Basics Quantum Mechanics

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Module No. # 03
Linear Harmonic Oscillator-1
Lecture No. # 04
Linear Harmonic Oscillator (Contd.)

We continue our discussions on the linear harmonic oscillator problem, and hopefully we have been discussing the harmonic oscillator problem from quite some time now, hopefully today we will be able to write the final result, and the complete solution of the one-dimensional Schrodinger equation corresponding to the linear harmonic oscillator problem.

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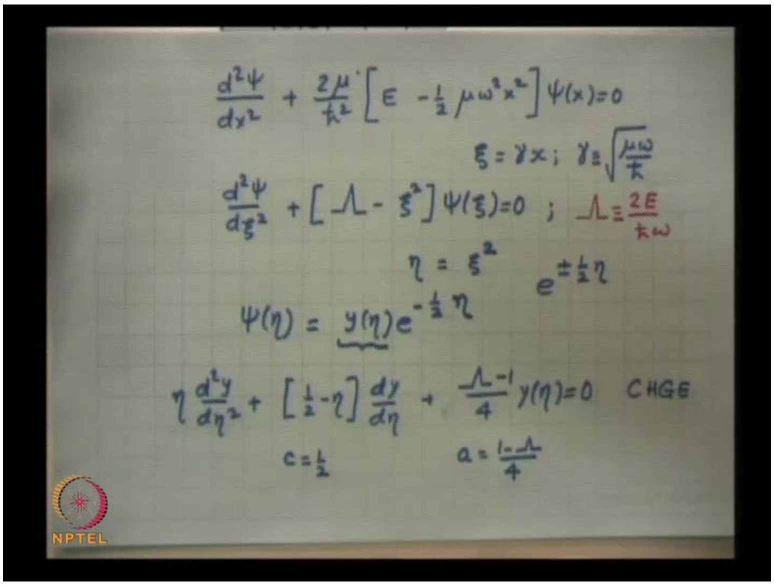

So, we start with the Schrodinger equation and as we all know that they Schrodinger equation. So, let me just summarize everything; 2 psi by dx square plus 2 mu by h cross square, I am sure that all of you are familiar with this now, half mu omega square X square psi of X is equal to 0.

So, we make a transformation psi is equal to gamma X, where gamma is equal to mu omega by h cross, if you do that the above equation becomes d 2 psi by d xi square, in terms of the new independent variable, plus lambda minus xi square psi of xi equal to 0. where lambda is equal to where the capital lambda is equal to 2 E by h cross omega.

Actually I should write the defined to be equal to this is also defined to be equal to gamma is defined to be equal to the omega, then what we did was first we had defined this independent variable eta, which is equal to xi square, we wrote down that equation, and then we found that the large xi value, large xi behavior is form of e to the power of plus minus half eta.

So, we said that psi of eta was equal to y of eta e to the power of minus half eta, and then we determine the equation that is satisfied by y of eta, and we found that the equation that is satisfied by y of eta, is given by eta d 2 y by d eta square plus half minus eta half minus eta dy by d eta plus lambda minus 1 by 4 y of eta is equal to 0.

So, this is the confluent hyper geometric equation, and the parameter c is the half, and the parameter a is 1 minus lambda by 4, now because this is confluent hyper geometric equation we said and because c is equal to half, the two independent solutions are y of eta, and so therefore psi of eta psi of eta is y of eta, multiplied by e to the power of minus I eta, and eta is I square. So, this we did in the last lecture carefully.

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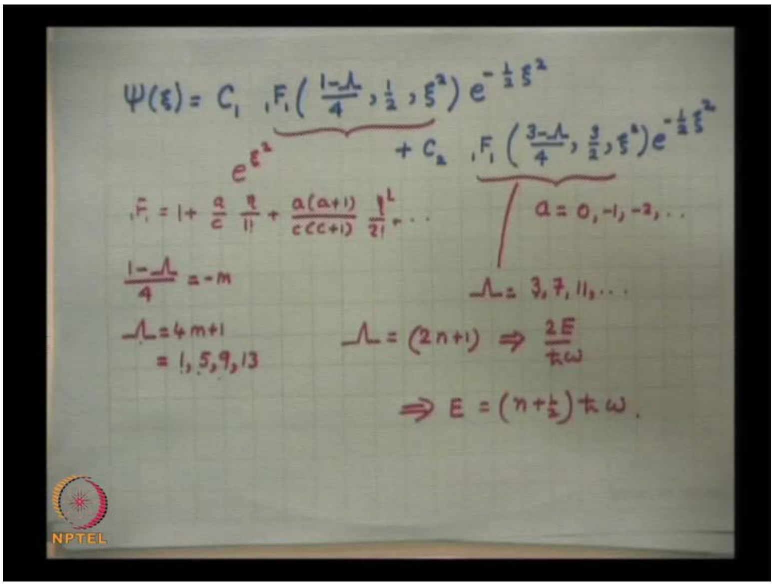

So, the psi of xi these the two solutions are C 1 this the 1 constant, F 1, 1, a that is 1 minus lambda by 4, c is half, tome xi square, and then e to the power of minus half eta. So, e to the power of minus half xi square, this is the first solution and both are represent convergent series, plus C 2, F 1, 1, then a minus c plus 1, then a minus c plus 1, if you do that this will become 3 minus lambda by 4, 2 minus c; c is half.

2 minus c that is 3 by 2 into xi square e to the power of minus half xi square. So, we said that this series although it is convergent for all values of xi, but it behaves as e to the power of xi square.

So, for the wave function to be integrals to be well behaved this must become a polynomial, and if you recall the F 1, 1, function was 1 plus a by c into eta by factorial 1 plus a into a plus 1 into c into c plus 1 eta square by factorial 2 etcetera.

So, this can become sorry let me write it down this will become a polynomial only when a is 0 minus 1, minus 2 etcetera. So, when 1 minus lambda by 4, becomes equal to minus m, that is lambda is equal to 4 m pus 1, that is equal to equal to 1, 5, 9, 13 only for these values of lambda this becomes a polynomial.

Similarly, in this case this will become a polynomial only when lambda becomes 3, 7, 11 etcetera. Now, let me we had done last time that lambda equal to 1, so therefore I can you can see that lambda can takes values 1, 3, 5, 7, 9, 11, 13 so lambda will take only odd integers, this will imply lambda is equal to 2 E by h cross omega, so this implies that E is equal to n plus half h cross omega. Now, let me write down these two solutions again, so the we had consider lambda equal to 1, let me consider lambda equal to 3.

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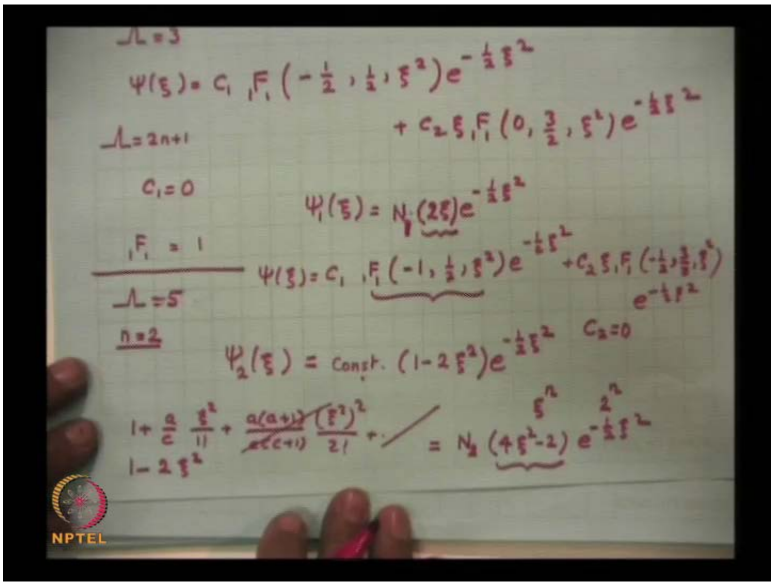

So, let me consider lambda equal to 3, then what will happen is psi of xi will become C 1, this will become F 1, 1, if lambda is 3 1 minus 3 by 4, that is minus 2 by 4.

So, this will become minus half half xi square e to the power of minus half xi square plus C 2 and this will be if lambda is 3 this is 0, there is a xi here there is a xi here because eta raise to the power of 1 minus c eta rest to the power of 1 minus c; c is half, so eta to the power of half eta is xi square, so there is a xi sitting there, so C 2, xi, F 1, 1, if lambda is 3, then this becomes 0, comma 3 by 2, into xi square, e to the power of minus half xi square.

Now, this series is an infinite series, so we must have C 1 is equal to 0, and the wave function will be at this will be F 1, 1, if a is 0, then that is only 1. So, the solution is or the Eigen value psi 1 of xi, is equal to some multiple of xi e to the power of minus half xi square.

The coefficient I will come back to that in a moment, actually I will put here a factor n's of 2 n's of one which is the normalization constant, and I will put a factor of 2 which will become clear in a moment.

Let me go beyond this, let me do one for lambda equal to 5, lambda is equal to 5 and as you can see I go back to the solutions again, so you will have psi of xi, please see this C

1, 5 means 1 minus 5 is minus 4, minus 4 by 1 is F 1, 1; F 1, 1. minus 1, half xi squaree to the power of minus half xi square plus C 2 xi F 1, 1.

Now, this is lambda is 5, so 3 minus 5 by 4, that is minus 2 by 4, is minus half 3 by 2 xi square, and e to the power of minus half xi square. So, if you see that this is a polynomial, but this is not. So, I must choose C 2 equal to 0, and so therefore the wave function will be if I write lambda is equal to 2 n plus 1, then n here is 2, so I write psi 2 of xi is equal to some constant, some constant and you remember that F 1, 1 function was 1 plus a by c xi square by factorial 1 plus a into a plus 1 into c into c plus 1 xi 4 by factorial 2 xi square whole square by factorial plus 1.

But a is 1, so this term and the remaining terms all vanish, a is 1 and this is half, so this becomes a 1 minus 2 xi square, so this becomes 1 minus 2 xi square e to the power of minus half xi square.

I choose the constant here, such I multiply this by a factor such that the coefficient xi square, xi to the power of maximum, the maximum power n, in this case xi square, the coefficient is 2 to the power of n, so I multiply by 2 and divide by 2, actually minus 2 if I multiply this by minus 2 this becomes constant which I write as n 2.

You see if I multiply this by minus 2, then it will become 4 xi square minus 2 e to the power of minus half xi square. This quantity is the hermit polynomial h 2 of xi h 1 of xi is 2 xi, let me do one more.

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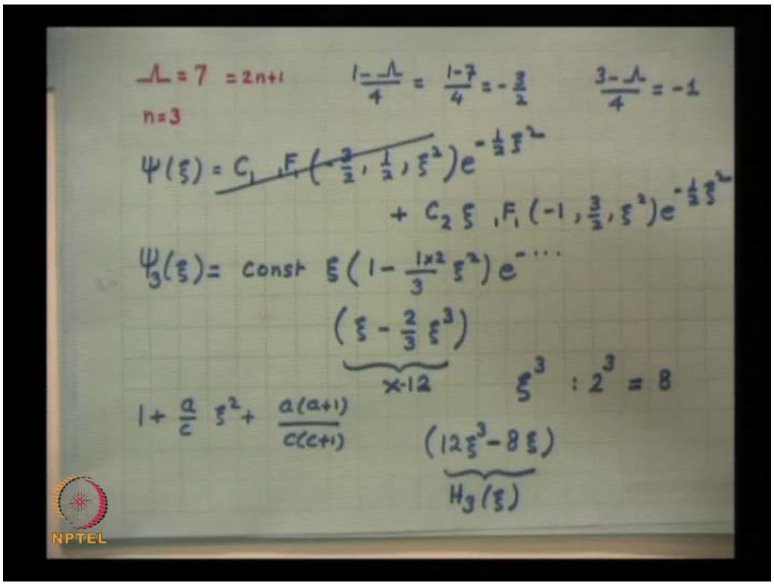

Let me do one more and that is lambda is equal to 7, lambda is equal to 7, so lambda is equal to 2 n plus 1, so n is 3, so this is the 3rd wave function. So, what is my psi of xi, so you will have 1 minus lambda by 4, this will be equal to 1 minus 7 by 4, so this is minus 6 by 4, so that is minus 3 by 2, and 3 minus lambda by 4, will be 3 minus 7 by 4, which is minus 1.

So, I will obtain I will obtain the solution as psi of xi, please see this let me put the solution here, so that you can see for yourself, psi of xi is equal to C 1 F 1, 1, minus 3 by 2 half xi square e to the power of minus half xi square, plus C 2 xi, F 1, 1, and this will become minus 1, minus 1, 3 by 2 xi square, e to the power of minus half xi square. So, this is not this can this is an infinite series, so it will behave as e to the power xi square, and so therefore the function will blow up, therefore we must take C 1 equal to 0.

So, this function will be removed, so my psi 3 of xi, will be a is minus 1. So please recall that my infinite series is 1 plus a by c into xi square plus a into a plus 1, so this will cancel out this will be 0, c plus 1 this will be 0, and you will have some constant, xi into 1 plus a, a is minus 1, so minus 1 divided by 3 by 2, that is 3 into 2 xi square into e to the power minus this thing.

If I multiply this out, so I will get xi minus 2 by 3 xi cubed, the highest power of xi is xi to the power of 3, and I want its coefficient to be 2 to the power of 3, so 8, 2 to the power of 3 is 8. So, I multiply this by 12, if I multiply this by 12 actually minus 12, so what will happen is 2 into minus 12 minus 24, divided by 3 is 8, and this is minus, so you get 12 xi cubed, minus 8 xi, this is the 3rd hermit polynomial. Similarly I will just tell you the if I do for lambda is equal to we have done for 7.

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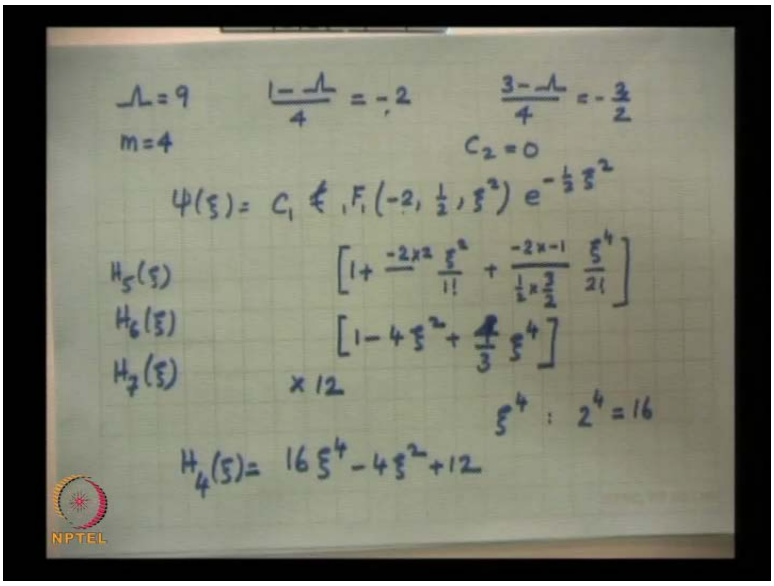

So we have lambda is equal to 9, lambda is equal to 9 means m is equal to 4, so you have 1 minus lambda by 4 is 1 minus 8 by 4 is minus 2. And 3 minus lambda by 4 is 3 minus 9 is 6 minus 2 by 3, something like 3 by 2 something like that.

So, once again since this since this becomes minus 2, this series will become a polynomial, this series is not, so you take C 2 equal to 0, and you will have the solution as psi of xi, is equal to C 1, sorry F 1, 1, minus 2 half xi square, this is a polynomial. So, if you can see that please see this sorry this is a, this is c, so what will be my polynomial 1 plus a, that is minus 2 by c, that is 1 by 2, 1 by 2, xi square by factorial 1, so 1 minus 4 xi square, then plus a into a plus 1, so therefore minus 2 into minus 1 divided by c into c plus 1 half into 3 by 2 divided by multiplied by xi 4 by factorial 2.

Next term will be a into a plus 1, into a plus 2, but a plus 2 is 0, so that term will not be there and all subsequent term will vanish. So, you will have 1 minus 4 xi square plus 2 2 into 2 into 2 that is 8. I hope I have done it correctly 8 by 3 divided by 2, that is that is 6, 2 this will become 4 by 3 you do have to do by patiently, 4 by 3 xi 4.

Now, I want the coefficient xi to the power of 4 to be 2 to the power of 4 equal to 16. So, I multiply the whole thing by 12, if I multiply by 12 so I will get 16 xi 4, minus 48 xi square, plus 12 H 4 of xi.

In fact, you ask me to evaluate any hermit polynomial unless it is too big, I know the fact that in any hermit polynomial there are either even powers or odd powers, and by because I remember the confluent hyper geometric function, I can immediately write the polynomial within a multiplicative constitute and I choose multiplicative constant such that the power of xi to the power of n, is 2 to the power n. So, I leave it is an exercise to for you to find out what is H 5 of xi, what is H 6 of xi please do this.

And this will help you to understand the solution the H 7 of xi is worked out at the book and I would like you to find out what are H 5 of xi, and H 6 of xi, the final solutions of harmonic oscillator problem.

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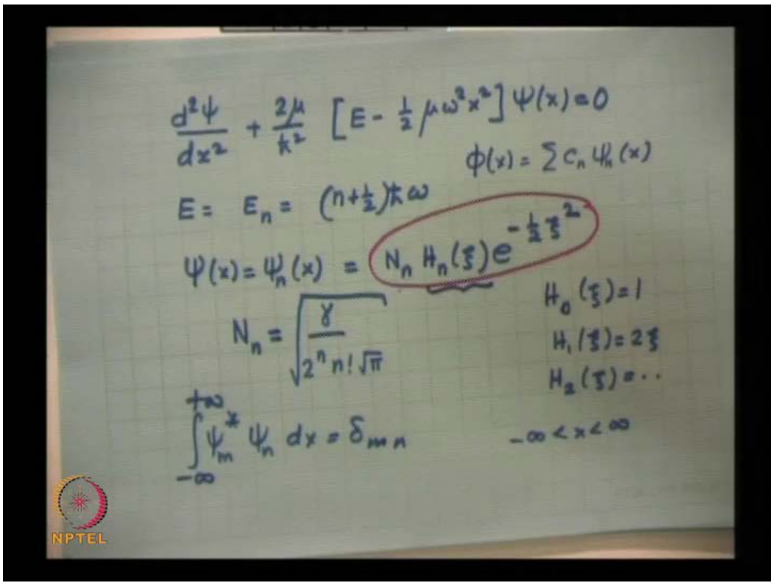

Is therefore that the solution is once again my Schrodinger equation is d 2 psi by dx square plus 2 mu by h cross square E minus half mu omega square X square psi of X is equal to 0, well behave solution, well behave site.

Solutions of this equation exist only when the Eigen values of the problem are E is equal to n plus half h cross omega, and the corresponding wave functions are psi of X is equal to psi n of X, is equal to .N’s of n H of n of psi e to the power of minus half xi square, when H n of psi are the hermit polynomials, some people call it hermit polynomials H 1 of xi is 2 xi, H 2 of xi we have found out and H 3, H 4 I have actually found out all hermit polynomials up to H 4 of xi.

The normalization constant that of course it takes a little bit algebra you have to use the generating function. So, that is gamma so you must remember this 2 to the power of n; n factorial square root of pi, based in the normalization constant. So, you will have psi n star psi n dx, is equal to delta m n, and this set of functions all are extremely important and in the domain from minus infinity less than X less than infinity it is a complete set of function.

This form a complete set of functions, and any well behaved function any well behaved single behaved function can be expanded in terms of this function, that is any wave function any function phi of X can be expanded as c n of x. So, there is completeness condition also. So, that really completes one of the most important and one of the most beautiful problems in quantum mechanics, and that is the linear harmonic oscillator problem.

So, now we have done we have obtained exact solutions of the Schrodinger equation for 3 problems the first problem was.

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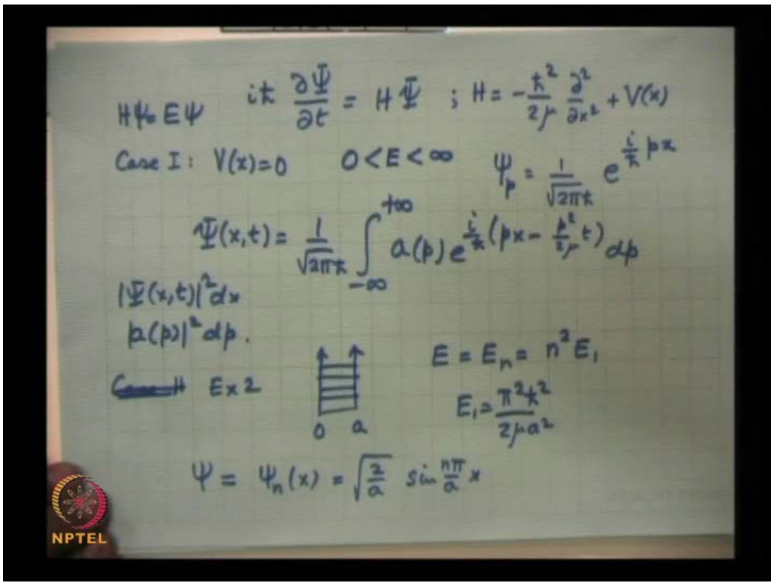

So, we have obtained my time depended Schrodinger equation is i h cross delta psi by delta t, for the 1 dimensional problem h psi, and h is equal to minus h cross square by 2 mu delta 2 by delta X square plus V of x.

So, in the first case one we had obtained we consider the free particle problem, we found all values, so the Eigen value equation is h psi is equal to E psi, we found all solutions, all values of E to valid these are actually the continuum solutions, and what are the wave functions psi p is equal 1 over under root of 2 pi h cross e to the power of i by h cross p x.

And what is the most general solution I have psi of x t is equal to is equal to because this are continuum solution, so 2 pi h cross, minus infinity to plus infinity a p e to the power of i by h cross p x minus e t , that is p square by 2 mu t dp, and psi x t mod square dx, represent the probability of finding the particle in the space dx, between x and X plus d x.

Similarly, a p mod square dp is the probability of finding the particle, and then even find out the expectation values and things like that, then we consider the second example actually it is example two example two the particle in a box problem, there we have a set of infinite number of discrete energies n square of E 1, where E 1 was equal to pi square h cross square by 2 mu a square.

The particle was confined between the region 0 less than a, these are the complete set of functions and we have found that the wave functions were psi of X is equal to psi n of X, and this must be equal to 2 by a sign of n pi by a X, this form a complete set of wave functions in the domain 0 to a, and these are the Eigen values.

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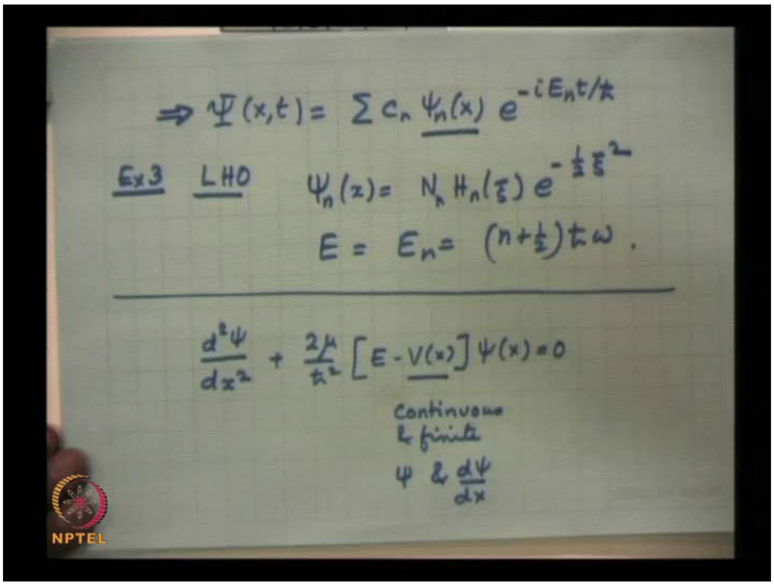

And the most general solution of the Schrodinger equation will be psi of X t, as I have tried to demonstrate through the software psi psi n effects, e to the power minus i E n t, even for the linear harmonic oscillator problem you have you obtain and infinite number of discrete Eigen function just as particle in a box problem.

You obtain an infinite number of discrete states, the only thing is my psi n of the 3rd example that we worked out, I am working out for last 2, 3 days will be was the linear harmonic oscillator problem, in which the in which the psi n of x, was the normalized hermized gauss function, h this thing and the corresponding Eigen values also we have found out n plus half h cross omega.

So, these are wave functions and ah the Eigen values energy Eigen values and then we said that even the classical oscillator the classical pendulum that you see in first year laboratory that corresponds to the superposition of different states, and the solution corresponding to that is described by this particular equation.

Now, in the following 1 or 2 lectures we will discuss one more aspect, but before that let me mention one that if there is a if i try to obtain the solution of d 2 psi by dX square plus 2 mu by h cross square E minus V of X psi of X is equal to 0.

Then if V of x is continuous and finite everywhere that is thus is continuous and finite then psi and d psi by X, must necessarily be the continuous everywhere, must necessarily be continuous everywhere and the proof of this is very simple.

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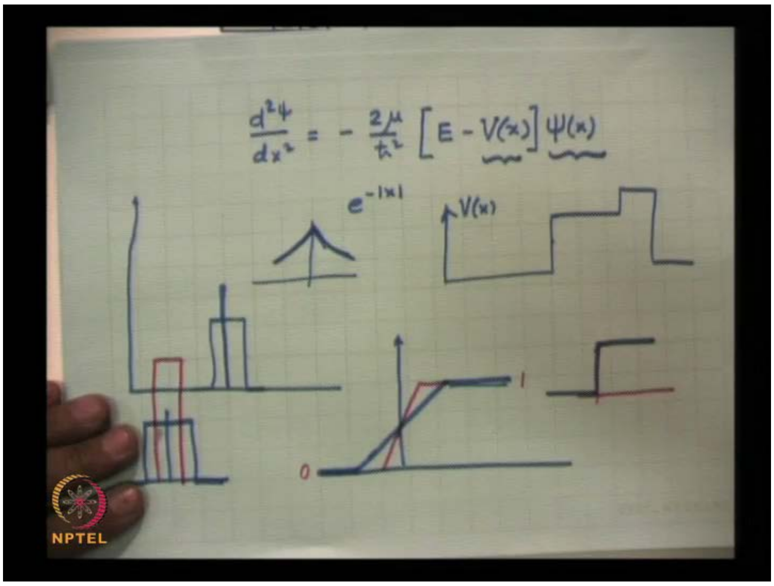

Let me rewrite this equation as like this d 2 psi by dX square, is equal to minus 2 mu by h cross square E minus V of x psi of x, let us we are assuming that V of x is continuous and finite, it can have a discontinuity for example, V of x can may be like this like this like this like this like this like this like this can be the variation of V of x, it can have discontinuities but the value is finite.

Now, you may recall that we have told you right in our first lecture the deduct delta function was the limiting form of the rectangular function, so it is a spike it is a rectangle with an unit area, the width is extremely small, the height is extremely large, so that the product is finite.

Now, we remember that we consider we have consider another function which is the rand function, that is the function is constant and then it has a constant value, the derivative of this function if you plot this is 0, this is constant, this is 0 so it is something like this. So, the derivative of the rand function we had shown this to be a rectangle functions.

Now, let us suppose this value is 0, this value is 1, let us suppose I make this rand stepper, I had discussed this in great detail, so this will become sharper in the limit this becoming a step function the derivative is a delta function, and the delta function the value of the function at that point is infinity.

So if there is a discontinuity in the function, if a function let us suppose I have the unit step function which looks like this is derivative its delta function here, its derivative is infinite here, so let us suppose we assume that the wave function is continuous but its derivative is not something like this we had consider this also.

I have wave function like this, something like e to the power of minus mod X, then at X is equal to 0, it has 1 value here, but the derivative here, and derivative here, are discontinuous.

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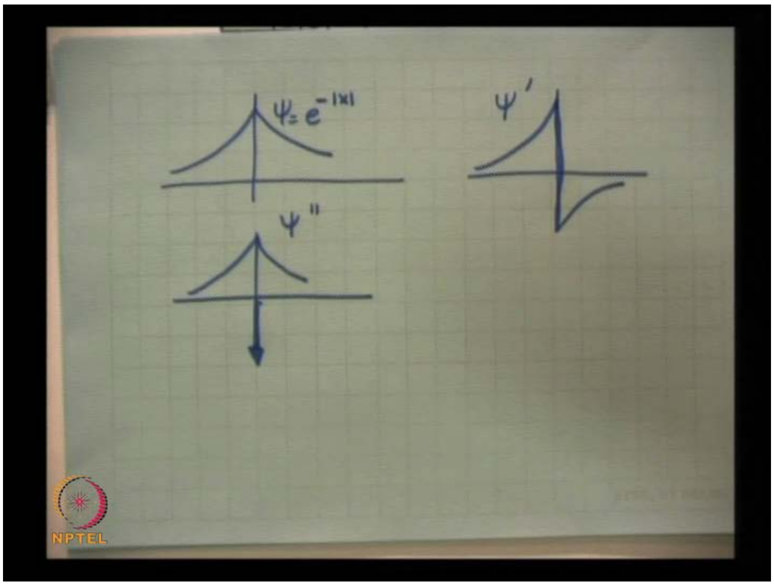

So, let me plot this carefully I have done this before that if you plot e to the power of minus mod X, so it will be something like this, this is e to the power of minus mod X, if you plot (( )) this is psi, if you plot the wave function and the derivative of the wave function, so it will have a discontinuity and so therefore this is double psi prime, and the double derivative psi double prime, will be like this only, but at this point they will be the value will be infinite, because there is a infinitely negative derivative here, this a minus jump.

So therefore, if the derivative is discontinuous then the double derivative has the delta function.

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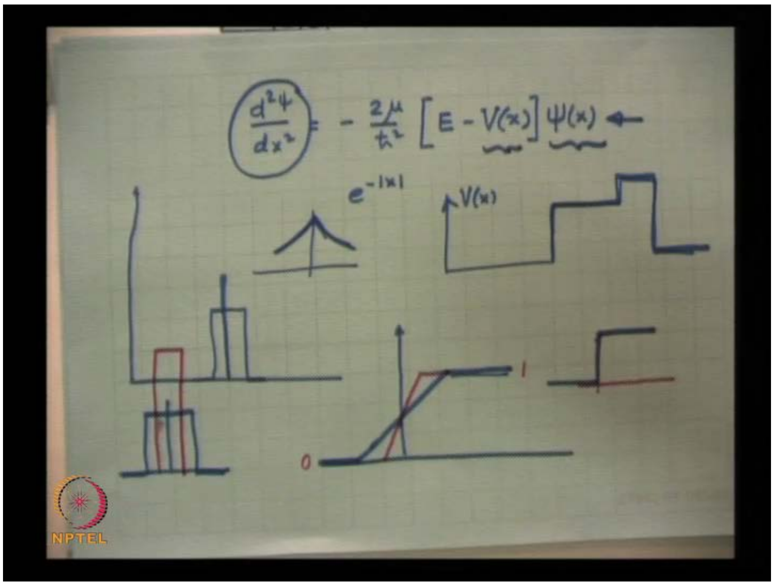

So, we come back to this equation and we say let us supposed psi of x is discontinuous, but d psi by dx is not discontinuous, d psi by dX is psi of x is continuous, but its derivative is not.

So, then this is finite and continuous this is finite and continuous, so the right hand side is finite and continuous, but the double derivative was just continuous, so that is not possible, so derivative have to be continuous, an n fact, if the wave function is discontinuous then its derivative is discontinuous, and its double derivative is more discontinuous,

So, therefore if V of x has a step discontinuity, a step discontinuity then the wave function has to be continuous at this discontinuity, and its derivative also have to be discontinuous has also be to continuous, I am sorry. So, the very fact the psi of x and d psi by dx are continuous, is a consequence of fact that the psi of x satisfies a second order differential equation.

With this introduction I start on a different class of solutions, and that is let us suppose that there is a free particle approaching a potential step I will try to calculate the probability of reflection and transmission.

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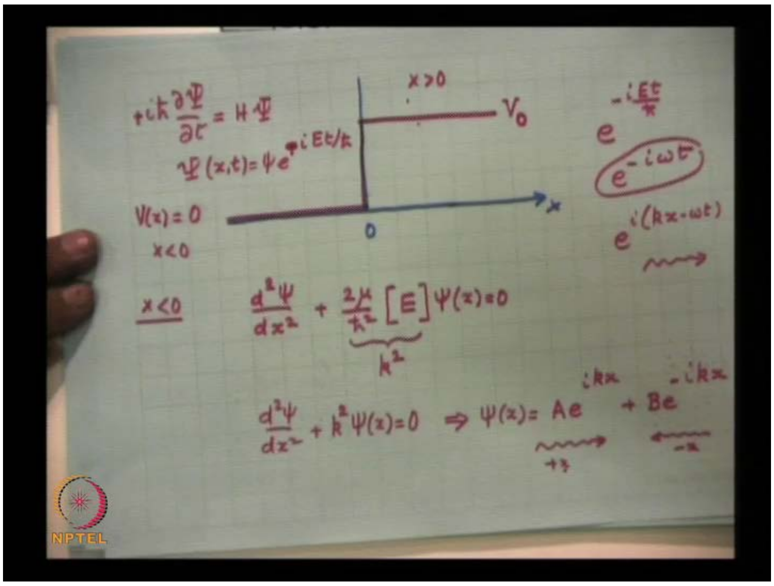

So let us suppose that at x is equal to 0, this is my x axis, and this is the origin, at x equal to 0, there is a step potential like this, so V of 0, V of x is equal to 0, for x less than 0, and V of x let us suppose V 1, for x greater than 0, this is the domain, sorry I will write this as V 0. I will write this as V 0

Now, a particle is approaching particle like electron, or a proton, or a neutron with a certain velocity. So, therefore, the solution the Schrodinger equation in this region for x than 0, the solution of this the Schrodinger equation in this region is d 2 psi by dx square plus 2 mu by h cross square, E minus V of x, but V of x is 0, in the region X less than 0.

So, my Schrodinger equation becomes like this, this I put equal to k square, so i obtain d 2 psi by dx square plus k square, psi of x is equal to 0. I can write the solutions in terms of plain waves, so I can write it down psi of x is equal to A, into e to the power of i k x plus B into e to the power of minus i k x.

Now, this represents a plain wave propagating in the plus x direction, this represents a plain wave propagating in the minus x direction, I would like you to think for a moment why doers this term represent a wave propagating in the plus x direction, and y does this term represents a wave propagating in minus the x direction.

May be most of you are familiar aware of that the reason that this is because in quantum mechanics as you know that the time dependence we have taken to be equal to minus i E t by h cross, so if I replace E by h cross omega, so the time dependence of wave function is e to the power of minus i omega t, because of that this term this complete term it becomes e to the power of i k x minus omega t, so this is a wave propagating to the plus x direction.

If in quantum mechanics this was taken to be plus sign here, plus sign here then this could have maintain wave propagating in the this minus x directions, the question is in quantum mechanics could I have chosen that of course could have the entire quantum mechanics could have remain the same.

I would have been replaced by minus i, that is it, but since in all you see the Schrodinger equation s give by i h cross delta psi by delta t, excuse me is equal to h psi, so I assume a method of separation of variable and I find that psi of x t, is psi of x e to the power of minus i E t, if a minus sign would have been chosen then it would have been become plus i E t, but since convention is it is a plus sign here, so there is a minus sign here, and the time dependence is of the form of e to the power of minus i omega t.

So, in the region x less than 0, I have 2 waves, 2 terms, the first term representing a wave propagating towards the barrier and of course there is a reflection by this barrier which is represented by B.

Now, I want to write the solution in the seconds region then the first question you are going to ask me is the total energy less than (( )) 0 or greater than (( )) 0, we will consider both the cases we first consider the case where x is greater than 0 sorry E is greater than B 0.

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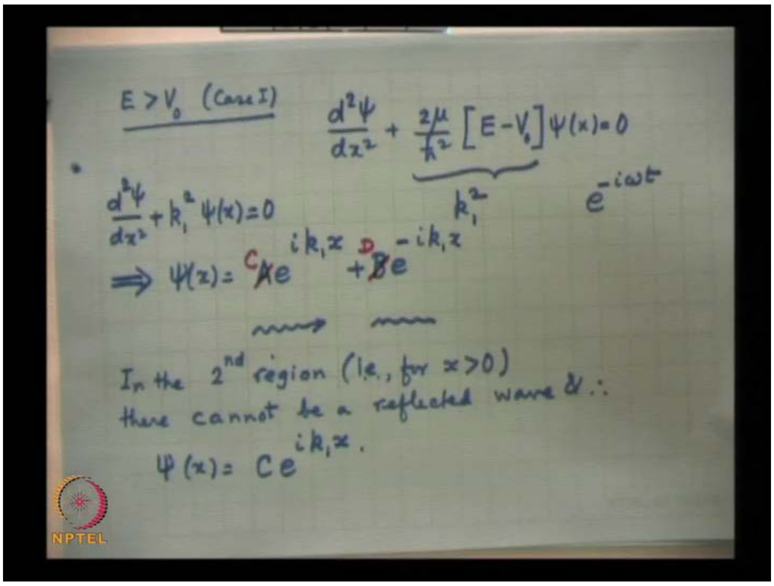

So, you will have let me have E greater than case 1, so this is my case 1, and the case 2 will be E less than B 0. So, my solution is d 2 psi by dx square, then the Schrodinger equation 2 mu by h cross square, E minus V 0, psi of x is equal to 0, this I represent by k 1 square, so my equation becomes d 2 psi by dx square, plus k 1 square, psi of x is equal to 0.

Again I will have 2 solutions psi of x is equal to a, e to the power of I k 1 x plus B e to the power of minus i k 1 x, and as I mention before because the time dependencies is of the form of minus i omega t, this term represents a wave propagating to the right, and this term actually since I have use A and B earlier so let me replace this by C and D, I am sorry C and D, I have used A and B for this in the solution corresponds to x less than 0.

Now, a wave is propagating in this direction, and this potential extends to infinity, so there is no reason why there should be a reflected wave here. So, therefore we can write that in the second region in the second region that is for x greater than 0, there cannot be there cannot be a reflected wave, and therefore the solution is given by psi of x is equal C, e to the power of I, k 1 x.

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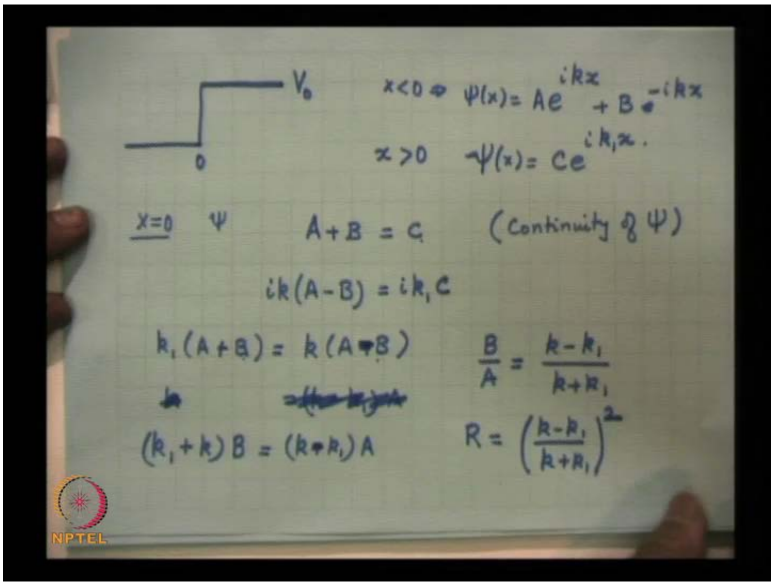

So, therefore let me write down the solutions in the 2 parts, I have this barrier, this is V 0, this is x equal to 0, for X less than 0, you have psi of x is equal to A to the power of i, k x plus B into e to the power of minus i k x, and for x C greater than 0, you will have psi of x is equal to C into e to the power of i k 1 x.

At X is equal to 0, psi should be discontinuous as I have discussed just now, and the derivative also has to be discontinuous, derivative also has to be continuous. So, you will have at X is equal to 0, the wave function is A into e to the power of i k x, plus B e to the power of minus i k x, at x is equal to 0, it will be A plus B is equal to C.

So, this is this is this is equation that we get from continuity of the wave function, then continuity of the derivative will be if I differentiate this i k and here it will be minus i k, so i k, a minus B is equal to i k 1 into C.

So, we obtain these are 2 equations. So, i, i cancels out, so we multiply the top equation by k 1, so I will get k 1, a minus B is equal to k 1 C and k 1 C is equal to k into a minus B. So, you will have you take B in this side, so you will get k minus k 1 into a and if we take B in this side, so you will get k I am sorry this is k a plus B.

So, it will be a k minus k 1, so I have here I multiply this by k 1, so k 1 into a I am sorry this is so I have multiply this by k 1, k 1 into a plus B is equal to k 1 C, this is equal to k into A plus B. So, therefore I will bring the B here, so you will get k 1 plus k into B is equal to k plus k 1 into A.

So, this gives me that B by A, B by A is the coefficient the amplitude of the reflected wave, amplitude of the incident wave, so this will be equal to B by A, will be equal to k, I again made a mistake so this is B will be k 1 plus k, this will be k minus k 1, so B by A will be k minus k 1, divided by k plus k 1.

So, the reflection coefficient will be k minus k 1, dived by k plus k 1 whole square, so this is one expression, then we have we can calculate that we may rewrite this one step more.

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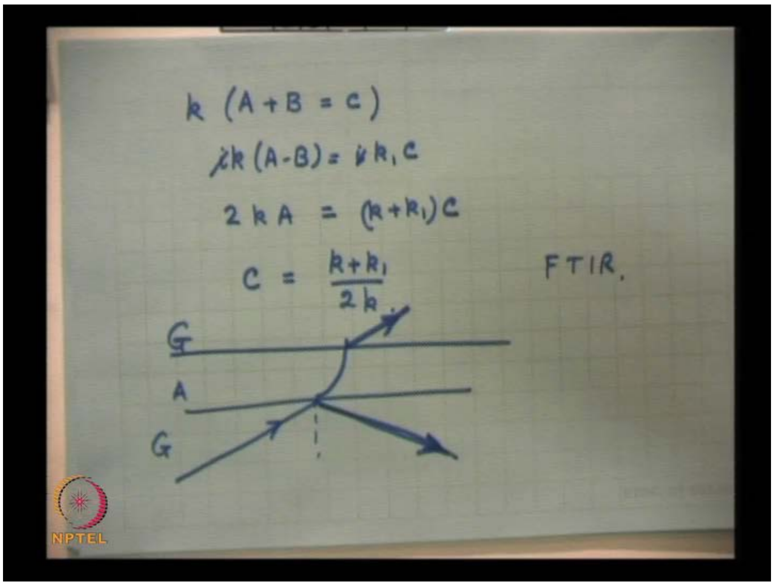

So, A plus B is equal to C, so we will have and i k A minus B is equal to i k 1 into C, so what we do is now multiply the top equation by k and I remove the i here, so k B appears here k B appears here and then I add them, so B is cancels out.

So, you get 2, k times a, is equal to k plus k 1, into c. So, you will obtain C is equal to k plus k 1 divided by 2 k. So, I have then being able to find out the coefficient B in terms of a, and obtained a expression for the reflection coefficient, I will I have also been able to find out the coefficient C in terms of a, which will be related to the transmission coefficient.

What now I have to do is and which I would like to leave as an exercise for all of you to solve, which will do in the next lecture, calculate the current density associated with the solution in the second region, we as current density associated with the incident wave, current density associated with reflective wave, and from there we will consider the reflection and the transmission coefficient.

Before I conclude in next 1 minute or 2 minutes, we will then consider the case E less than V 0, when I consider E less than V 0, then there will be not oscillatory solution in this region, there will be exponential solutions, this is something like the evanescent wave which is present here.

In optics or electrometric theory when you have a beam coming in here, and undergoing total internal refection and according to the ray optics the total energy get reflected, but when you solve Manxman's equation, then although the energy the reflection coefficient is 1 the total energy is reflected, but there is an exponentially decay in wave here this wave is known as evanescent wave.

So, let us suppose this is glass, this is air, and if you put another glass surface here then there is a possibility in fact it does happen the through the evanescent wave a beam can lick out this is in optics this is known as frustrated total internal reflection F T I R.

In quantum mechanics also we will show that there exist a evanescent wave and which will eventually lead to the phenomenon of tunneling. Thank you.