Basic Quantum Mechanics

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Module No. # 05

The Angular Momentum - I

Lecture No. # 01

The Angular Momentum Problem

In my last lecture, near the end of that lecture, we had start we had started the Angular Momentum Problem in Quantum Mechanics. And we had, we will continue our discussion on that, I discussed the Eigen values and corresponding Eigen functions for the angular momentum.

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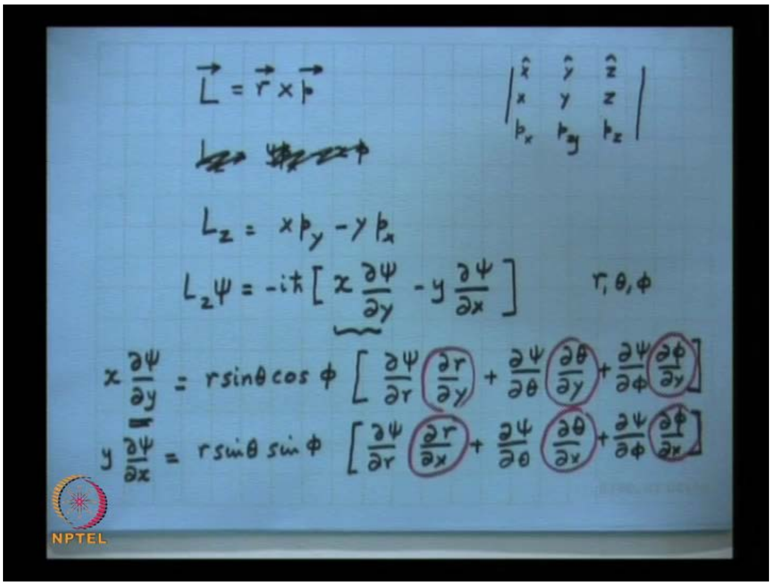

We had said that, we represented as in classical mechanics by the r cross p but, now p is a differential operator, so for example, L z will be equal to y p x minus x p y, so the cross product is x cap y cap and z cap and x y z p x p y p z. So, p x p y so I'm sorry, so this will be L z will be L z will be x p y minus y p x and similarly, L x similarly, L y. So, this if I write the differential represent operator representation. So, this becomes minus i h cross x delta, so L z operating on a wave function psi will be delta psi by delta y minus y delta psi by delta x.

Now, I want to express this in terms of the spherical polar coordinates r theta phi, so that we know what is x that is r sine theta cos phi, so the first term, so x delta psi by delta y will be equal to r sine theta cos phi multiplied by. Now I want to express this in terms of spherical polar coordinates.

So, it will be delta psi by delta r time's delta r by delta y plus delta psi by delta theta into delta theta by delta y plus delta psi by delta phi into delta phi by delta y, this is the first term. And the second term will be y delta psi by delta x and this will be r sine theta sine phi and delta psi by delta x will be delta psi by delta r y here will be replaced by x delta r by delta x plus delta psi by delta theta delta theta by delta x plus delta psi by delta phi although it looks very combustion but, the analysis is quite straight forward.

So, as you can see we require therefore, delta r by delta y, delta theta by delta y, delta theta by delta x, delta phi by delta y, delta phi by delta x and delta r by delta x. So these are the expressions that, we would like to express in terms of the spherical polar coordinates.

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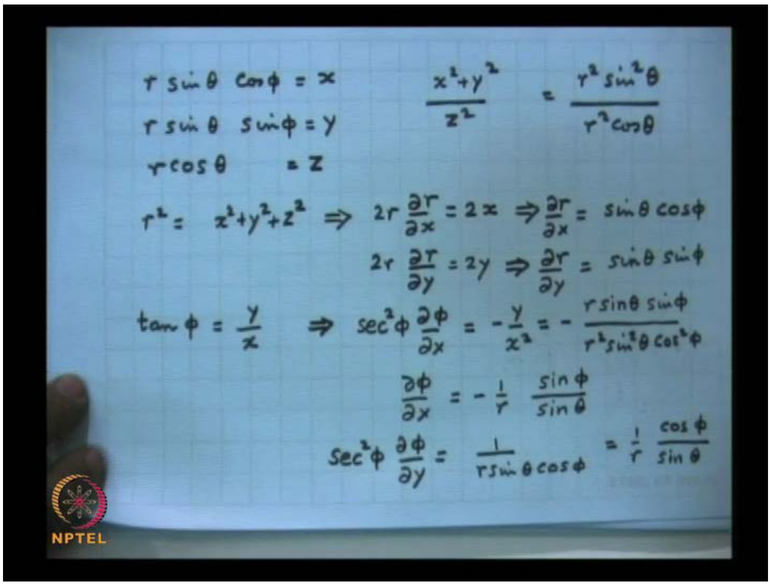

So, as we had said that, the spherical polar coordinates were defined as r sine theta cos phi was equal to x, r sine theta sine phi was equal to y and r cos theta was equal to z. So, if we square and add then it will become sine square theta cos square phi sine square theta sine square phi, so if we add them it become sine square theta plus cos square theta.

So, r square is equal to x square plus y square plus z square, so if I differentiate with respect to x, so it becomes 2 r delta r by delta x is equal to 2 x therefore, we will have delta r by delta x will be equal to x by r but, x is equal to r sine theta cos phi; so this will be sine theta cos phi. Similarly, 2 r delta r by delta y now, when I write this partial differentiation, when I differentiate partially with respect to y, then x and z have to be kept constant. So, this will be equal to 2 y, so this will imply that delta r by delta y is equal to y by r that is sine theta sine phi.

So, you can see these are not that difficult, then let me let me write the expression for tangent of phi, so I divide this equation by this equation so I get tangent of phi becomes equal to y by x y by x. So, this equation if I differentiate this, so we will get secant square, secant square phi delta phi by delta x will be equal to if I differentiate this with respect to x, so this will be minus y by x square; so this will be minus y is r sine theta r sine theta sine phi divided by x square that is r square sine square theta cos square phi.

So, as you can see if I multiply secant square phi to cos square phi, it will become 1, so I obtain delta phi by delta x is equal to minus 1 over r sine phi over sine theta, because sine theta and sine square theta one sine theta cancels out; so this is one result, if I differentiate with respect to y that is very simple.

Secant square phi delta phi by delta y will be just 1 over x, and 1 over x is r sine theta cos phi, so if I multiply this one cos phi will cancel out with secant phi and then cos phi will come on the top; so I will have 1 over r cos phi over sine theta this is one expression and the last expression is that if I square these two.

So, x square plus y square is r square sine square theta x square plus y square is r square sine square theta and z square is r square cos square theta; so r square r square cancels out, so you are left with tan square theta sorry this is tan square theta is equal to x square plus y square divided by z square.

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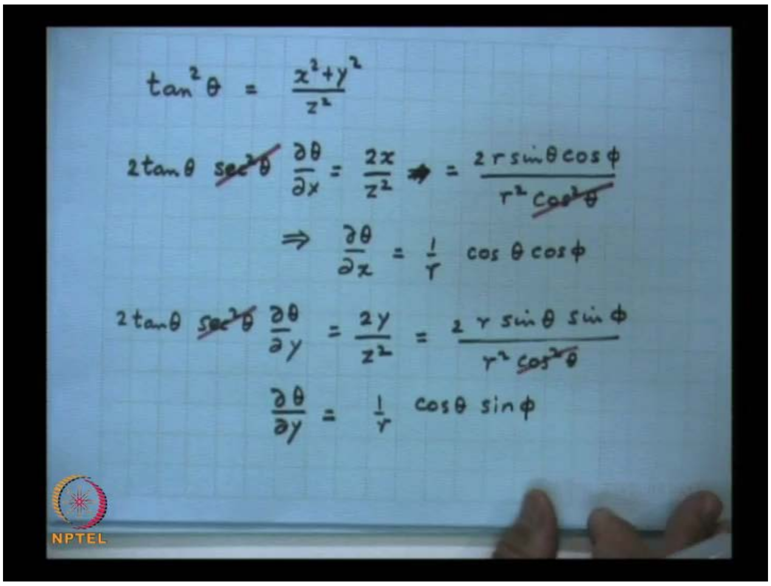

So, if we differentiate this with respect to x or y, let us let us differentiate with respect to x plus 2 tangent theta secant square theta delta theta by delta x is equal to 2 x by z square. So, this implies that that this is the right hand side is equal to 2 r sine theta cos phi and divided by r square cos square theta.

So, r square cos square theta this cos square theta and secant square theta cancel out and 2, 2 cancels out therefore, this implies that delta theta by delta x will be 1 over r the 2 also cancels out sine theta cos phi by tan theta tan theta is sine theta over cos theta, so this will be just cos theta cos phi. Finally if I differentiate with respect to y, then again two tangent of theta secant square theta delta theta by delta y this is equal to 2 y by z square that is 2 r sine theta sine phi divided by r square cos square theta.

Once again, this term will cancel out with this term and therefore, this will be delta theta by delta y will be equal to 1 over r cos theta sine phi, so we have now, expressions for delta r by delta y delta r by delta x delta theta by delta y delta theta by delta x delta phi by delta y and delta phi. So, I just have to substitute it here before we proceed further, let me tell you, let me warn you a little bit about the partial differentiation that you see; let us suppose I want to calculate delta r by delta x then y and z have to be remaining remain constant.

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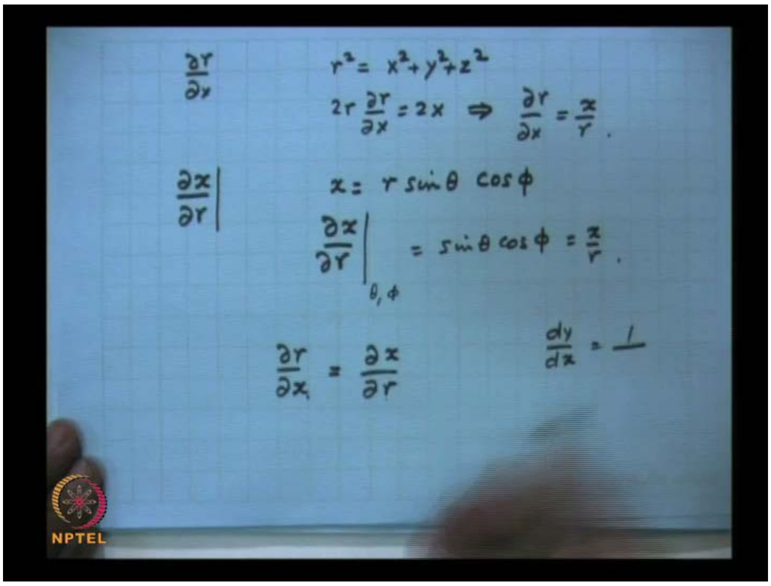

So therefore, I must express r in terms of x y z and now I differentiate with respect to x delta r by delta x becomes 2 x and this becomes this gives delta r by delta x is equal to x by r. Now let us suppose I wanted to differentiate delta x by delta r, then I must express x because, when I differentiate with respect to r theta and phi remains constant. So, I must express x is equal to r sine theta cos phi and if I differentiate this delta x by delta r and here, theta and phi remains constant; so this becomes sine theta cos phi and this is also x by r, so you can see that delta r by delta x happens to be equal to delta x by delta r.

In total differential you know that d y by d x is equal to 1 over d x by d y but, in partial differentiation one has to be very careful as to when your differentiating partially with respect to x then y and z have to remain constant. And when your partially differentiating with respect to r then theta and phi are to remain constant, so these are some of the tricks therefore, the our objective was to calculate to obtain the operator representation of L z in the Cartesian format it is x delta psi by delta y minus y delta psi by delta x.

But I wanted in terms of the polar coordinates and therefore, you have to evaluate this which we have evaluated all these are evaluated say for example, delta r by delta y is given here, delta r by delta x is given here, delta theta by delta y delta phi by delta y is given here, delta phi by delta x is given here (Refer slide time: 15:34), so everything is there

So, we just have to substitute those expressions in this carry out a simple manipulation and one finally, obtains this remarkable result that L z psi becomes equal to minus i h cross delta psi by delta phi.

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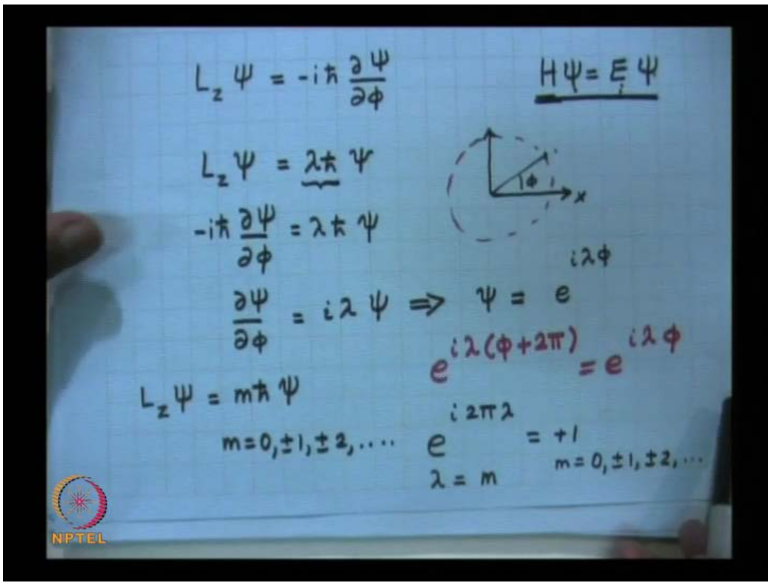

It simplifies to this particular relation, now let me let me try to find the Eigen values of L z, so what is an Eigen value equation if you recall that the for the Hamiltonian the Eigen value equation is H psi is equal to E psi that is this is the operator operating on a wave function, E is a number multiplied by the same wave function, then this equation is known as the Eigen value equation.

So, I would like to find out say L z psi the Eigen values and Eigen functions of the operator L z, so let me write it down as let me try to solve Eigen value equation lambda h cross i introduce h cross just for the sake of simplicity delta psi. So, lambda z psi sorry L z psi is equal to minus h cross is just a constant delta psi by delta phi, the Eigen value of the operator x z I represent it by lambda H cross the Eigen value of the Hamiltonian that we have been solving till now are the energy given by E.

So, this is equal to lambda h cross psi h cross h cross cancels out, if I multiply both sides by I then I get delta psi by delta phi is equal to i lambda psi, this is a very simple integration that psi becomes the phi dependent. One cannot say anything about the theta or r dependent if phi dependent becomes e to the power of I lambda phi. Now, any wave function has to be well behaved, has to be single valued that is on the x y plane you see on the x y plane this is the angle phi if I go around the origin and I make phi 2 phi plus 2 pi I arrive at the same point and the wave function must have the same value.

So, therefore, therefore, e to the power of i lambda phi plus 2 pi must be equal to e to the power of i lambda phi therefore, we obtained the result that e to the power of i 2 pi lambda should be equal to plus 1 and therefore, from this we immediately obtain that lambda has to be equal to a positive or negative integer, lambda must be positive or negative integer, that m can take the values 0 plus minus 1 plus minus 2 and so on.

So the Eigen value of the operator L z are given by L z psi is equal to m h cross psi, where m is equal to 0 plus minus 1 plus minus 2 and so on. And what are the corresponding wave function.

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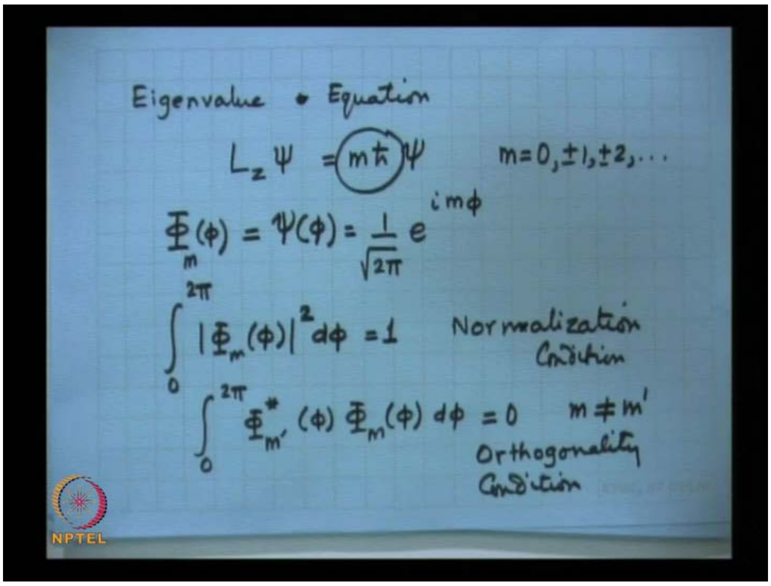

The the therefore, the solution of the Eigen value equation the solution of the Eigen value equation L z psi is equal to m h cross psi, where m will take the values 0 plus minus 1 plus minus 2, etcetera.

And the corresponding phi dependence the phi dependence only one cannot say anything about the r and the theta will be e to the power of i m phi and to normalize it you will have under root of 2 pi, these wave functions are usually denoted as capital phi subscript m as phi.

And because of this normalization constant if you have phi m square d phi from 0 to 2 pi phi goes from 0 to 2 pi this will be one this is known as the normalization condition. And the second is that if you have 0 this is this can be also true that very easily phi m star times phi multiplied by phi m phi d phi this will be 0 for m not equal to m prime this is known as the orthogonality condition.

So therefore, we have been able to find that the operator L z we have been able to solve this equation L z has the Eigen values m h cross multiples of h cross, that m can take we have used the condition, that the wave functions have to be single valued, that the wave functions have to be single valued that as I go from the point phi to phi plus 2 pi the wave function was remained unchanged.

Using this single valued condition, the fact that the wave function should be single valued we obtained lambda should be either a positive or a negative integer or a 0 (Refer slide time: 23:11), so these are the so what are the Eigen values of the operator L z. The Eigen values are m h cross that m is equal to 0 plus minus 1 plus minus 2, etcetera; now we have obtained the operator representation of the operator L z exact very similarly, you can obtain for L x and L y.

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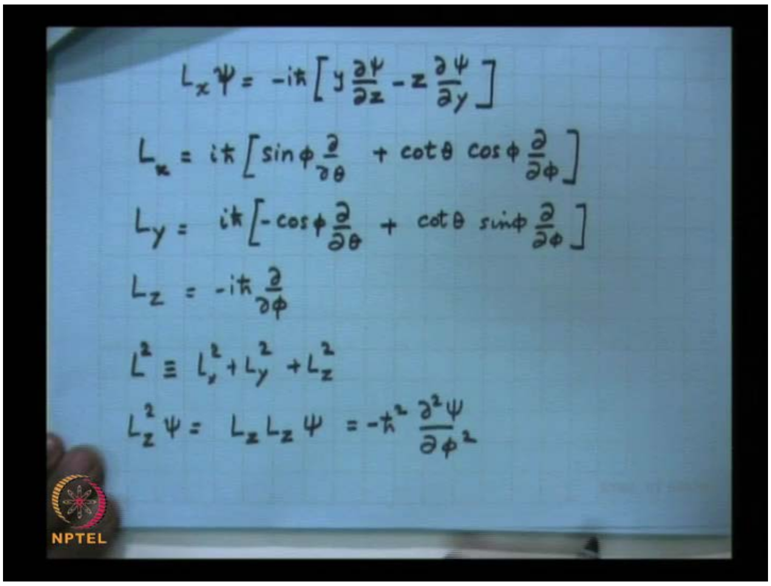

So, L x as you know will be L x operating on psi will be minus i h cross y p z, that is y delta psi by delta z minus z p y that is delta psi by delta y. And again you expressed this in terms of spherical polar coordinates and if you do that algebra then, you obtain a slightly combustion just it is not at not combustion just a little detailed algebra one has to keep track of the factors; i h cross sine phi delta by delta theta plus cot theta cos phi delta by delta phi. And L y is equal to i h cross minus cos phi delta by delta theta plus cot theta sine phi delta by delta phi and of course, we had obtained that L z is equal to minus i h cross delta by delta phi.

Now, I want an operator presentation of L square and L square is defined as L x square plus L y square plus L z square L z square is very easy to obtain, let me do this L z square psi square of of an operator is just L z operating on L z tab psi. So, if you do that this will be minus h cross's square delta 2 psi by delta phi square del by del phi and then again del by del phi but, for others it is not that simple but, fairly straight forward.

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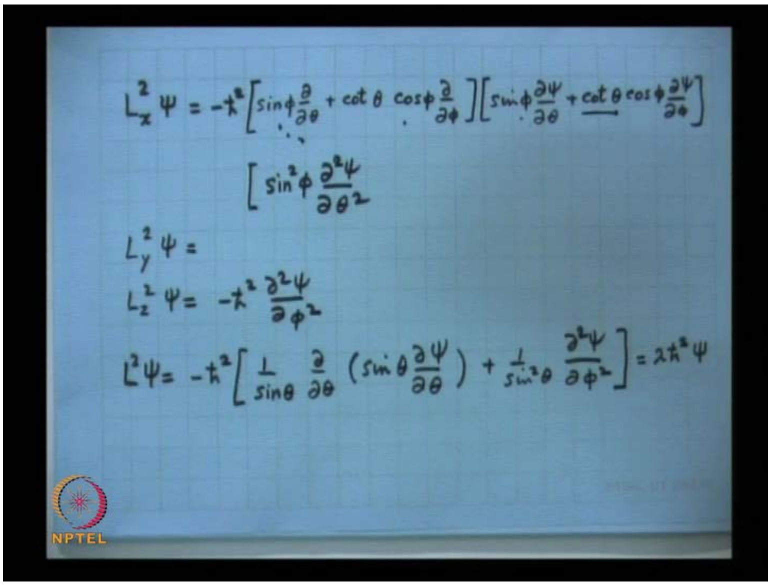

So, L x square will be L x square psi I will just write down the expression that will be equal to minus h cross's square. And then you will have sine phi delta by delta theta plus cot theta cos phi del by delta phi, this is L x times L x that is sine phi delta psi by delta theta plus cot theta cos phi delta by delta psi by delta phi.

When I will operate this on this, operate this on this, operate this on this, operate this (Refer slide time: 26:46) and we have to be very careful, when we differentiate with respect to theta then of course, phi can be kept constant, so if I operate this on this the first term will be very simple sine square phi sine square phi delta 2 psi by delta theta square. But, when we operate this on this whereas, there is a tail here, depending on theta so one has to be a little careful. Similarly, I can it is advisable that you do this once and it will allow you to get used to the way in which one deals with these operator algebra.

Similarly, one can calculate L y square and we are already L z square psi which was the easiest to calculate which was h cross's square delta 2 psi by delta phi square, if you add this up then, surprisingly this L square psi which is L x square plus L y square plus L z square; this comes out to be minus h cross's square 1 over sine theta delta theta sine theta delta psi by delta theta plus 1 over sine square theta delta 2 psi by delta phi square.

So, this is the expression that comes out for the operator L square, now our object is to find the we have found out the Eigen values and Eigen functions of the operator L z and that was very simple we have found out that that the Eigen values (Refer slide time: 28:59). Eigen values of m h cross and the Eigen functions of 1 over root 2 pi to the power of i and phi. Our next step which is not that easy is to find out the Eigen values and Eigen functions of the operator L square.

So, I write this down as equal to lambda h cross's square psi and I want to solve this, so I our objective now, is to solve this particular equation I have introduced h cross's square for the sake of convenience. So, the h cross's square, h cross's square which are constants gets cancelled and I bring this term to the left hand side.

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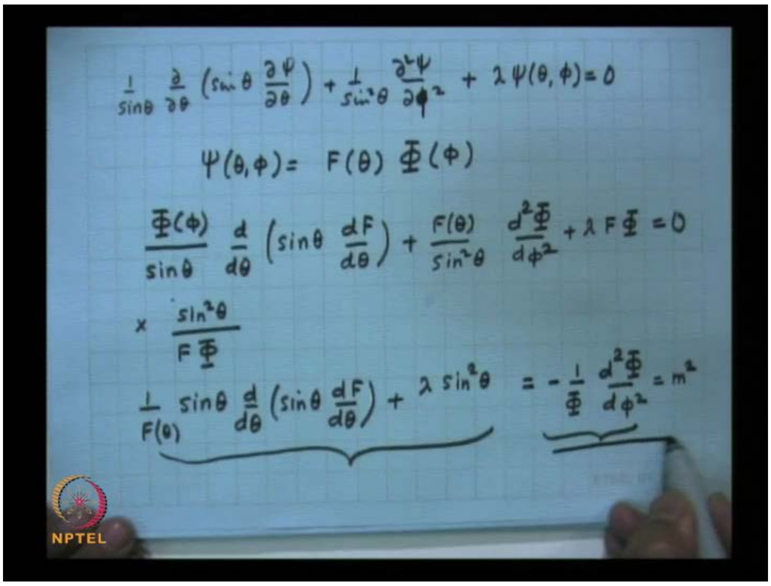

So I obtain I obtain 1 by sine theta delta by delta theta sine theta delta psi by delta theta plus 1 over sine square theta delta 2 psi by delta theta square plus lambda psi, which is now a function of theta and psi is equal to 0 I want to solve this equation. Our objective is to find this value of lambda and the corresponding wave functions that is a very important problem. Now, we use the same method method of separation of variables psi of theta and phi, we write down as f theta multiplied by capital phi of phi i'm sorry this is phi square.

So, I substitute this, so I get if I substitute it here, let me do it step by step phi of phi divided by sine theta and now, I can write it total differentiate d by d theta sine theta d F by d theta plus 1 over sine square theta. So, F will come outside, now F of theta sine square theta d 2 phi by d phi square plus lambda F into phi have the variable separated out not yet.

If this involves phi and theta this involves phi and theta this involves phi and theta (Refer slide time: 32:03) but, what we do is let me, multiply the whole equation by sine square theta divided by F times phi. So, please see if I multiply the whole equation, then I get 1 over F, because phi this phi will cancel out with this 1 over F sine square theta by sine theta that is sine theta d by d theta sine theta d F by d theta what I will do is; I will write this term first and take this term to the right hand side. So, I write plus lambda sine square theta is equal to minus 1 over capital phi d 2 phi by d phi square capital F is assumed to be to a function of theta.

So, now as you can see the variables have indeed separated out the left hand side is a function of theta the right hand side is a function of phi only, so a function of theta cannot be equal to a function of phi unless both of them are equal to a constant. So, I put this equal to m square a square of number and the reason is that it will come out in a moment.

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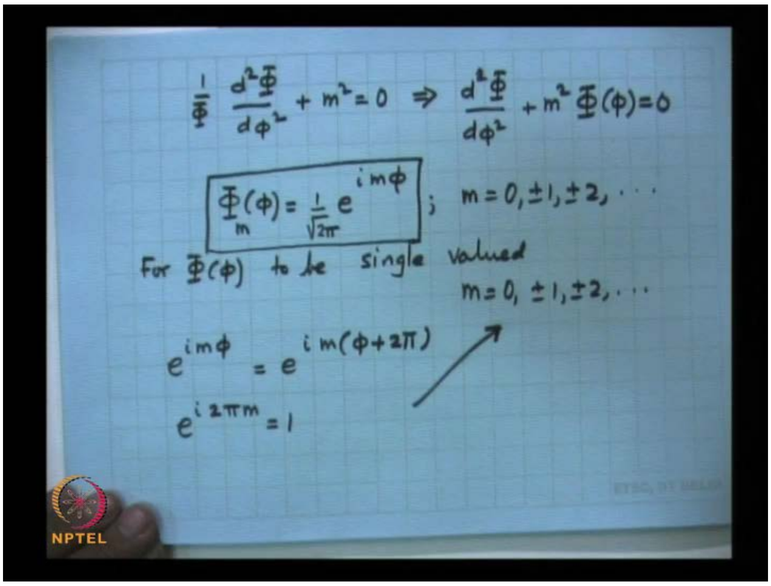

So, let me solve this part first, so this part will come out if I just look at the phi part, so I obtain 1 over phi d 2 phi by d phi square, plus if I bring it here, then it is minus minus plus m square is equal to 0 this will imply d 2 phi by d phi square plus m square capital phi of phi is equal to 0. The solution of this is extremely simple we have phi of phi is equal to again e to the power of i m phi and as we have just just discussed few minutes back if I if for the wave function to this, for phi of phi to be single valued to be single valued m must be equal to 0 plus minus 1 plus minus 2, etcetera.

That is if you increase phi to phi plus 2 pi, it must give me the same wave function that is e to the power of i m phi must be equal to e to the power of i m phi plus 2 pi, as I increase phi by 2 pi, I was get the same value of the function; otherwise the wave function will be multiple value. So, you will have e to the power of i 2 pi m must be equal to 1 and therefore, m must be 0 plus minus 1 plus minus 2, etcetera. So we have found one part of the solution and to normalize it I this form a orthonormal set of complete set of orthonormal wave functions.

So, these are which we had obtained, these are also Eigen functions of the L z operator the Eigen function of the L z operator m is equal to 0 plus minus 1 plus minus 2, etcetera. So, we come back to the equation and we find that m square must be this square of this integer can I put this as a negative constant the answer is of course, we can but, if you solve this then the solutions will be on the form of e to the power of m phi which are not single value function.

And so therefore, this has to be put equal to a positive constant if I put into a negative minus m square, then the solution will be exponential and those will not be single valued. So therefore, once we have solved the phi part of the equation rigorously, now let me solve the theta part of the equation, so we have here.

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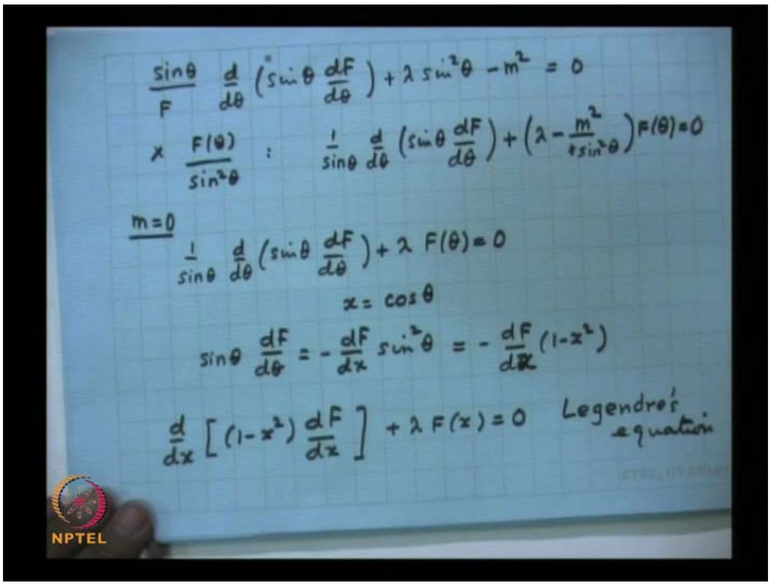

So, let me write the theta part of the equation and it will be something like this, so minus m square, so sine theta divided by F of theta d by d theta sine theta d F by d theta plus lambda sine square theta minus m square is equal to 0. I multiply the above equation by F of theta divided by sine square theta and I will get 1 over sine theta d, d theta of sine theta d F by d theta plus lambda minus m square by sorry sine square theta f of theta equal to 0; this is known as the associated Legendre equation associated Legendre equation.

The solution of this equation is little complicated but, of course, people have found the solution, what we will do is find the solution for m equal to 0; for m equal to 0 for m equal to 0 the above equation becomes 1 over sine theta d d theta of sine theta d F by d theta plus lambda F of theta equal to 0.

Now I introduce a new variable x which is defined to be equal to cos theta, so I write this in terms of this, so d F by d theta will be equal to d F in terms of the x variable x d x by d theta, that is minus sine theta. So, if I multiply by sine theta, so then this becomes sine square theta and that is equal to minus d F by d theta sorry d x 1 minus x square and then you can calculate what is d by d theta, I have just done that.

And final result will be that d of d x of 1 minus x square d F by d x plus lambda times F of x is equal to 0, this is very simple this is known as the Legendre's equation; which you must have studied but, in any case, we will obtain the solution of this particular equation.

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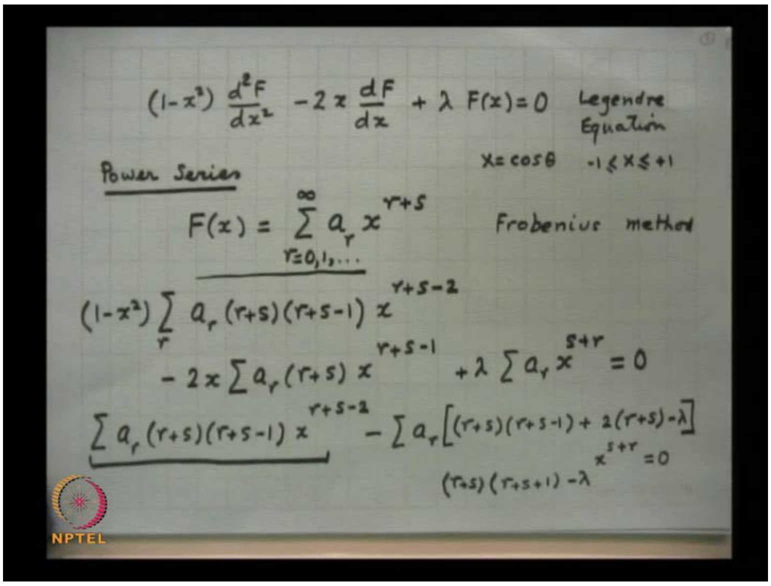

We rewrite the first the Legendre's equation, we differentiate the first term we obtain 1 minus x square d 2 F by d x square and the differentiation is minus 2 x d F by d x plus lambda F of x is equal to 0, this is also another form of the Legendre equation; here as we know that x is equal to cos theta And therefore, x lies between plus 1 and minus 1 Now, we solve this Legendre's equation by the power series method, by the power series method which is also known as the Frobenius method.

And we assume a solution of the form F of x is a sum a r x to the power of r plus s and the summation is over r, r goes from 0, 1, 2 to infinity this power series method which we had encountered while, solving the confluent hyper geometric equation is one of the very powerful methods for solving a second order differential equation.

This is also known as the Frobenius frobenius method, now I substitute the solution in this differential equation, so I will get 1 minus x square and if I differentiate this equation this equation twice this expression twice. So, I will get a r first differentiation will give me r plus s and the second differentiation will give me r plus s minus 1 x to the power of plus s r plus s minus 2 and the summation is over r minus 0 to infinity minus 2 x and if I differentiate this once.

So, you will get a r into r plus s into x raise to the power of r plus s minus 1 plus lambda and summation a r x to the power of s plus r is equal to 0 as you can see if I multiply x here so this becomes r plus s and if I multiply x square here so this again becomes r plus s, so essentially we have two terms first I multiply one by this, so I obtain this expression only.

So, summation a r r plus s into r plus s minus 1 x raise to the power of r plus s minus 2 minus and if I take to the other side or let me put the minus sign here, minus a r, now if I multiply x square here, as I just now mention becomes x raise to the power r plus s. So, it becomes r plus s into r plus s minus 1 and I have taken the minus sign out. So, this is plus 2 into r plus s and since I have taken the minus sign outside, so this is minus lambda minus lambda into x raise to the power of s plus r is equal to 0.

So, now this expression if you take r plus s outside, so this becomes r plus s multiplied by r plus s minus 1 plus 2, so this becomes r plus s plus 1 minus lambda and so since this minus this is 0, so I take to the other side of the of the equation.

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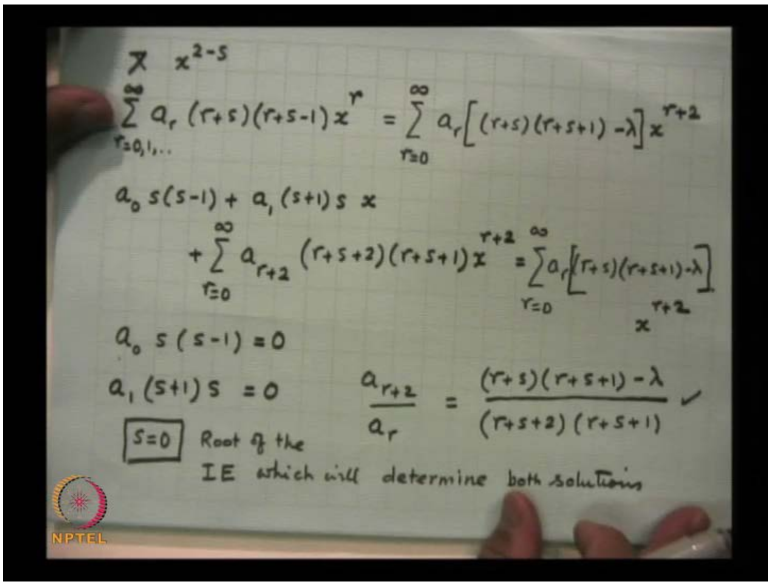

So, I will obtain I will obtain summation and let me multiply the equation the entire equation, we multiply entire equation by x to the power of 2 minus x, so the left hand side becomes summation a r r plus s r plus s minus 1 into x to the power of r, because I multiplied by x raise to the power 2 minus s. So, this term goes off so r is equal to 0, 1 to infinity and in my right hand side, becomes a r r plus s this term plus r plus s minus 1 plus 1 minus lambda times x raise to the power of r plus 2; because I have multiplied by x raise to the power of 2 minus s so this becomes like this.

So, both the sums are from 0 to infinity, now this equation as we have mentioned earlier is valid for all values of x, so I make an expansion, so the first term is a 0 r equal to 0 s into s minus 1 x to the power of 0 plus a 1 a 1 s plus 1 into x multiplied by x and then we will have plus summation a r plus 2, I replace r by r plus 2; so then r goes from 0 to infinity you say I have taken out the first two terms outside.

So, r plus 2 that means r plus s plus 2 and r plus s plus 1 x to the power of r plus 2, this is equal to the same, what is written above that is summation r equal to 0 to infinity a r r plus s the same term, within brackets r plus s plus 1 minus lambda multiplied by multiplied by x raise to the power of r plus 2.

Now, each term the coefficient this is an equation which has to be valid for all values of x, so the coefficient of x to the power of 0 must be 0 coefficient of x to the power 1 must be 0, coefficient of x to the power 2 must be 0 and so on.

So, the first term gets a 0 s into s minus 1 must be equal to 0, the second term will give a 1 s plus 1 into s is equal to 0 and the third term will get a r plus 2 multiplied by this will be equal to a r multiplied by this; so I obtain a r plus 2 divided by a r will be equal to r plus s r plus s plus 1 minus lambda divided by r plus s plus 2 into r plus s plus 1, this is known as the recurrence relation, because using this equation I can determine a r plus 2 in terms of a r.

Now, in this equation there are two roots s is equal to 0 and s is equal to 1 and the root s is equal to 0 makes a 1 indeterminate; so there is a theorem in the theory of differential equation that is one of the roots makes a 1 indeterminate, then that particular root is the root s equal to 0 will determine both the solution.

So, this is the root of the indicial equation, which will determine which will determine both solutions and we will show this in a moment, so we will just assume s is equal to 0 and if I assume s is equal to 0, then my recurrence relation becomes very simple.

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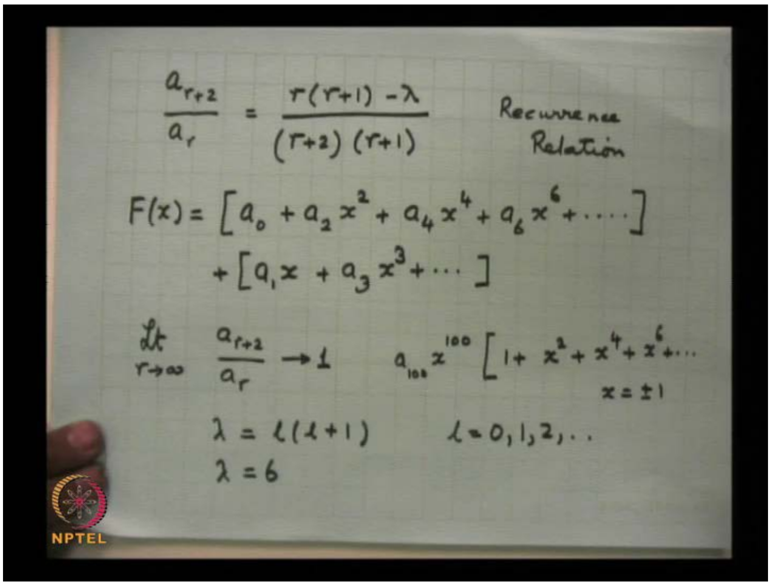

So, if I substitute s is equal to 0, then the recurrence relation will become a r plus 2 a r is equal to r into r plus 1 minus lambda divided by r plus 2 multiplied by r plus 1. Since a 0 will be related to a 2 and a 2 will be related to a 4 and so on we will have therefore. So, this is the recurrence relation, this is the recurrence relation and this is the root of the indicial equation; so my solution will be the solution F of x can be written as like this two independent solutions, the first term consists of only even powers a 2 x square plus a

4 x 4 plus a 6 x 6 only the even powers plus a 1 x plus a 3 x cubed plus a 5 x 5 and so on; Because a 2 is related to a 0 a 4 is related to a 2.

So, we have the odds even series and then we have the odd series, now we can see from this from the recurrence relation that as r tends to infinity for large terms this the dominating terms becomes r square the dominating terms in the denominator becomes r square.

So, a r plus 2 divided by r square tends to 1, so they are equal, so if I choose a larger value of r that is suppose x to the power of 100, then beyond that and the coefficients are equal; that means, let us suppose after x to the power of 100 I can write this down that a 100 and then it will be 1 plus x square plus x 4 plus x 6 this is a divergence series of x equal to plus minus 1. And therefore, it will be of at x equal to plus minus 1 the divergence at x equal to plus 1 and so therefore, for the solution to be well behaved we must make terminate the series, we must we must turn this infinite series to a polynomial and that will happen if lambda is equal to L into L plus 1, if lambda is equal to L plus 1.

That is L equal to 0, 1, 2, 3 then and then only will the will one of the infinite series become a polynomial, let me illustrate this; let us suppose I take L equal to 2, so lambda is equal to 6 and therefore, we will have we will have from here, if lambda is equal to 6.

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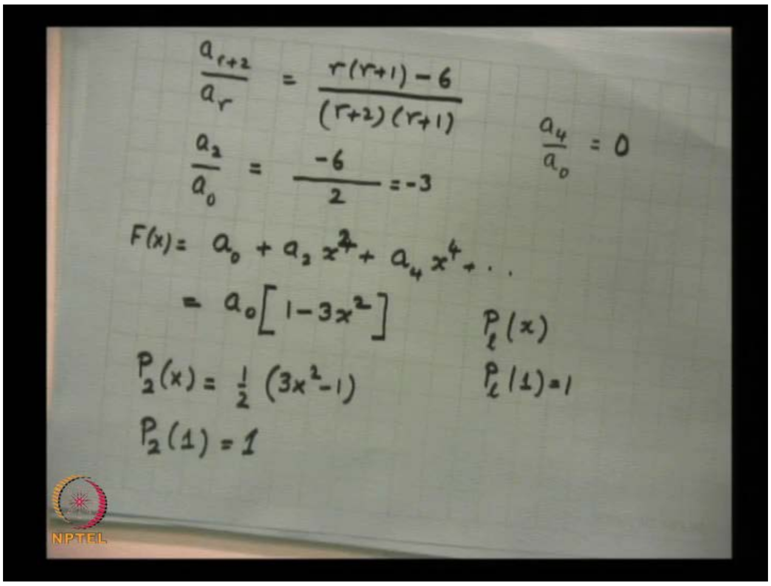

So, then we will have a r plus 2 divided by a r is equal to r into r plus 1 minus 6 divided by r plus 2 into r plus 1 and let me take the just the even series, so a 2 by a 0 that is r a 0. So, this becomes minus 6 r is 0 so 2, so this is equal to minus 3 and a 4 by a 0 will be equal to r s 2. So, 2 into 3 6 minus 6, so this is 0 therefore, the the even series, become a polynomial and we will have a 0. So F of x the even series will become a 2 plus a 2 x square plus a 4 x 4, so a 0 is a 0, let us suppose and a 2 by a 0 is 1 minus 3 x square plus a 4 is 0; so this is the polynomial solution.

And the polynomial solution is known as the Legendre polynomials, p l of x we assume that p l at x equal to 1 is 1, if I do that then p this becomes this p 2 of x this becomes 3 x square minus 1 divided by 2. When we have chosen the value of a 0, such that at x equal to 1 p 2 of 1 is 1; so we will continue from this point onwards in my next lecture.