Basic Quantum Mechanics

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

We will continue our discussions on the solution of the Linear Harmonic Oscillator problem, solution corresponding to the linear harmonic oscillator problem.

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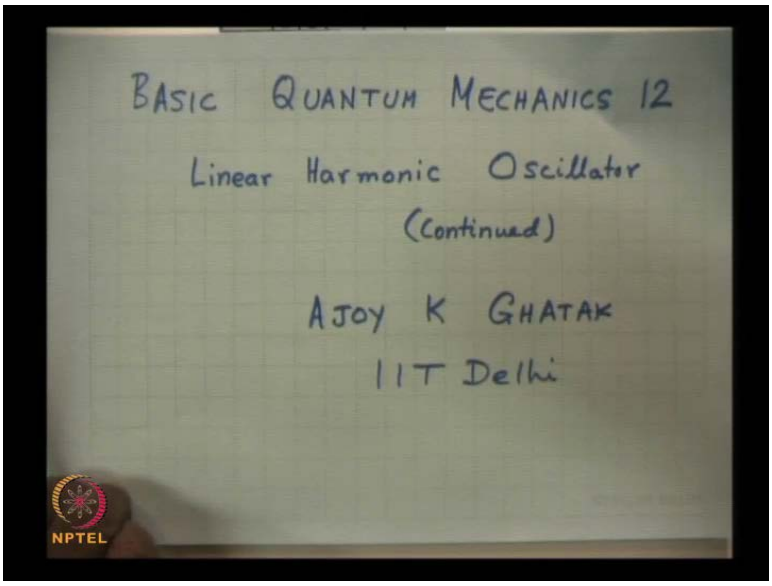

Once again we will be solving the Schrodinger equation and so, this lecture will be again on obtaining the solution for the linear harmonic oscillator problem.

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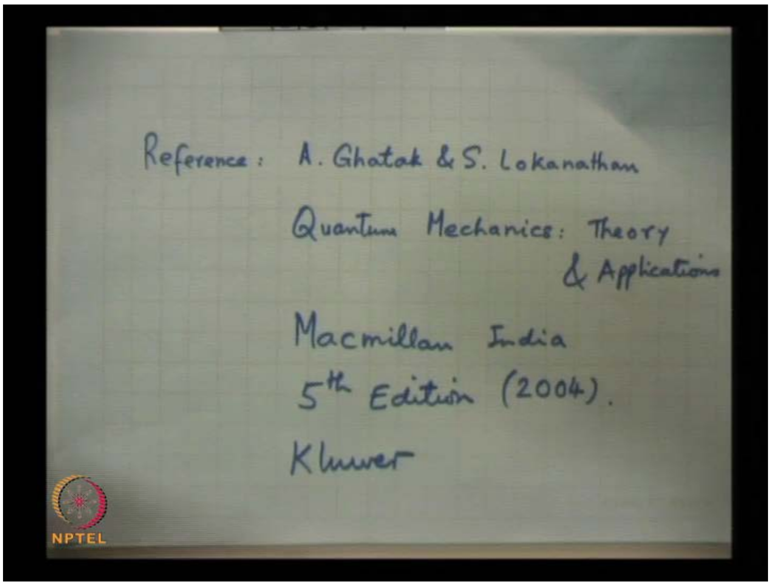

And as I had mentioned before, the reference for this and even my earlier lectures is our book on by myself and professor Lokanathan on quantum mechanics theory and applications, and published by Macmillan India, in India and also by Kluwer in Netherlands by Kluwer in Netherlands and this is the 5th edition, so that will be our reference.

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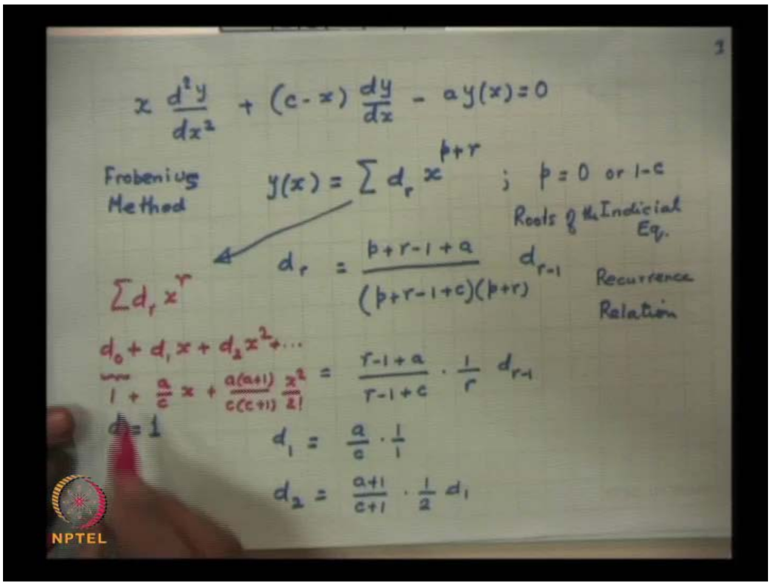

So, in my last lecture, we had discussed the solution of the confluent hyper geometric equation. Now, as we know that the confluent hyper geometric equation is x d 2 y by d x square plus small c minus x d y by d x minus a y of x.

So, we try to solve this equation by using the power series method, this method is also known as the Frobenius method. And this Frobenius method in this method, Frobenius method, we assume a power series expansion of this. Hence, usually it is in c, but since c appears here, so we will write d of r x to the power of p plus r. When we substitute it, this equation, the solution in this equation, we found that p will be either 0 or 1 minus c, these are the roots of the indicial equation these are the roots of the indicial equation these are the roots of the indicial equation.

Then we had also found that that d r over d r minus 1, that is d r was equal to p plus r minus 1 plus a divided by p plus r minus 1 plus c into p plus r times d r minus 1. So, the coefficient d r and d r minus 1 are related through this equation and this equation was known as the is known as the recurrence relation this equation is known as the recurrence relation.

So, let me take p equal to 0 first, and so, we have this is equal to r minus 1 plus a divided by r minus 1 plus c divided by r multiplied by d r minus 1. So, we calculated using this relation, we calculated d 1 in terms of d 0, d 2 in terms of d 1 and so on. So, if I assume, for example that d 0 is equal to 1, if I assume d 0 is equal to 1, so I assume r is equal to 1. So, I get d 1 if I put r equal to 1, so this becomes 1 minus 1 is 0, so a by c into 1, d 2 will become 2 will be a plus 1, so a plus 1 divided by c plus 1 multiplied by 1 over 2, multiplied by d 1 multiplied by d 1. So, that is a into a plus 1 divided by c plus c into c plus 1 into factorial 2 and so on. So, we get the solution, these p is 0 p is 0.

So, therefore, for p equal to 0, this equation becomes d r x to the power of r. So, we will have d 0 plus d 1 x plus d 2 x square plus so on. We are assuming d 0 is equal to 1, so this becomes 1 plus a by c x plus a into a plus 1 into c into c plus 1 x square by factorial 2, 1 into 2 and then it be 2 factorial times 3, so factorial 3, so this is the infinite series.

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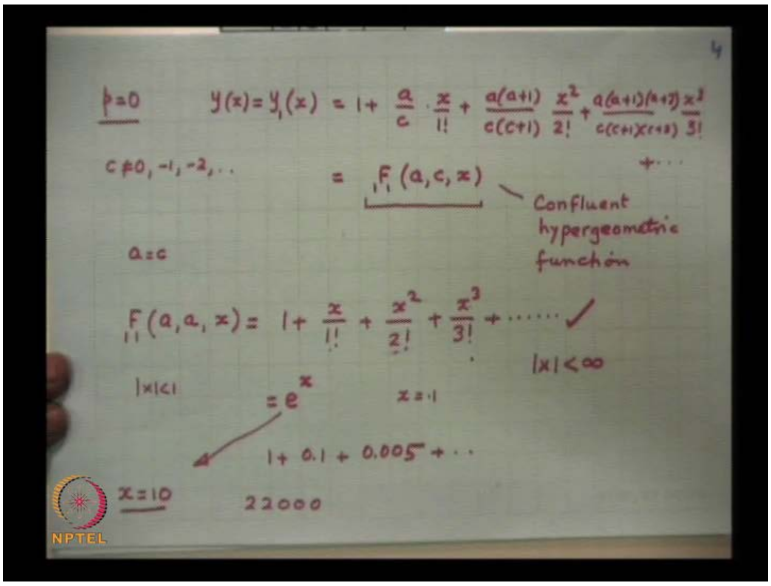

So, we obtained as one of the solution corresponding to p equal to 0, one of the solution as say y of x, the first solution y 1 of x, this will be equal to 1 plus a by c into x by 1 factorial plus a into a plus 1 into c into c plus 1 x square by 2 factorial plus a into a plus 1 into a plus 2 divided by c into c plus 1 into c plus 2 x cube by factorial 3 plus 1. So, let me write this down, a into a plus 1 into a plus 2.

This equation, this infinite series is usually denoted by F 1 1 a comma c comma x and this is known as the confluent hyper geometric function confluent hyper geometric function, it is an extremely important function and I would like all of you to understand this very carefully.

Now, let me consider this special case, I will I will consider the p is equal to 1 minus c also in a moment. But before that, let me tell you an important property let me tell you an important property of this confluent hyper geometric function, and that is let us take this simple case when a is equal to c when a is equal to c this factor is 1, this factor is 1, this factor is 1 (Refer Slide Time :8:57).

So, F 1 1 when a is equal to c a a x, this is equal to 1 plus x by factorial 1 plus x square by factorial 2 plus x cube by factorial 3. I usually ask my students, what is the domain of convergence of the series that means, for what value of x is this series convergent, if you would like to think for a moment.

Normally, students reply may back that this series is convergent for mode x less than 1, now that is not quite true, this series as you know is e to the power of x. And so, therefore, this series is convergent for all values of x, in fact for all complex values of x. If you take x equal to say 0.1, then it converges very rapidly.

So, it will be 1 plus 0.1 plus 0.01 divided by 2 that is 0.005 or something like that and so on. So, it converges very rapidly for x is equal to 1, then what will happen is that the, first the numbers are large, but then it will come down.

Even if you take a value let us suppose x is equal to 10, then eventually the factorials take over, initially the value of each term increases, first term will be 10, then this will be 100 divided by 2, this is 50, this is 1000 divided by 6, that is our 100 and something. So, even for a value x is equal to 10, it will take a very large number of terms, but the series will converge and that if you use your calculator, it will be a number which is very close to 22000, 22000 plus, (()) or something like that.

So, that means even if you take a value of x is equal to 1000000, the value of the function e to the power x will be finite, it will be extremely large number, but it will be finite. So, this series, this infinite series is convergent for all value of x and you use to write convergence for mode x less than infinity, all values of x this series convergent.

However, the values of the series increases with x so that the series is convergent, but the value of the function will increase as I had told you that for x is equal to 10, the value becomes extremely large, I hope I have been able to convey you. So, this infinite series, this infinite series is convergent for all value of x (Refer Slide Time: 12:55). So, therefore, this is a valid solution of the confluent hyper geometric equation, for all value of x, except for c naught equal to 0, minus 1, minus 2, etcetera. Because for c equal to 0 or negative integer, these denominator will be 0 and therefore, the function will blow up.

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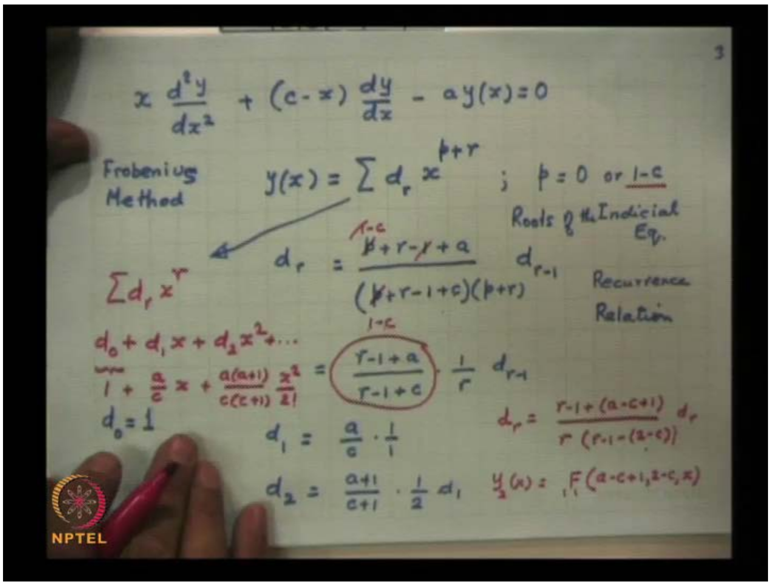

Now, let me look at the other solution let me look at the other solution, now I go back to my recurrence relation which I had written down here and I now assume p equal to 1 minus c. So, if I assume p equal to 1 minus c, then I will have d r is equal to, please see this, this equation will be equal to r minus 1 plus a minus c plus 1 and divided by r into r minus 1 minus 2 minus c. If you just do a little bit of algebra, this will come out, because if you put p is equal to 1 minus c, so this becomes this becomes 1 minus c, this becomes 1 minus c.

So, 1 and 1 cancel out, c and c cancel out, and r comes out, and this comes out to be 1 minus c plus r. So, I write this as r minus 1 minus 2 minus 1 c. So, 1 minus c, 1, 1 cancel out, so this is a plus r minus c. And I write this down as a plus r minus c and I have added and subtracted 1.

So, I just related it slightly, the reason why I have related in this form is because, you can see now that if I compare this with this expression, I hope all of you can see this, a will be replaced by a minus c plus 1 and c will be replaced by 2 minus c.

So, therefore, the second solution y 2 of x will be, therefore, F 1 1, for a I must write a minus c plus 1, for c I will write 2 minus c and x.

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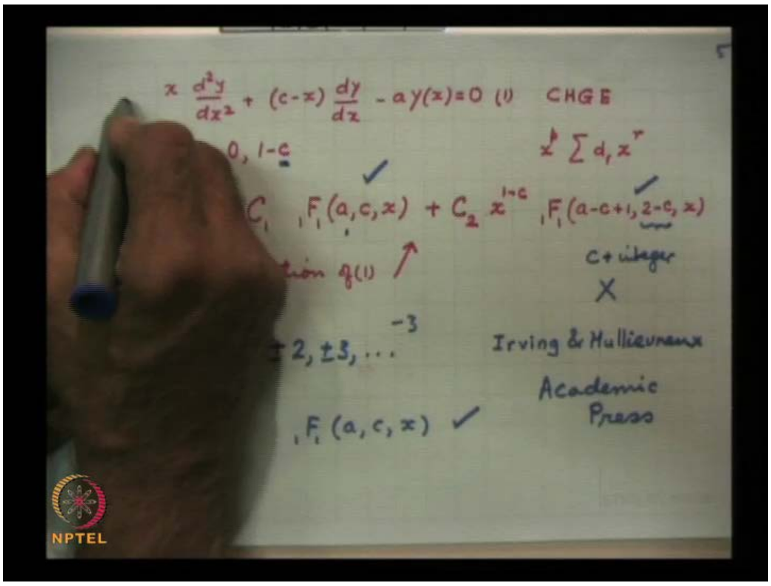

So, therefore, the two independent solution of this equation that is x d 2 y by d x square plus c minus x d y by d x minus a y of x is equal to 0, as I said this is the confluent hyper geometric equation.

So, we obtain p is equal to 0 and 1 minus c, these are the roots of the indicial equation and the two solutions are so the two solution are, also the general solution of this equation is c 1 x to the power 0 and then F 1 1 a comma c comma x plus c 2, you remember that we had summation d r x to the power of p plus r.

So, if I take r here, so x to the power p here. So, it will be x to the power of 1 minus c F 1 1 a minus c plus 1, 2 minus c comma x. So, this is the general solution so this is the general solution, because a second order differential equation will have two solutions. So, the general solution of equation 1 of the confluent hyper geometric equation is given by this, one more thing we had seen that when c becomes 0 or negative integer, then this solution does not remain valid, it becomes infinite and when c becomes a positive integer, then this quantity becomes a negative integer.

So, therefore, this solution blows up when c becomes positive, positive integer. So, the general solution of this equation, so I can write down that this is the general solution for c not equal to 0 plus minus 1 plus minus 2 is equal to some. Actually when c is equal to 1, plus 1, then this is a correct, this is alright. And when c is equal to let us suppose minus 3, then this is alright, but this is then not alright. I repeat that, let us suppose when c is equal 2, then this function will be ok, because c appears in the denominator, but this function this will be 0, so this will not be this will not be a valid solution.

Similarly, for c is equal to, let us suppose minus 3, this function will blow up, but this function will not. So, one of the solutions will be alright, for the other solution there are there are tricks to obtain that. This I have given in the appendix of the book that I have just now mentioned, but you can find it in any book or mathematical physics, a very good book on mathematical physics is by Irving and Mullieunux, m u l l i e u n u x mathematics for physics and engineering, this published by academics press, it is a very very nicely written books and has a lot of examples.

And if you want to study for example, the the solution of second order differential equations, Bessel functions, Legendre functions and other than that, this is a very good reference. Actually in the problem that we will be considering, c will come out to be half, therefore both of them will be valid solution.

So, I have obtained the general solution of this equation.

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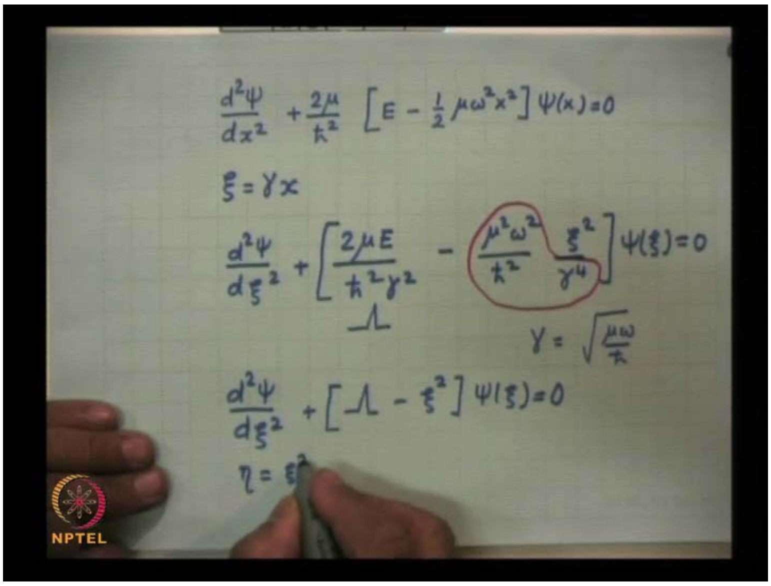

Now, why I am doing why am I doing all this, my overall aim is to solve the Schrodinger equation, so let me write down the Schrodinger equation. So, d 2 psi, the time independent Schrödinger equation d 2 psi by d x square, u is the mass of the particle, h cross is the Planck’s constant, e minus v of x, but v of x for harmonic oscillator is minus mu omega square x square psi of x is equal to 0. So, what I do, I think I had done this before, let me quickly in order to write it a convenient form, I write as xi is equal to gamma x, I have done this before.

So, we get this equation, the above equation becomes d 2 psi by d xi square plus 2 mu e by h cross, this becomes gamma square times this. So, I put gamma square here, minus mu square omega square, that is mu square omega square by h cross square xi square by gamma to the power 4.

So, I choose my gamma, I choose which I have done before, I choose my gamma so that this is 1. So, I obtain so I obtain and this I put as lambda, so I choose my gamma so that this equal to under root of nu omega by h cross. And so, therefore, Schrodinger equation becomes for the harmonic oscillator problem plus lambda, capital lambda minus xi square, psi of xi is equal to 0.

Now, what I do is that, I now want to solve this equation. So, because there is a xi square term appearing here, let me make a let me make a transformation that, let me define eta is equal to xi square, I define eta is equal to xi square.

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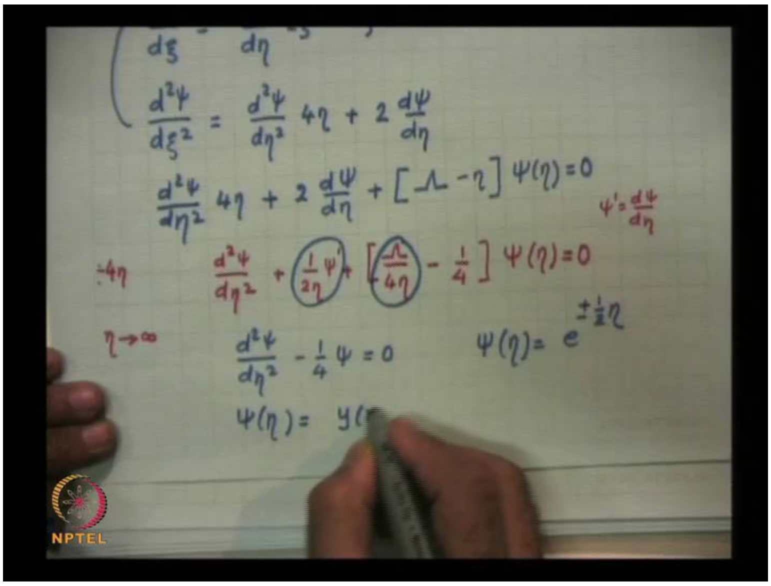

So, if I do that, then I will obtain sorry I will obtain, please see this carefully, d psi by d xi is equal to, I want to express this in terms of the new variable eta, d psi by d eta times d eta by d xi, so that is 2 xi.

I differentiate this again I differentiate this again, so I get let me write it in the next line, d 2 psi by d xi square. So, I get d 2 psi by d eta square plus multiply by d eta by d xi which is 2 xi. So, this becomes 4 xi square xi square is eta, 4 eta plus I differentiate it with respect to xi. So, this is 1, so 2 d psi by d eta, so I substitute this in this equation (Refer Slide time 25:03).

So, I get d 2 psi by d eta square 4 eta plus 2 d psi by d eta plus lambda xi square is eta, so eta psi of eta is equal to 0. So, using this as the independent variable, I define the variable eta is equal to xi square and I make a simple transformation and the above equation becomes something like this.

So, I rewrite this I rewrite this, what I do is, I divide by 4 eta I divide by 4 eta, so to obtain d 2 psi by d eta square plus 1 over 2 eta plus lambda over 4 eta minus 1 by 4 psi of eta is 0. Everything till now is rigorously correct, there is no approximation that I have made anywhere, sorry 1 over 2 eta d psi by d eta I am sorry this is psi prime that is, this is psi prime is psi prime is d psi by d eta, I miss that.

Now, for large values of eta, that is for large value of xi square, this term will be very small, this term will be because there is eta which is coming in the denominator, this term will become very small. So, you will have just these two terms, d 2 psi by d eta square minus 1 by 4 psi of eta is equal to 0. And I know the solutions of this psi of eta, this will be e to the power of plus minus half eta.

So, this suggests this suggests that the try out a solution, psi of eta which is equal to y of eta a to the power of minus half eta, e to the power of plus half eta that is plus half xi square will blow up at xi is equal to infinity.

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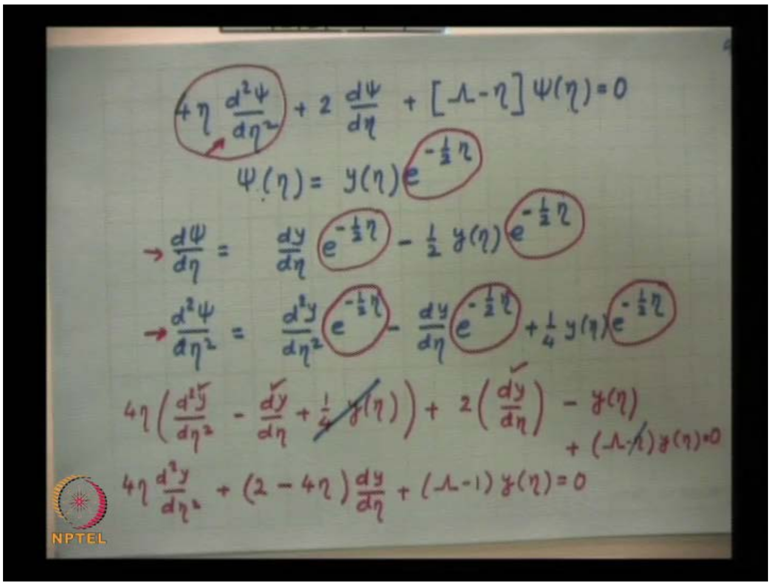

So, we try out a solution like this we try a solution like this, so we write this equation 4 eta d 2 psi by d eta square plus 2 d psi by d eta plus lambda minus eta psi of eta is equal to 0. And we solve this equation by assuming because the, for large eta, it is given by this.

So, we substitute the solution in this equation, it is very straight forward, I differentiate it once, d psi by d eta will be equal to d y by d eta e to the power of minus half eta minus half y of eta e to the power of minus half eta. Then I differentiate it again, very straight forward derivation, d 2 psi by d eta square, this is equal to d 2 by y d eta square. I differentiate this, again e to the power minus half eta and then when I differentiate the second term, I will get minus half d y by d eta e to the power of minus half and here when I differentiate this term, I will get minus half.

So, those two terms will be equal, as I am sure all of you would know. So, you will get d y by d eta e to the power of minus half eta and then if I differentiate this term again, I will get minus half, so plus 1 by 4 y of eta e to the power of minus half eta.

Now, next what I do is that, I substitute this here, this here, and this here, and as you will see, all the terms involve e to the power of minus half eta (Refer Slide time 30:07). So, that term e to the power of minus half eta, this term which appears in all the terms will just cancel out, these term, this term will when I substitute for d 2 psi by d eta square, d psi by d eta and psi of eta in this equation, this term will be common to all of them and then it will cancel out (Refer Slide Time: 30:30).

So, I obtain 4 eta, please see d 2 y by d eta square minus d y by d eta plus 1 by 4 y of eta, this is the first term, this was the this term and then plus 2 d psi by d eta. So, plus 2 bracket d y by d eta minus 2 times this, so therefore, minus y of eta, because 2 into minus half is minus 1 plus lambda minus eta y of eta, this is equal to 0.

So, you can now see that, please see this, 4 eta times 1 by 4, that is 4, 4 cancels out, this terms is eta y of eta and there is a minus eta y of eta. So, these two terms cancels out, I hope you are able to understand. So, this term will cancel out with minus d y by d eta.

So, we will obtain we will obtain 4 eta, let me do it in carefully, d 2 y by d eta square plus 2 here, minus 4 eta d y by d eta. So, this term is taken care of, this term is taken care of, this term is taken care of, plus lambda minus 1 y of eta equal to 0 (Refer Slide Time: 33:00).

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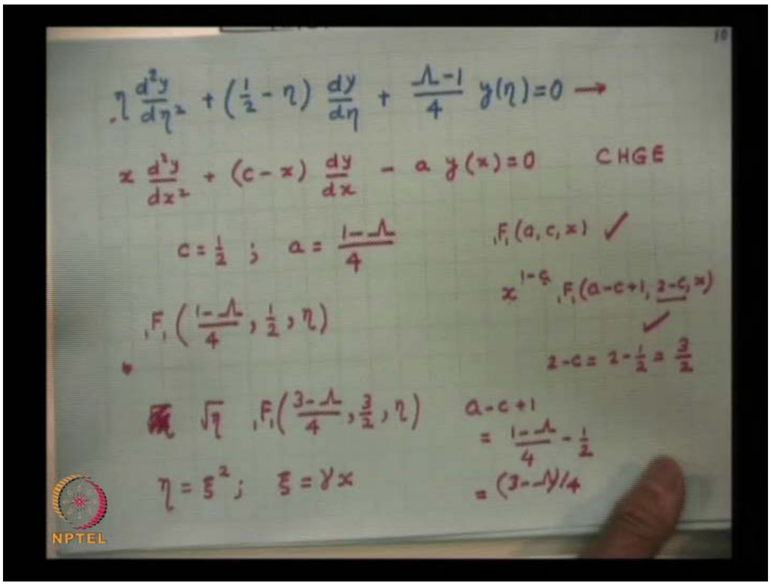

What I do next is, I divide by 4 I divide by 4 to obtain; if I divide by 4, then I obtain eta d 2 y by d eta square plus 2 by 4 is half minus eta d y by d eta plus lambda minus 1 by 4 y of eta.

So, this Schrodinger equation gets transformed to this equation, and let me now write down the confluent hyper geometric equation. The confluent hyper geometric equation if you remember, x d 2 y by d x square plus c minus x d y by d x minus a y of x is equal to 0. So, this is my confluent hyper geometric equation.

So, we find that we have actually obtained a confluent hyper geometric equation, so c is equal to half and a is the minus of that, so a is equal to 1 minus lambda by 4. So, since c is half, both the solutions, one solution was F 1 1 a comma c comma x, this was one solution. And the other solution was if you remember x to the power of 1 minus c F 1 1 a minus c plus 1 comma 2 minus c comma x, both solutions are convergent series and they represent the most general solution of this equation, the complete solution of this equation.

So, please see this that I have here, I have here the complete solution is, so let me write down what is a minus c plus 1 or first write let me write down what is 2 minus c, 2 minus c is equal to minus half. So, this is 3 by 2 and a minus c plus 1 is equal to a 1 minus lambda by 4 minus half plus 1, so that is minus half.

So, this will be to 2 3 minus lambda by 4 3 minus lambda by 4. So, my two independent solutions are F 1 1 F 1 1 a that is 1 minus lambda by 4 comma c that is half and eta which is actually xi square, this is one solution, and the other solution is x to the power of 1 minus c, c is half 1 minus half is half.

So, that is square root of x square root of x sorry of eta I am sorry square root of eta F 1 1 3 minus lambda by 4 into 3 by 2 into eta and as you know, eta is equal to xi square and xi we have said was equal to proportional to x, so eta is actually gamma square x square.

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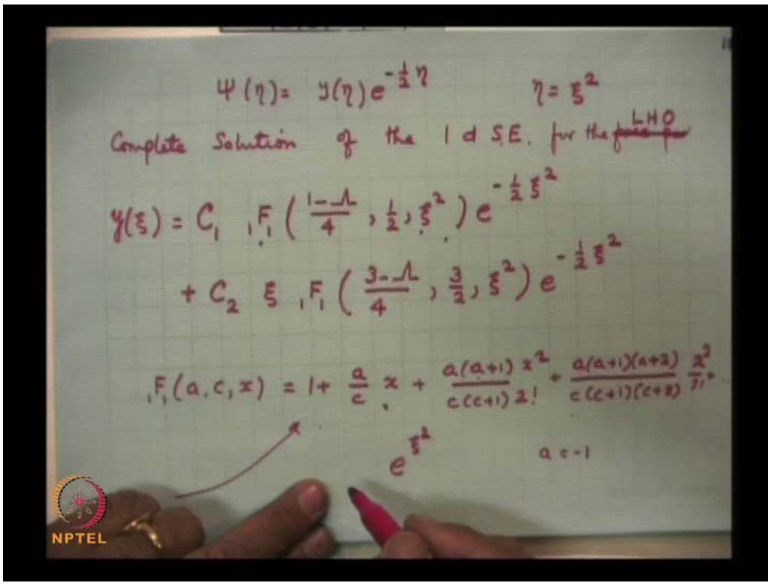

So, now you remember that we had taken, we had assumed psi of eta was equal to y of eta e to the power of minus half eta and eta is equal to xi square. So, the complete solution complete solution of the one dimensional Schrodinger equation for the free particle sorry sorry for the linear, I am sorry for the linear harmonic oscillator will be y of xi, please see this some constant C F 1 1 a as we said.

So, 1 minus lambda by 4 a, this is a, c is half psi square e to the power of minus half xi square plus C 2 square root of eta, square root of eta is just xi F 1 1, 3 minus lambda by 4 comma 3 by 2 to xi square e to the power of minus half xi square.

This is the complete solution, rigorously correct and valid for all values of xi, but there is a problem and the problem is that, you remember that we have said that F 1 1 a comma c comma x is equal to 1 plus a by c x plus a into a plus 1 into x square by factorial 2 plus a into a plus 1 into a plus 2 into c into c plus 1 into c plus 2 x cube by factorial 3.

If this series, understand this point carefully, if this series is allowed to go to infinity, that is, if this series remains an infinite series, then although the series is convergent, it will behave as e to the power of plus xi square which is obvious, because e to the power of plus x and x is xi square.

Actually, I should write eta here, does not matter, this function behave as e to the power of x. So, therefore, if this remains an infinite series, then it will behave as e to the power of xi square. So, the total function will behave as e to the power of plus half xi square and so, the wave function will blow up at infinity and therefore, the wave function will not be normalisable.

This can be averted if you make this a polynomial, if you make this, you can make this polynomial only if a is a negative integer. So, for example if a is equal to minus 1, then this term will be 0, this term will be 0, all the remaining terms will be 0 and only this term will survive, these two terms will survive (Refer Slide Time: 08).

So, therefore, so therefore for this function that is for F 1 1 a comma c comma xi square multiplied by e to the power of minus, let me repeat what I have just now said. If this infinite series is not terminated is not terminated, then it will behave as e to the power of xi square for large values of xi. And so, therefore, the function will, the product will behave as e to the power of half xi square and so, therefore, the wave function will blow up at infinity, it will be a valid wave function, but it will not be a square integral wave function, because the wave function will have a very large value at infinity.

This can only be averted if this infinite series is made into a polynomial and because there is a into a plus 1 into a plus 2, this can be made into a polynomial only if a is a negative integer negative integer that is either 0 or 0. If it is 0, then 0, minus 1, minus 2, minus 3, etcetera; only then, you will have that.

So, therefore, I have these two solutions, this series will become a polynomial if 1 minus lambda by 4 is a negative integer or 0, or this series will become 0, will become a polynomial if this coefficient becomes a negative integer or 0.

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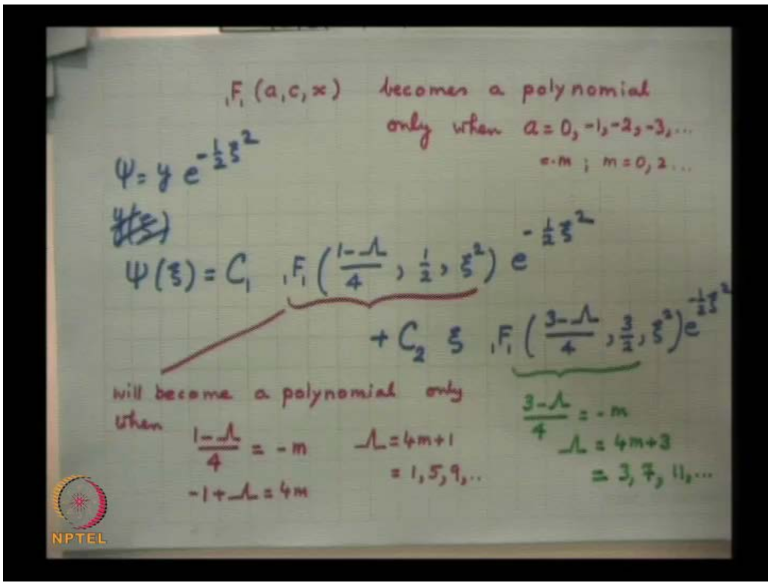

So, let me summaries this, that is that is F 1 1 a c x becomes a polynomial polynomial only when a is equal to 0, minus 1, minus 2, minus 3, etcetera, or equal to m, minus m where m is equal to 0, 1, 2, 3, etcetera. And now, what we had done is that y of xi, the solution the the the actually psi of xi, I am sorry psi of xi the wave function wave function was y into e to the power of minus half eta eta is xi square.

So, psi of xi will be equal to y of xi that is C 1 F 1 1 1 minus lambda by 4 in half that is the value of c into xi square into e to the power of minus half xi square, I will illustrate this in terms of examples, this is the general solution, square root of eta that is square root of xi square. So, xi F 1 1, 3 minus lambda by 4, 3 by 2 you have to remember this, these 2 formula you have to remember, then it will become very easy. I remember, so I think you can also remember.

So, what we have found is this infinite series will become a polynomial, only when this is a 1 minus lambda by 4 is equal to minus m, so therefore, this is if you take lambda on this. So, this will be, if you multiply by both sides by minus 4, so minus minus 1 plus lambda is equal to 4 m. So, it take 1 to this side, so lambda is equal to 4 m plus 1 which is may equal to 0. That means, 1, 5, 9, etcetera, and then we see that this will become a polynomial when 3 minus lambda by 4 is a negative integer. So, simplify that and you will get lambda is equal to 4 m plus 3.

So, this will be m equal to 0, 3, 7, 11, etcetera, these are the Eigen values of the product these are the Eigen values of the product

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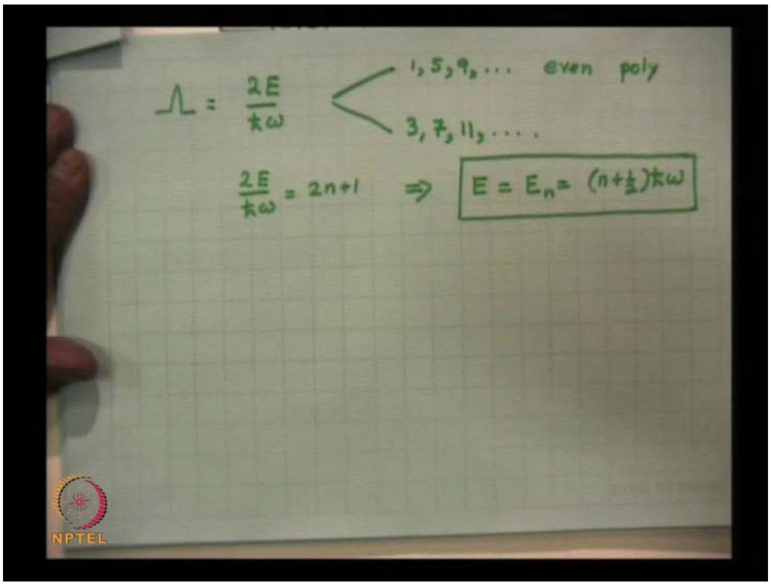

And let me tell you that we had said that lambda is equal to 2 E by h cross omega. So, this can take values 1, 5, 9, etcetera and the first solution will be a polynomial solution and this will be 3, 7.

So, the solution will be an even polynomial and this as I will show you in a moment 3, 7, 11, it will be an odd (()) the second solution. So, we will have an odd integer, so therefore, 2 E by h cross omega must be 2 n plus 1.

So, this implies E is equal to E n is equal to n plus half h cross omega, this is an extremely important result that we have been able to find out, these are the discrete energy Eigen values of the harmonic oscillator problem.

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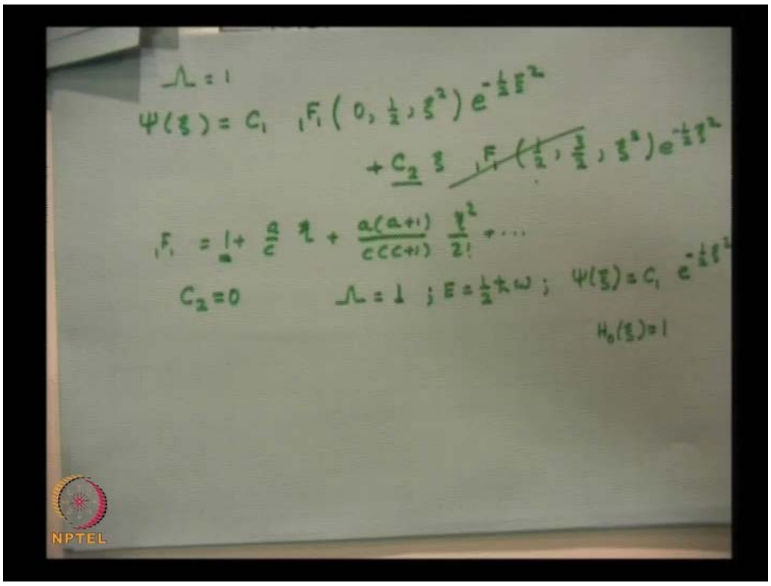

Now, let me go back now let me go back now let me go back that to our solution to to this solution to the solution that we written, now let me go back and we assume that that these are the two solutions. So, let me assume that lambda is 1, if lambda is 1, then psi the general solution of the equation Schrodinger equation is psi of xi becomes C 1 F 1 1, this is 0 half xi square e to the power of minus half xi square plus there can be another solutions C 2 xi F 1 1, 3 minus 1 that is 2 by 4, that is half, 3 by 2 psi square into e to the power of minus xi square.

Now, you see this here a is half and as you know F 1 1 is equal to 1 plus a by c x sorry here xi square that is eta by factorial 1 a into a plus 1 into c into c plus 1 eta square by factorial 2. So, this will not be become a polynomial and therefore, we must choose C 2 equal to 0 and therefore, this we should neglect, we should assume C 2 equal to 0, because then the the the this series will become a polynomial and the first series will be equal to only a 0, so only a constant term will survive.

So, for for lambda is equal to 1 that is E is equal to half h cross omega, my psi of xi will be equal to C 1 constant that is 1 into e to the power of minus xi square. So, I will this is h 0 of xi, h 0 of xi is 1.

So, this is the first Eigen function of the solution. Now, in my next lecture, what I will do is using these two equations, we will find out the Eigen functions corresponding to different Eigen values, thank you.