is equal to a k square of x is 0. So, in this region, k square is small and therefore, the JWKB solutions are not valid.

In this region k square of x is less than 0. So, you have exponential solutions. In this region, k square of x is positive. So, you have exponential solutions, I mean sinusoidal solutions. So, what are the connection formula, what solution will go over to an exponentially decaying solution and what solution on the left will go over to an exponentially amplifying solution? I am just giving you the answer without proof. Hopefully, I will give you the proof later and the answer is that 2 by root k x sin x to a k d x plus pi by 4 goes over to an exponentially decaying solution. This I had written down in the previous slide also and this 1 over root k. If you have a term like this, then this will go to an exponentially amplifying solution.

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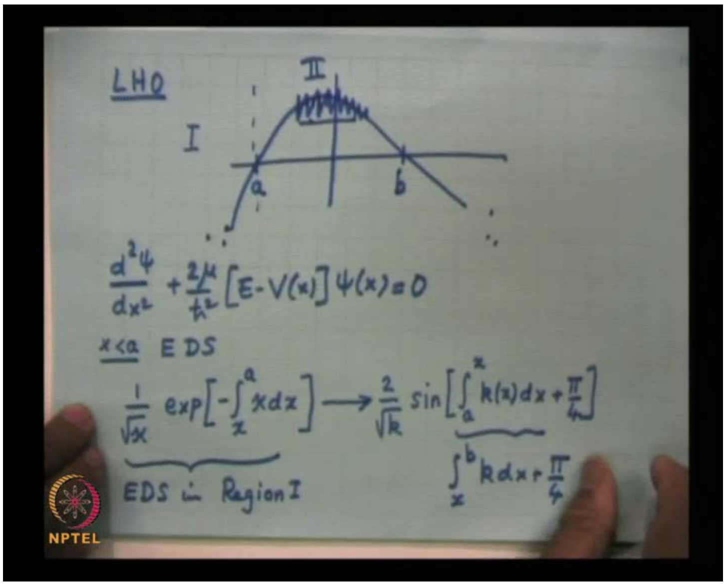

Now, let us solve a problem. Let me consider the linear harmonic oscillator problem which we have been doing large number of times, the linear harmonic oscillator. So, you have linear harmonic oscillator type. So, you have a k square of x variation which is something like this as I had discussed. So, it has two turning points at x is equal to a and at x is equal to b. Now, I want to find out the Eigen values of the problem. Eigen values correspond to the bound state. That means, d 2 psi by d x square plus 2 mu by h cross square e minus v of x. I am solving this problem. So, the boundary conditions are that x must go to 0 as x tends to infinity and as x tends to minus infinity, so I must start. I must have an exponentially decaying solution here and I must have an exponentially decaying solution here.

So, the trick is that in region 1, that is x less than a, I start with an exponentially decaying solution here. I then go over to this region and then, I look towards this turning point and go over to this region and find the coefficient of the exponentially amplifying solution and that we must set equal to 0. Let me do this. So, for x less than a, if you want to have an exponentially decaying solution, then the solution is 1 over root kappa as we discussed just a few minutes back minus x to a kappa d x.

This is the exponentially decaying solution in region 1. I write this. It goes over to in region 2. In this region far away from the turning point to 2 by root k sin of a to x k of x d x plus pi by 4. So, I have stated with an exponentially decaying solution here and using the connection formulae, I have been able to get a solution here. Now, I want to get a solution in this region. So, for that if this is let us suppose the point b, then I must write the solution in terms of x to a or this turning point x to b k d x plus pi by 4. The argument has to be like this and then only I can hop over this turning point and go to this side.

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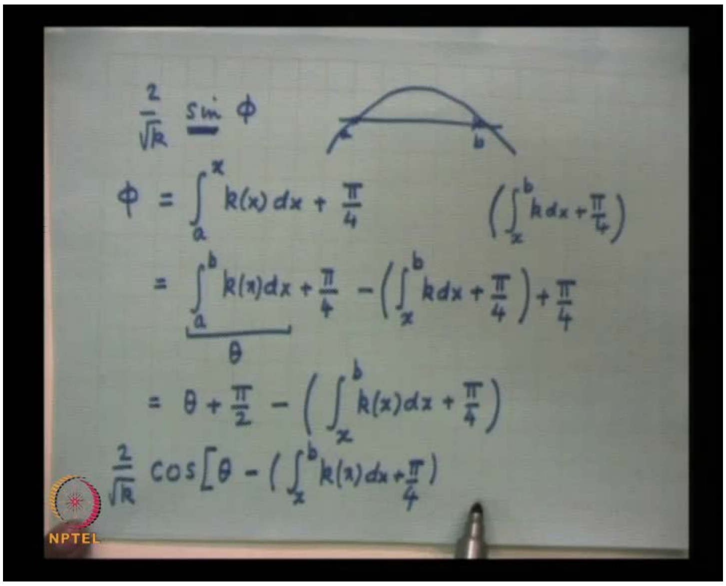

So, let me tell you. So, instead of this, I must have expression like x to b k d x plus pi by 4. So, it will become clear in a moment. So, in the second region, my solution is 2 by root k sin of phi, where phi is equal to integral a to x k of x d x plus pi by 4. So, a point is here and b point is here. So, I want to now write the integral in terms of x to b k d x plus pi by 4. So, what I do is I write this down as a to b k of x d x plus pi by 4 and then, I write minus x to b k d x plus pi by 4. I have added a term minus pi by 4. So, this I add pi by 4.

So, what I had done is I have written integral a to x as a to b minus x to b. So, this becomes let me put this is equal to theta. So, this becomes theta plus pi by 2 pi by 4 plus pi by 4 minus integral x to b k of x d x plus pi by 4. So, if I take the sin phi, if I take the sin of this thing sin of pi by 2 plus alpha is cos alpha, so I will get 2 by root k. This term, please see this 2 by root k cos of theta minus this whole quantity x to b k of x d x plus pi by 4. So, now I will write this as cos a cos b plus sin a sin b. We will continue from this point onwards in our next lecture.