Basics Quantum Mechanics

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Module No # 09

The JWKB Approximation and Application

Lecture No # 02

The JWKB Approximation: Use of Connection Formulae to solve Eigen value Problems

In the previous lecture, we had discussed the solution of the Schrödinger equation of the one dimensional Schrödinger equation, in the JWKB approximation. We had written down the solutions when k square of x is positive and when k square of x is negative and we wrote down the connection formulae.

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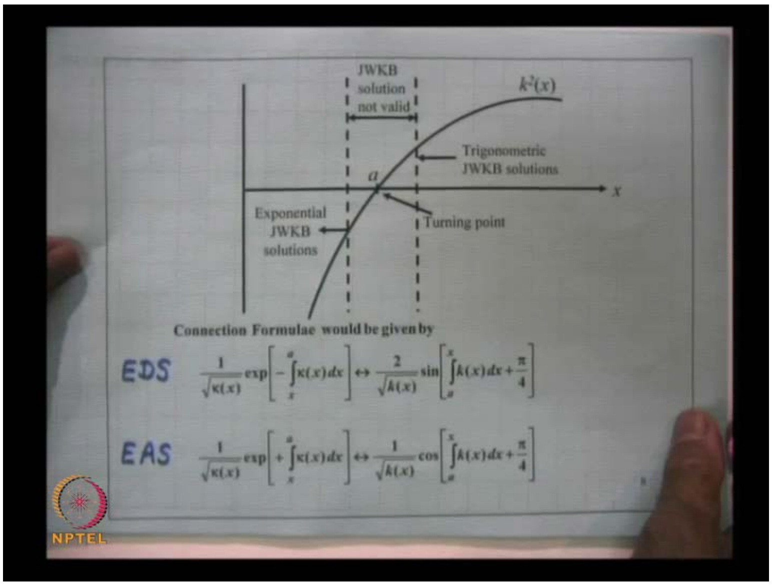

We said that if k square of x, variation is like this, so that the oscillatory solution is to the right of the turning point. This point x is equal to a, is the turning point where k square of x is equal to 0. So, in this region, we have exponential solutions and in this region we have trigonometric solutions. So, these are the connection formulae, 1 over root kappa of x, exponential... You must be careful for the limits. In this region, x is less than a, so x to a kappa of x goes over to 2 by root k x, sine of a to x.

In this region x is greater than a. So, it is a to x, k d x plus pi by 4. This is the exponentially decaying solution similarly, we have the connection formula that I had written down for the exponential and we find the solution. On the left, on the right, are the JWKB solutions. Near the turning point, k is extremely small. In fact, I have at the turning point, k square of x is 0 and the JWKB solutions are not valid.

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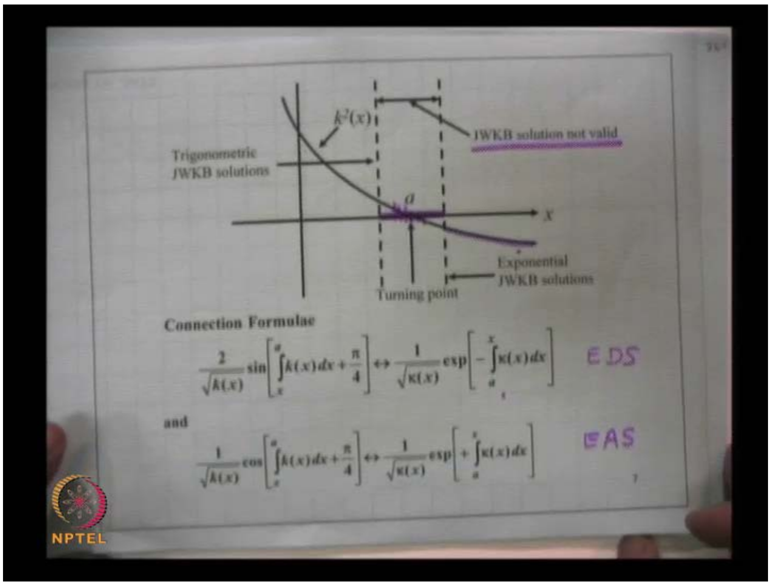

On the other hand, if I have a situation, in which you have k square of x becomes negative to the right of the turning point, and we have just to reverse this. So, near the vicinity of the turning point, JWKB solutions are not valid, and we will explicitly show that probably at the end of today’s lecture. On the left are oscillatory solutions, so you have on the left side x to a, because in this region x is less than a, and in this region x is greater than a. So, the limits are from a to x.

So, this is the exponentially decaying solution, so 2 by under root of k sine of x to a k of x d x pi by 4 goes over to a exponentially decaying solution and cosine of this thing goes over towards exponentially amplifying solution. So, with this, we will now use the connection formulae to obtain, to derive an eigen value equation, to derive an equation which will determine the eigen values of the problem.

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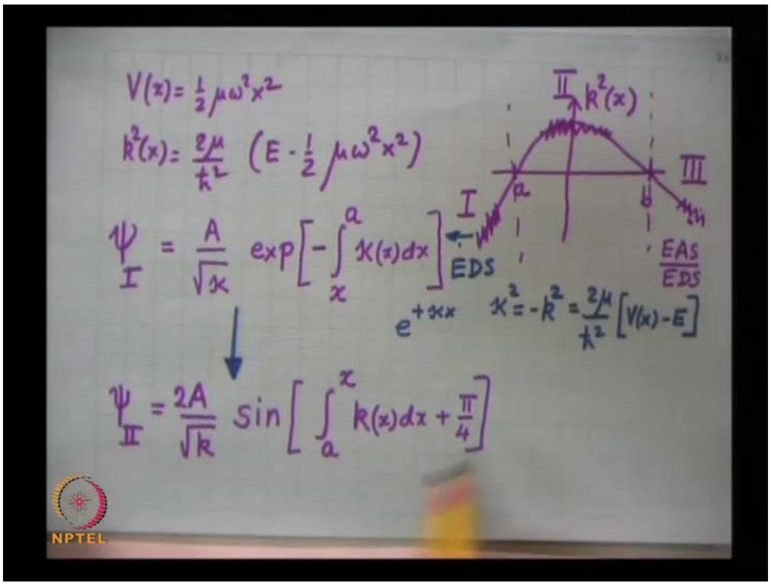

We consider for example, V of x is equal to half m omega square x square, harmonic oscillation, something like that. So, my k square of x is equal to 2 mu by h cross square E minus half mu omega square x square. So, as I discussed in my last lecture, you will have a variation of k square of x; something like this.

So, we start with a exponentially decaying solution here. We hop over this turning point, let us suppose this is x equal to a, and go to this region, then the WKB solutions is really valid in the entire region from here to here (Refer Slide Time: 04:58) and then we use the correction formulae with respect to the turning point b, and hop over to this region, and we will find that in this region, we will have the both exponentially amplifying solutions as well as exponentially decaying solutions.

We will, for a bound state, an exponentially decaying solution should go over to exponentially decaying solution. So, the coefficient of the exponentially amplifying solution will be set equal to zero and that will lead to the eigen value equation. So, let us do this. So, the exponentially, this is region 1 for x less than a, x between a and b is region 2, and x greater than this is region 3. So, these are the 3 regions in which we will discuss in WKB solution.

So, let me first write down psi 1 in the first region. We will, in the first region we have an exponentially decaying solution, so you will have say some constant or A by root of kappa, exponential minus, here it is x is less than a, so this is x to a kappa of x d x. So, what is the kappa? kappa is; kappa square is equal to minus k square of x and in this case this is equal to therefore, 2 mu by h cross square V of x minus E, because if for x less than a, V of x is greater than E and therefore, this is the variation of k square of x, as we had discussed in our last lecture.

This is the exponentially decaying solution. This is the exponentially decaying solution and that is because if kappa was constant, this will be minus e to power of minus kappa x and at the lower limit, it will be e to the power of plus kappa x, as x goes to minus infinity, this is an exponentially decaying solution (Refer Slide Time: 07:48).

So, we will now use the connection formula that we had mentioned a minute back, and this then goes over to psi 2 equal to 2 into A upon root k. This is the connection formula, which I had told you without proof, but we will prove that. Sine of, in this region x is greater than a, a to x, k of x; k is a function of x. But, in future, I will not write k of x, just k plus pi by 4. Therefore, this solution is in this region (Refer Slide Time: 08:39).

Now, I must look towards the turning point x is equal to b. Now, I must look towards the turning point x is equal to b and therefore,

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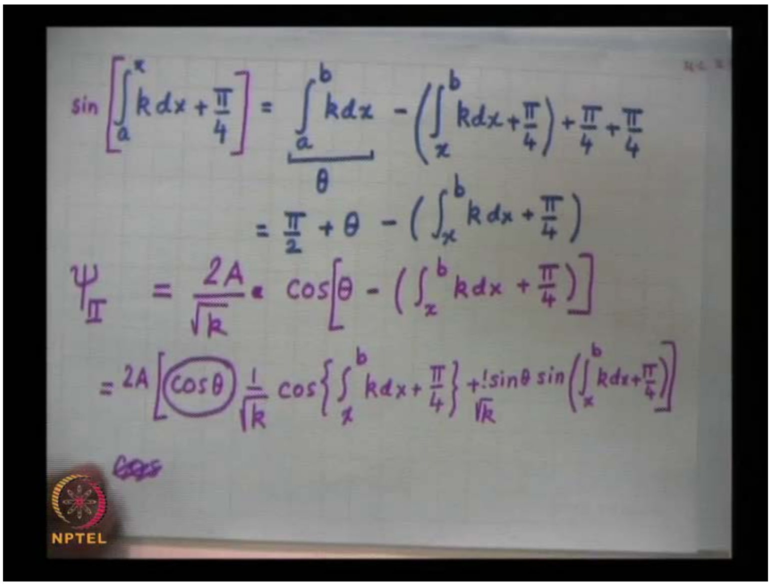

I should write this integral as, a to x, k d x plus pi by 4. This is the phase term. This I write as a to b k d x, minus x to b k d x. But, in order to use the connection formula, I must add pi by 4. this is the…So, you have here for example, x to a k d x plus pi by 4, this goes to our exponentially decaying solution. We will have x to the turning point I have denoted by b, so x to b k d x plus pi by 4 (Refer Slide Time: 10:08). So, here there is a pi by 4 and this is minus pi by 4. So, I have 2 pi by 4, plus pi by 4 to take care of this and plus pi by 4 to take care of this.

Let us suppose this, I put equal to theta (Refer Slide Time: 10:28). So, this becomes pi by 2 plus theta, minus integral x to b k d x plus pi by 4. Now, in the WKB solution, we have to take the sine of this expression. So, let me write it down. Sine of this will be therefore, sine of the whole quantity and that will be equal to cosine of theta minus the whole quantity, x to b k d x plus pi by 4. So, my WKB solution, as we had written down will be psi 2 will be equal to 2 A by root k multiplied by this. So, this is my WKB solution.

Now, this is cos of a minus b, so cos a cos b plus sine a sine b. So, let me write it down carefully, 2 A, I take outside, and you will have cos theta times one over root k, cos of, now this is very important, x to b k d x plus pi by 4, plus sine theta and sine of the entire quantity. I hope this can fit in inside this; sine of integral x to b, k d x plus pi by 4.

Now, therefore, I have obtained the solutions in this region (Refer Slide Time: 13:13) and here k of x is 0, so these solutions are really, sorry there is a 1 over root k factor here (Refer Slide Time: 13:24). So, I have now the solutions here and now I must use the turn connection formulae to go from here to here, and I have those connection formulae; the sine term x to a pi by 4 goes over to a exponentially decaying solution, and the cos term goes over to a exponentially amplifying solution. Therefore, the coefficient of the cos term must be 0.

Otherwise, the wave function will blow up for x greater than b. Once again, if I have the cosine term in this region, then that will go over an exponentially amplifying solution. So, therefore, that will not correspond to a bound state problem and therefore, the coefficient of the exponent cosine term must be zero. So, therefore, this term must be zero. So, we must have cos theta.

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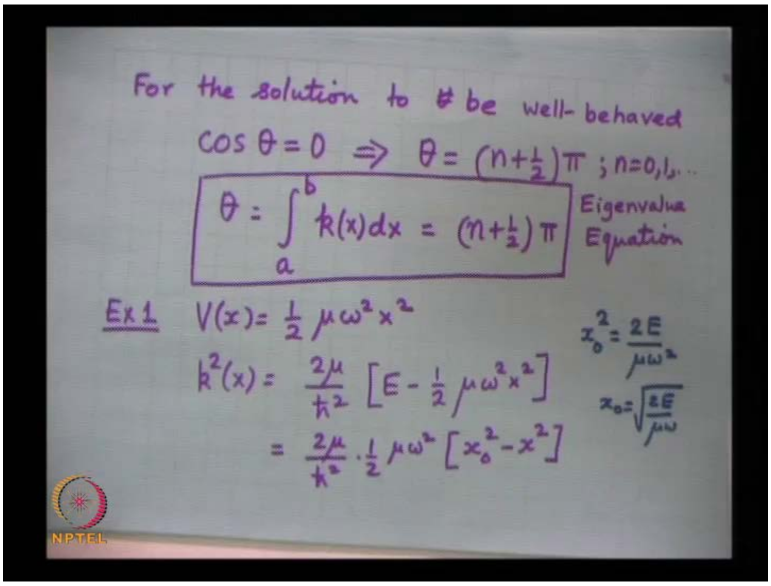

Let me write it down that for the solution to be exponentially; to be well behaved that it should not go to infinity. The coefficient of the exponentially amplifying term must be zero and therefore, cos theta must be zero, because it is this term (Refer Slide Time: 15:30), which goes over an exponentially amplifying solution. This term goes over to a exponentially decaying solution. So, therefore, this cannot happen for as bound state, therefore, cos theta must be zero. So, this implies, theta is equal to n plus half pi where n is equal to 0, 1, 2, 3 etcetera.

And what is my theta? Theta is equal to a to b k d x. So, theta is equal to integral from two turning points, a to b, k x d x, must be equal to n plus half pi. This is a very important result (Refer Slide Time: 16:26) that we have derived. This is the eigen value equation, the equation which determines the eigen values of the problem. I will consider a few examples now. So, example one I have. Till now our analysis was general, in the sense, it could be an arbitrarily variation of V of x as long as it is smoothly varying, so that our WKB approximation is valid.

We now consider our linear harmonic oscillator V of x is equal to half mu omega square x square (Refer Slide Time: 17:19). So, you have k square of x is equal to 2 mu by h cross square, E minus V of x, so E minus half mu omega square x square. If I take out half mu omega square outside, this becomes two mu by h cross square times half mu omega square, and I write x naught square minus x square, where x naught square is equal to 2 E by mu omega square. Actually, x naught is classical amplitude as we have discussed in our last lecture the classical amplitude. So, x naught is the turning point. So, this two and this two cancels out and you get mu square omega square by h cross square.

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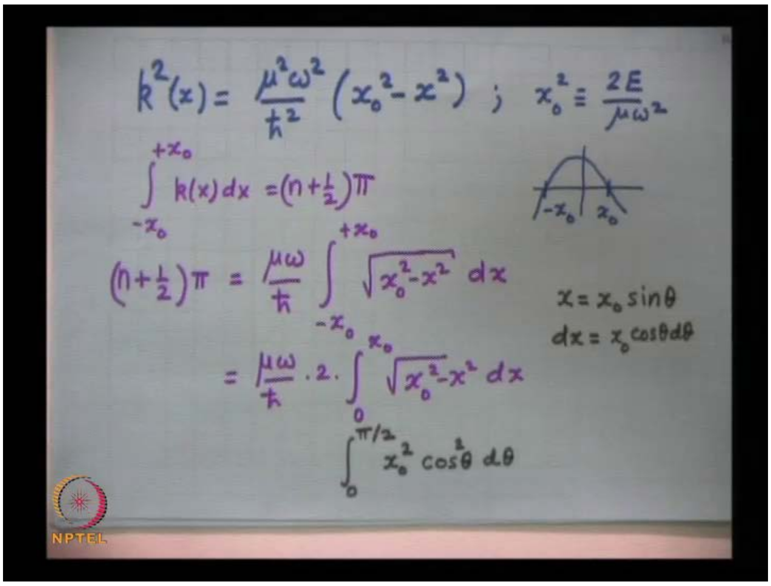

So, let me write down carefully that k square x is equal to mu square omega square by h cross square, x naught square minus x square, where x naught is x naught square is equal is defined to be equal to 2 E by mu omega square. This is the classical turning point where k square of x is 0, so that the kinetic energy is zero and the total energy is potential.

So, my eigen value condition, so the turning points are. So, the k square of x variation as you can see, it will be something like this. This will be plus x naught and this will be minus x naught. So, the eigen value equation will be from minus x naught to plus x naught, because those are the turning points, k of x d x is equal to n plus half pi. So, let me write the right hand side in the left hand side. So, n plus half pi is equal to, k of x will be mu omega by, this is a trivial integration, but let me do it, minus x naught to plus x naught under root of x naught square minus x square d x.

This is an even function of x. So, this will be mu omega by h cross 2 times, 0 to x naught, 0 to x naught under root of x naught square minus x square d x. Let me do this integral. Although, I know all of you will be familiar with this. I do this x is equal to x naught say sine theta. So, d x is equal to x naught cos theta d theta. This will be from when x is 0, this is 0. When x is equal to x naught, theta is pi by 2. So, this will be x naught square, this will be x naught outside and 1 minus sine square theta, so this is cos theta and d x is equal to x naught cos theta, so cos square theta d theta. I hope I have done it alright.

So, you can carry out this integration very, because the integration will be.

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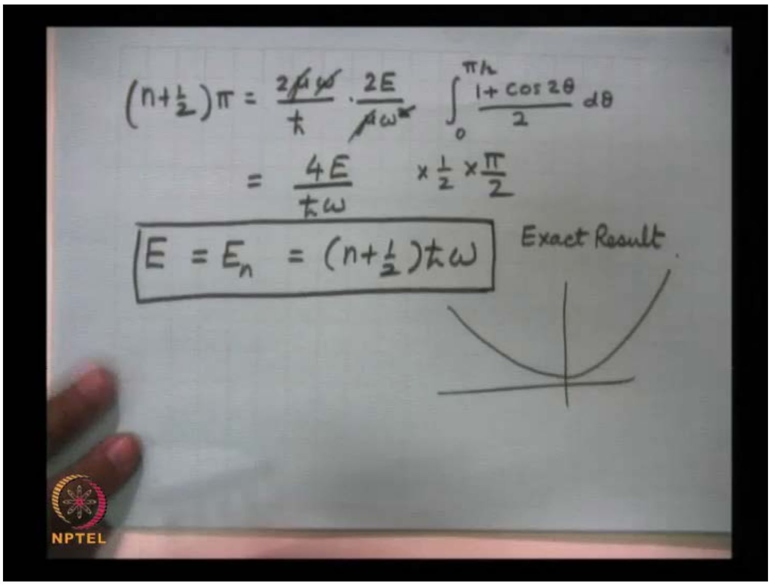

Therefore, n plus half pi, so let me do it like this, so that you can see. The n plus half pi is equal to 2 mu omega by h cross multiplied by x naught square. So, x naught square is 2 E by mu omega square, and this will be cos square theta; so 1 plus cos 2 theta, divided by 2, d theta. The second integral will come out to be zero. I leave it as an exercise. So, half into d theta, half into pi by 2, this will be into half into pie by 2. Here mu and mu cancels out and omega and omega cancels out.

This will be 4 E, 4 and 4 cancels out, therefore, 4 E by h cross omega. So, this 4 cancels out with this, pi cancels out with this. You get the result that the energy eigen values for the harmonic oscillator is n plus half h cross omega. So, we can get exact result (Refer Slide Time: 23:52). We have derived it using the Bra-Ket algebra, and also by solving the Schrödinger equation. So, we get the exact result and this is for (( )) exact result and one of the reason is that the parabolic potential, with the parabolic potential is a very smoothly varying function. So, therefore, we get very accurate result.

But, it is for (( )) that we get the exact result. So, this is the recipe for obtaining the eigen values. Let me do one more problem. Actually, we will do and this was example number one and we will do another problem, two more simple problems to tell the tricks of using the connection formulae.

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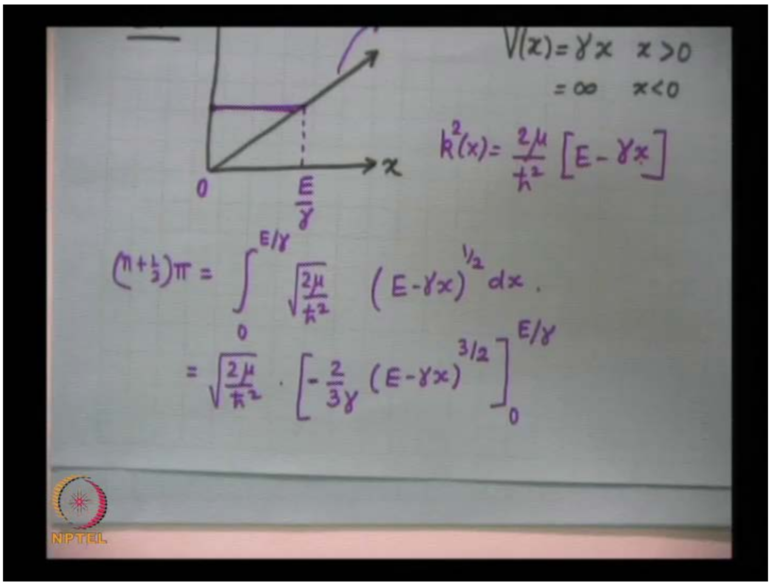

So, example number two is a linear potential. I assume a particle such that at x is equal to 0, it is infinity, and as for x greater than 0 it is equal to gamma x, for x greater than 0, and is equal to infinity for x less than 0. So, it is a triangular potential, and this is my x axis, and this is V of x. Now, I assume any value of energy. So, let me assume, E can never be negative. So, this is gamma x and this is the line. So, I assume E, where e is equal to V of x, those are the turning points. So, my k square of x will be 2 mu by h cross square, E minus gamma x.

So, one turning point is at x is equal to zero, and the other turning point is at x is equal to E by gamma. I hope this is clear. At x is equal to E by gamma k square of x is zero, and let me solve this. This is very simple. So, here k of x that is here, n plus half pi, will therefore be equal to, between the two turning points, zero to E by gamma, k of x that is under root of 2 mu by h cross square, and then e minus gamma of x raise to the power of half d x.

So, this is an equation which is extremely easy to solve. So, you have two mu by h cross square, two by three with a minus sign, because as you integrate, so E minus gamma x raise to the power of three by two, with the gamma sitting in the denominator, and this will be from zero to E by gamma. There will be a minus sign because this is a minus.

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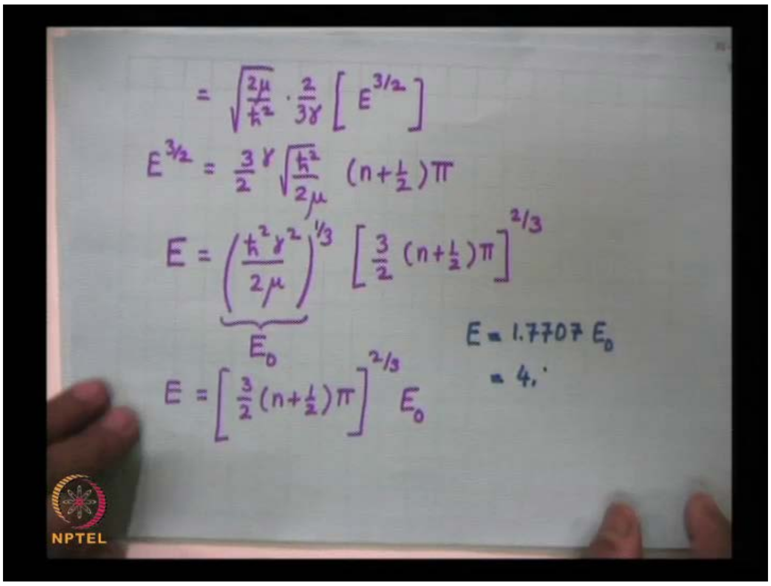

This is a very simple integration. So, if I take gamma outside, we will get two mu h cross square multiplied by 2 by 3 gamma. This is equal to and then if you take the limits, at the lower limit, it will be E, E to the power of 3 by 2, and that is it I think. So, this comes out to be E to the power of 3 by 2 and therefore, you will get E to the power of 3 by 2 is equal to 3 by 2 gamma h cross square by 2 mu n plus half pi.

So, you can put gamma square inside. So, you can write down h cross square gamma square by 2 mu, raise to the power of 1 by 3, because this is half multiplied by 3 by 2 n plus half pi, raise to the power of 2 by 3. So, these are the energy eigen values.

Now, let us suppose this (Refer Slide Time: 29:47) I put equal to E 0. So, you get E is equal to 3 by 2 of n plus half pi, whole raise to the power of 2 by 3, raise to the power of E 0. So, this is an analytical expression, and if you substitute the values of n equal to 0, you will find that E comes out to be, the allowed energy levels comes out to be 1.7707 of E 0. This is for n is equal to 0, this is n is equal to 0, then you will have 4 point 0 Let me write it down on a separate page.

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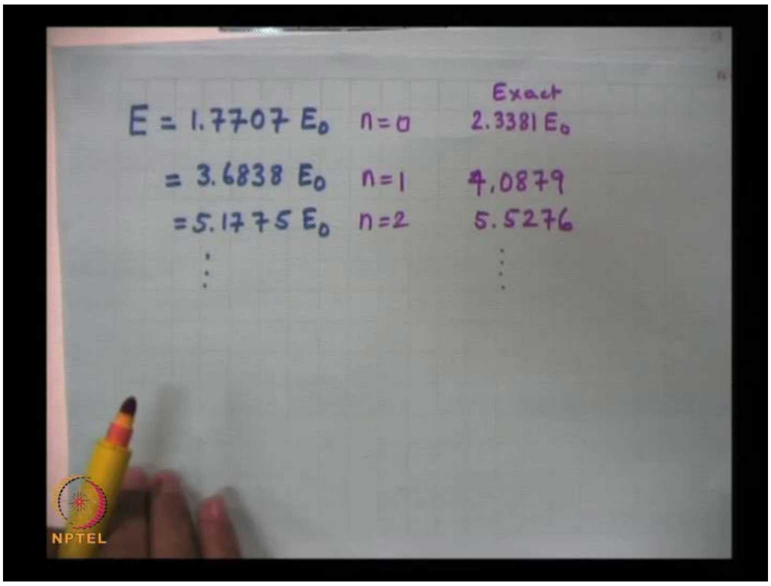

So, if you substitute n equal to 0, n equal to 1 and n equal to 2, you will get the following values. E is equal to 1.7707 E 0 and this is equal to 3.6838 E 0 and 5.177 E 0 and so on. This is for n is equal to 0, this is for n is equal to 1 and this is for n equal to 2.

This particular problem, the linear potential that I have considered, can be solved in terms of airy functions or other in terms of Bessel functions. I leave it is an exercise for those who want to do. So, you can solve it very easily with the help of airy functions. So, if I solve that problem, then the exact values comes out to be 2.3381 E 0. These are the exact and then 4.0879 and 5.5276.

So, you see that for the linear harmonic oscillator problem, you are fortunate to get good result, but here, if you compare these two numbers, this two set of numbers, this and this (Refer Slide Time: 32:32) then the agreement is not very good, and let us look at the reason why it did not work out. This is because of the fact that if we look at any potential, this is the potential then V of x is infinite here. So, from the value zero it becomes infinite.

So, there is an infinite change in the value of the potential energy and therefore, WKB approximation, you may, if you may recall was 1 over k d k by d x is less than k. So, around this region, the WKB analysis is not quite right. So, how to improve that? We say, we start thinking like this that we say that at this point V of x is infinite and therefore, the wave function must be 0. So, we think of a wave function which goes to 0 at x is equal to 0.

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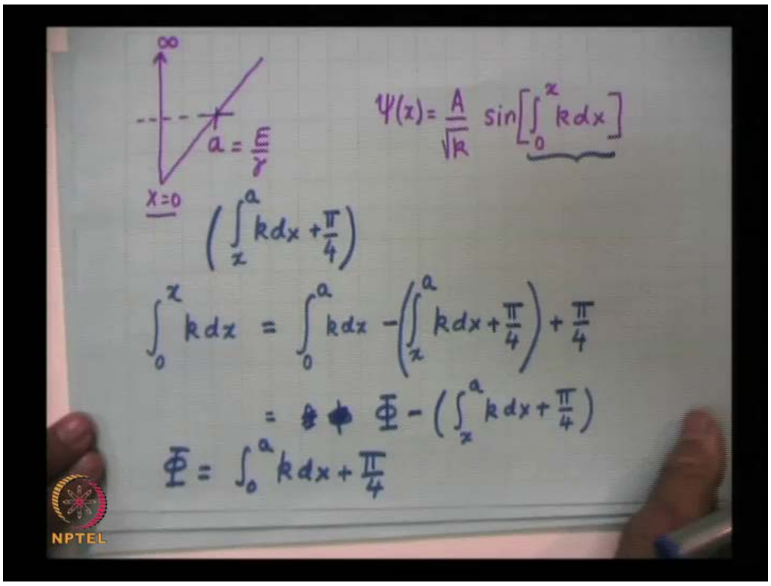

So, you have this as the potential, and you want a WKB wave function, which is 0 at x equal to 0, and that wave function is psi of x is equal to A by root k of x, sine of the, this point is 0, so 0 to x k d x. Now, this solution is therefore, vanishes at x is equal to zero. It satisfies the boundary condition at x is equal to 0. My turning point is at x is equal to a, let us suppose, which is equal to E by gamma. Now, I must put it, I must put the argument looking towards the turning point a, so the argument should be from x to a k d x plus pi by 4. This should be the argument.

So, I must write this, so that it has a term, which is equal to this, which is very simple, because 0 to x k d x is equal to 0 to a, a is E by gamma, k d x minus x to a, k d x. Then I must add pi by 4, so, I must add pi by 4 and because I have added pi by 4, so this minus pi by 4, so I must add pi by 4. So, you will have this and this will become, let us suppose this is theta. So, this is theta minus or let me put it as phi, so phi minus integral x to a k d x plus pi by 4 (Refer Slide Time: 36:39), where what is phi? phi is defined to be equal to integral 0 to a k d x plus pi by 4. Therefore, my solution will be… (No volume between: 37:03-37:14). So, the wave function is psi of x is equal to a by root k sine of this thing. So, this argument is equal to so much.

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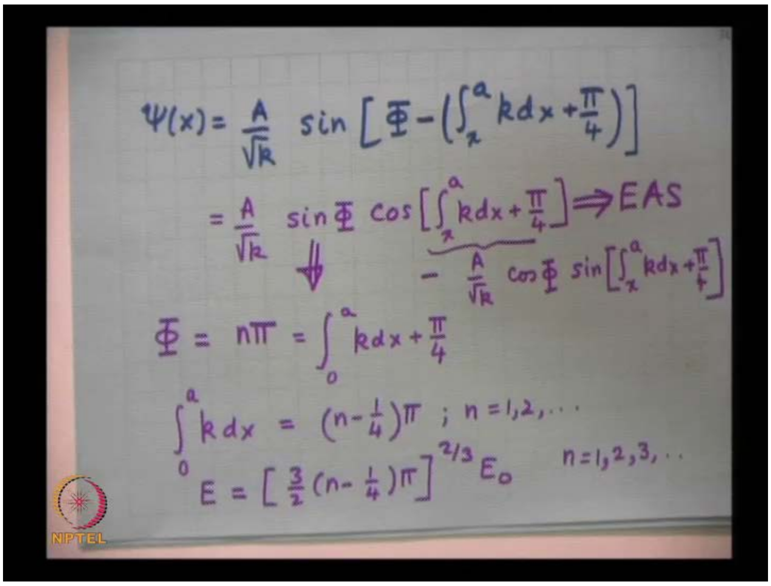

So, sine of the wave function becomes, so the wave function becomes psi of x is equal to A by root k sine of phi, this quantity, phi minus integral x to a k d x plus pi by 4. Let me align this properly. Now, this term becomes, I can write it expand the sine term. So, I get A by root k sine phi cos of x to a k d x plus pi by 4 minus A by root k cos phi sine of this term; sine of x to a k d x plus pi by 4.

Now, as we know from our connection formulae, which I had written down here (Refer Slide Time: 39:04) that it is the sine term which goes over to the exponentially decaying solution and cos whose argument is x to a k d x plus pi by 4, goes over to the exponentially undefined solution. So, this is the argument is now in the same form. So, this goes over to the exponentially amplifying solution. So, my sine phi should be zero. This should be zero; this will lead to the exponentially amplifying solution.

So, for the bound state its coefficient must be 0. Therefore, phi must be equal to n pi and what was my phi? Let me, just wrote it down, phi was equal to integral, phi was equal to integral zero to a k d x plus pi by 4. So, therefore, the eigen value equation condition will be zero to a k d x is equal to n minus 1 by 4 pi and n will of course, take 1, 2, 3 etcetera. So, it is not n plus half pi for such a problem. If you force the wave function, to vanish at the left turning point, then the eigen value condition slightly changes and so, therefore, you will have n minus 1 by 4 pi.

And therefore, corresponding energy values, you can immediately write down that instead of the previous result, it will be 3 by 2, n minus 1 by 4 pi raise to the power of 2 by 3 E 0. So, in my previous result it was n plus half pi. So, I must have n minus 1 by 4 pi

So, this is the difference in the result. Let me write it down the… If I now, in this expression, if I now put, I leave this is an exercise for you, n is equal to 1, 2, 3. So, instead of n plus half pi, if you put n minus a quarter pi, then the result will come out to be equal to (Refer Slide Time: 41:50). This is the modified JWKB result, slightly modified JWKB result and this will come out to be 2.3203 E 0, 4.0818, and 5.5172.

So, we can see now, that the results are extremely good and the only thing we did was that at the point x is equal to 0, the potential became extremely large. I make the wave function; I make the JWKB wave function go to 0. So, if you use the JWKB connection formulae with little bit of care, then as I said, as I showed you through this example it can give you very extreme, very good, very accurate results, provided of course, in between V of x does not vary very rapidly. So, if we use this method with care it is really one of the most powerful methods that is there.

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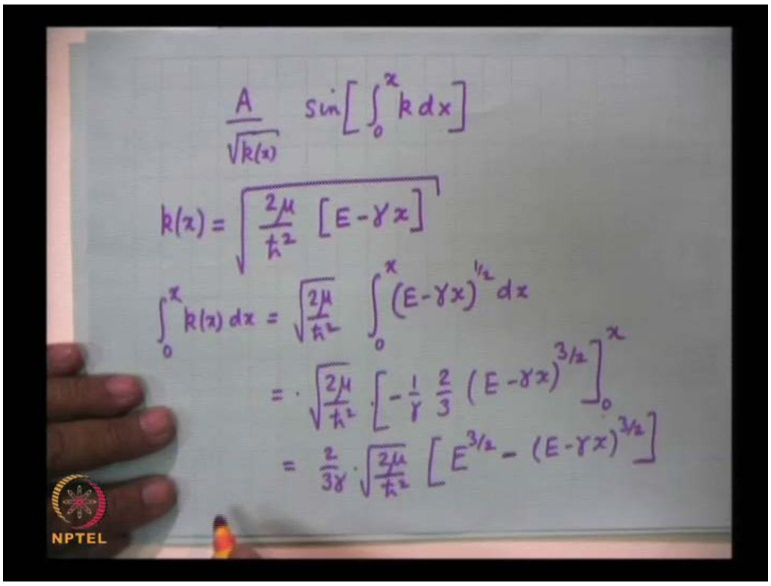

Let me conclude this part by mentioning that how to get the wave functions. The wave functions are A by root k of x, say something like sine of 0 to x, in this particular case there we make the wave function go to 0, and what was my k of x, k of x was equal to 2 mu by h cross square E minus gamma of x, E minus E minus v of x. So, k of x will be the square root of that.

This is k square of x. So, k of x will. So, integral of 0 to x k of x d x, will be under root of 2 mu by h cross square. This we had done before. So, integral of this quantity. So, integral 0 to x E minus gamma of x, raise to the power of half d x. So, once again it will be under root of 2 mu by h cross square minus 1 over gamma, 2 by 3 E minus gamma x raise to the power of 3 by 2 and so the limits are from 0 to x and you will write down say 2 by 3 gamma outside, under root of h cross square. And let me take the lower limit, because there is minus sign here. So, the lower limit is E to the power of 3 by 2, minus e minus gamma x raise to the power of 3 by 2, divided by k of x. So, divided by square root of k of x, so this will be sine of this function, let us suppose this as phi. So, sine of phi divided by under root of k x.

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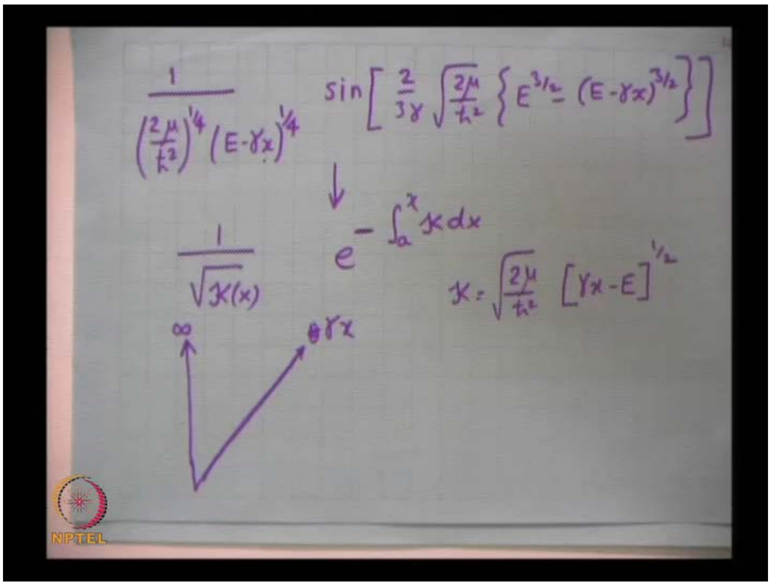

So, my wave function will be a by say 1 over root k, root k will be 2 mu by h cross square raise to the power of 1 by 4, E minus gamma x raise to the power of 1 by 4, sine of 2 by 3 gamma under root of 2 mu by h cross square and E to the power of 3 by 2 minus, whatever this is.

You can use a small program to calculate this, but, there is one point that I would like to mention, that at x is equal to E by gamma, the denominator becomes zero, and the function blows up. So, similarly, I can now use the connection formulae. So, write down the formula in terms of under root of kappa of x, and e to the power of minus say a to x, kappa of d x, and kappa is under root of 2 mu by h cross square. Now, V of x minus E, so therefore, gamma x minus E raise to the power of half and you can immediately integrate it and obtain an analytical expression, analytical expression for the JWKB solution

So, the wave functions are very easy to determine. This particular problem, as I mention to you that the potential like this. So, this is infinity and this is zero and this is gamma x. For this, in this region, I can write down the solution in terms of airy functions; a i functions and b i functions, which are related to the Bessel functions. So, for those who have not heard about the airy functions, let me mention that they are related to j 1 by 3 function. In fact, one can obtain the exact solutions of this problem.

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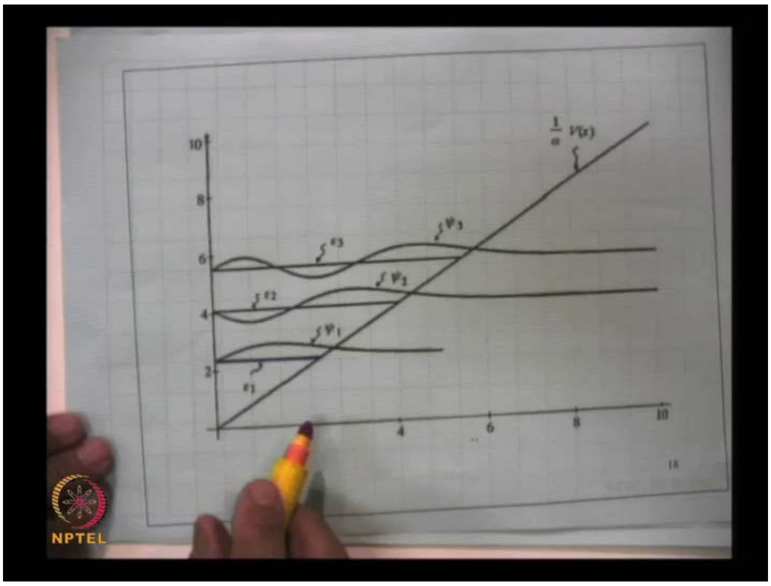

So, the exact solutions are this is the first energy level, this is first eigen function, this is the second energy level, this is the second eigen function, this is the third energy level and this is the third. Notice, that the first wave function does not have any zeroes, except the zero at the boundary, the second eigen function, this is the ground state wave function. First excited state has one zero, the second excited state has two zero and the third excited state has three zero.

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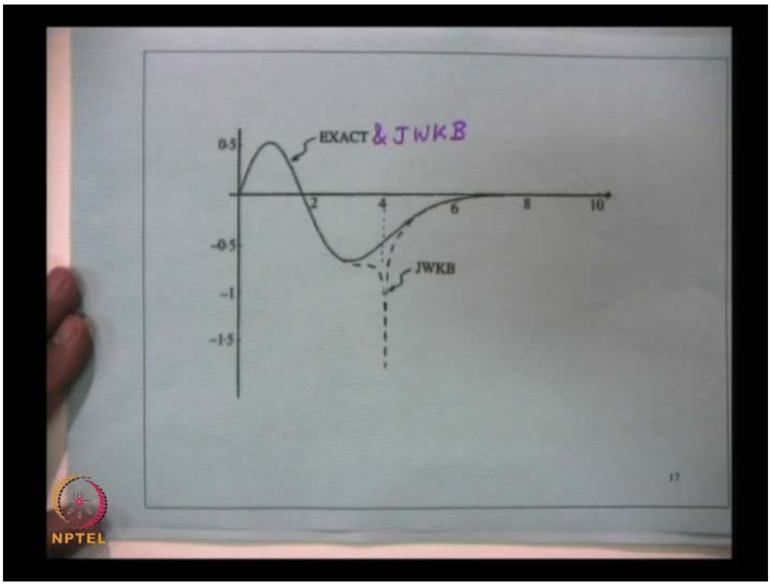

Now, using the WKB solution, the result comes out is something like this. That we had assumed the wave function to be WKB wave functions is to be 0 at x is equal to 0. So, it almost hugs the exact solution. So, this is exact and JWKB, for the linear potential, and notice only this is the turning point. This is the turning point and at the turning point, the WKB solution becomes infinity, but other than that far away from the turning point the WKB solutions are all right.

So, I hope, I have made myself clear that given the form of case V of x, you can calculate k of x; you can integrate that, and find out the approximate form of the wave function. Actually, the wave function is fairly good in agreement with wave function except at the turning point, because at the turning point, the JWKB solutions are not accurate and in fact, it goes to infinity.

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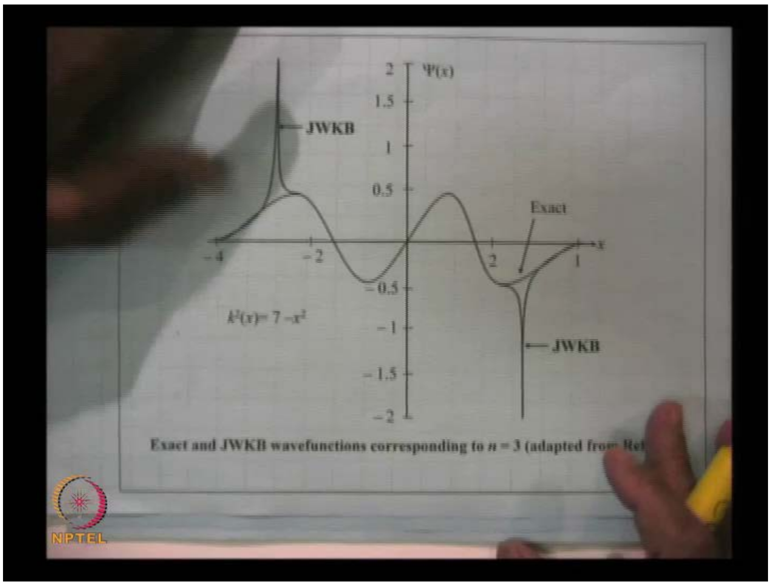

Let me also tell you that we have long time back discussed the exact solution for the harmonic oscillator problem.

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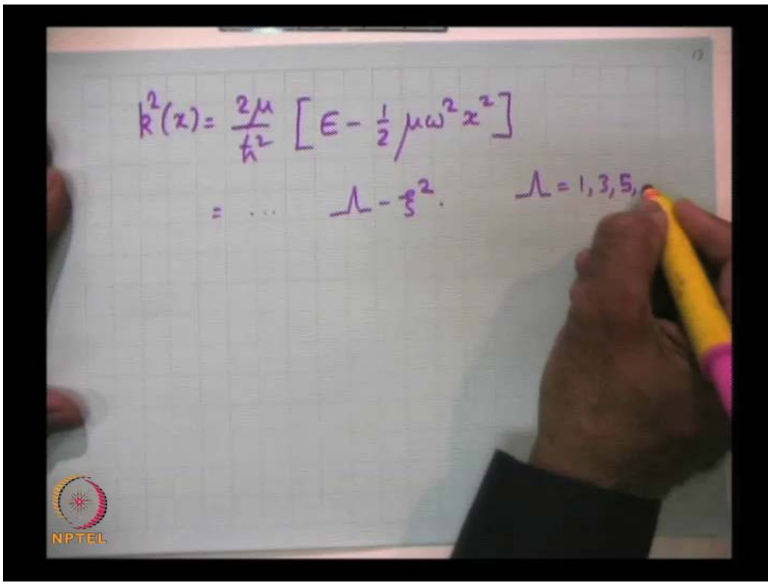

So, this is you remember for the harmonic oscillator problem, we had, let me brief you that k square of x is equal to 2 mu by h cross square E minus Vof x, so E minus half mu omega square x square. So, you can write this down in terms of dimensionless quantity, you may remember lambda minus xi square, and the eigen values are lambda is equal to 1, 3 , 5 etcetera.

So, for the 4th eigen value (Refer Slide Time: 51:03), 7 minus xi square, the exact functions are of course, the Hermit Gauss function and this is this actually h 3 of xi e to the power of minus half xi square, with some normalization constant. One can also, I leave this exercise for you, and it is done in our book on quantum mechanics on how to find JWKB solution. You can find out the JWKB solution and you will find that the JWKB solution goes to infinity at the two turning points. Otherwise, it agrees quiet well with the exact function. So, for the other, there is another this is.

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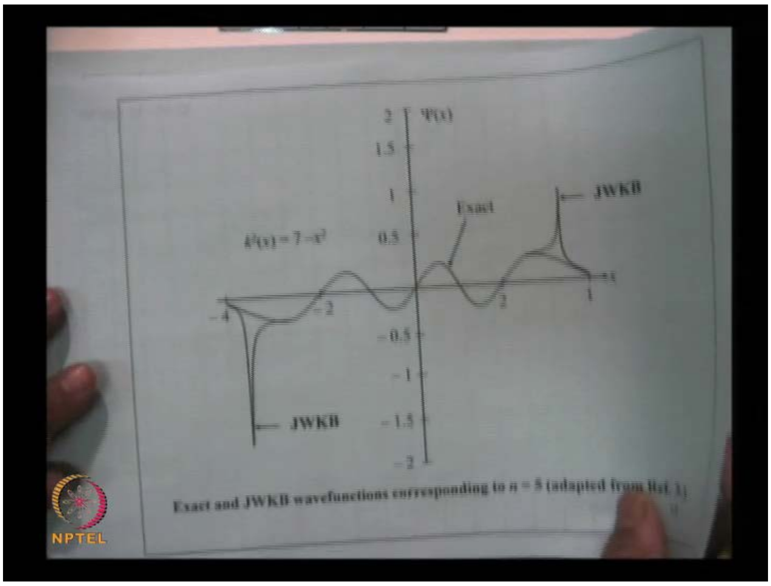

This is probably wrong, this is probably 9 minus x square and this is again for another eigen value for n is equal to 5. So, this is eleven, lambda is equal to eleven. So, it has 5 0s. 1, 2, 3, 4, 5; this is the fifth state. 0, 1, 2, 3, 4, 5, this is half h cross omega 3 halves, 5 halves, seven halves and so on. This is, a equal to 5 state, and a equal to 5 states will have 5 zeroes. 1, 2, 3, 4, 5, zeroes; this is the exact solution and this is the JWKB solution which agrees quite well with experiment, with the exact results.

So, what we have developed is a very powerful method, is a very powerful method for solving a second order differential equation, for obtaining the wave functions, and the eigen values for a smoothly varying potential.

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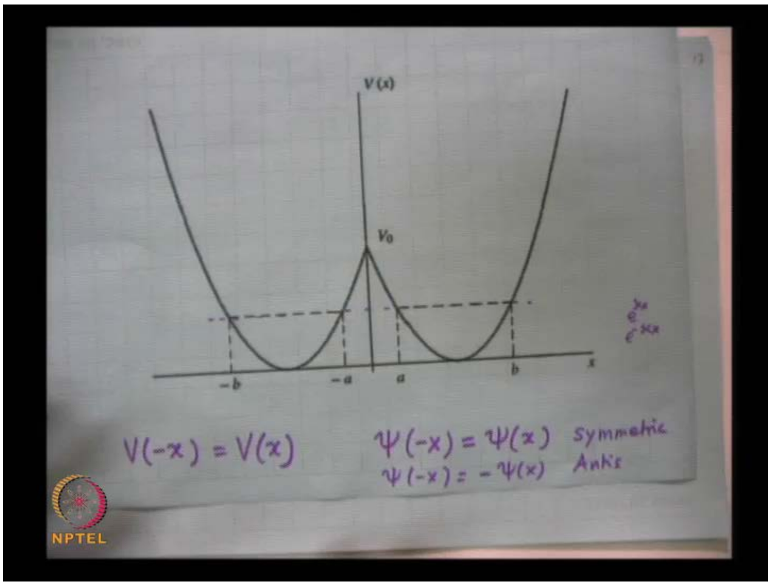

Now, I will do one more example and example 3 is for a symmetric double well potential, symmetric double well potential. Now, in which you have a potential energy variation, which look like this. It is symmetric about, such type of potential are of extremely important in molecular physics and even in other areas.

So, we will use the WKB methods, the JWKB formulation that we have found out to solve such a problem. Since, V of x is a symmetric function of x that is V of minus x is equal to V of x. Therefore, my wave functions are either symmetric or anti-symmetric. So, either psi of minus x is equal to psi of x or psi of minus x is equal to minus psi of x. So, this is a symmetric function of x or an anti symmetric function of x.

Now, let us suppose, I assume this as the energy eigen value. Now, in this region, the potential energy is greater than the total energy. So, k square is negative and if therefore, k square, I should write as minus kappa square, if I take this to be a constant, and I can write the solution as e to the power of plus kappa x or e to the power of minus kappa x.

Alternatively, in this region, if I assume a symmetric solution, it will be either cos hyperbolic kappa x or sine hyperbolic kappa x. So, we will either start with, if we discuss the symmetric solution, we will start with the cos hyperbolic function. if I start with If I discuss the anti symmetric solution, then I must use the sine hyperbolic solution. I will consider one of them and leave the other as an exercise for you. So, with that we end this lecture and we will continue with this point onwards in my next lecture. Thank you