Mathematics for Chemistry

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Module - 07
Lecture - 31
Power Series method for solving Legendre DE

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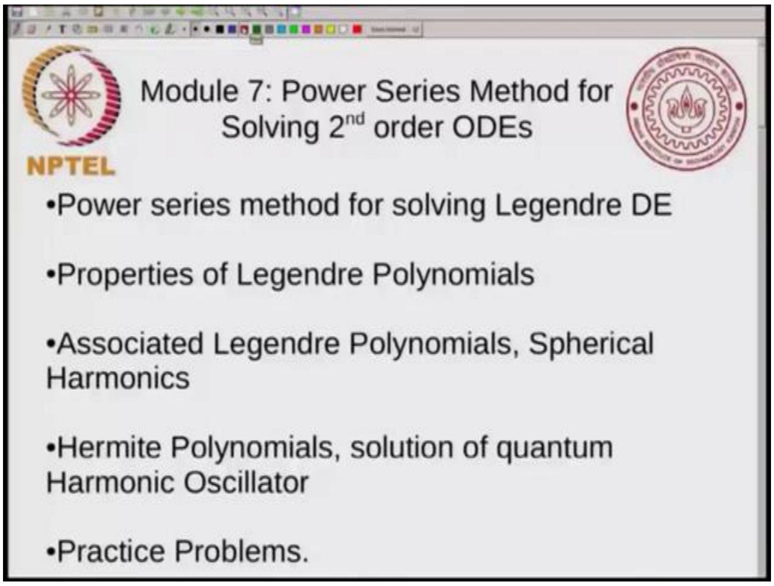

So today we will start module seven, and in this week the focus will be on using the power series method for solving second order differential equations. So, in this week there will be 5 lectures, the first one I will introduce the power series method, I will use the example of the Legendre differential equation then we will solve the Legendre equation using the power series method, and look at the properties of what are called Legendre polynomials. After that I will talk about associated Legendre polynomials and how these are collected to a spherical harmonics which is a problem that you encounter in quantum chemistry, and then I will take another problem that you encounter in quantum chemistry which is the quantum harmonic oscillator and how you will Hermite polynomials to solve this, and then we will finish with some practice problems.

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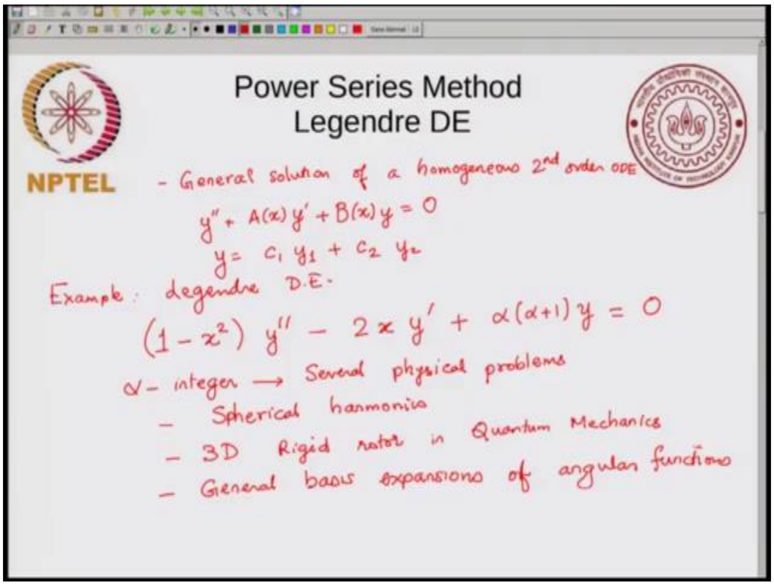

So, this will be the content of module 7. So, let us start with the power series method for solving ordinary differential equations. Now what does the power series method do it gives you the general solution of homogeneous second order ODE. So, typical homogeneous second order ODE is written in this form; so y double prime plus A of x, y prime, plus B of x y equal to 0. So, the general solution has this form y is equal to some constant arbitrary constant times y 1, which is one of the solutions plus some arbitrary constant times y 2. So, this is the general form of the solution and the power series method will show you how you can get the general solution of the homogeneous of a homogenous second order difference ODE, and I should mention that though we are talking about homogeneous second order ODE's, this method can also be extended to non homogeneous ODE's and also to higher order ODE's, but at least as far as this course is concerned, we will look at second order homogeneous ODE's.

So, the example that well that I will used to illustrate this, this is one example it is not a they can you can take many different examples; this how this is one example that we are using and this is called the Legendre differential equation. So, this is a differential equation I will write the differential equation, and we will solve it using the power series method. So, the differential equation is 1 minus x square, y double prime minus 2 x y prime plus n or I will use alpha here instead of n alpha, alpha plus 1 y equal to 0. So, this is the Legendre differential equation, and later on we will be interested in integer values of alpha. Later on we will look at integer values of alpha, but right now this is the form of the Legendre differential equation.

So, I will just mentioned that alpha being an integer, this is there are several physical problems. So, it is this is a form of solution of several physical problems. So, one of them will see later on which is what is called spherical harmonics, which is related to the solution of the rigid rotor in quantum mechanics. So, spherical harmonics and this is 3 D rigid rotor this is in quantum mechanics. So, the quantum mechanical 3 D rigid rotor is what will be solved using this Legendre polynomials. Also I should mention that this solution of this Legendre differential equation which leads some something called Legendre polynomials, these are also very important in general basis expansions of angular functions, and I am just writing this for now we will see later on how this is done, but the basic idea is that if you have a system when where you have an angular variable, and usually the angular variable has certain range of values let us say 0 to pi or 0 to 2 pi, then these Legendre these solutions of the Legendre differential equation these are very useful to get to as a basis for various problems with angular function.

So, now, what is the method of the power series method? So, what are the steps in the power series method, and keep in mind that we want to solve the Legendre differential equation.

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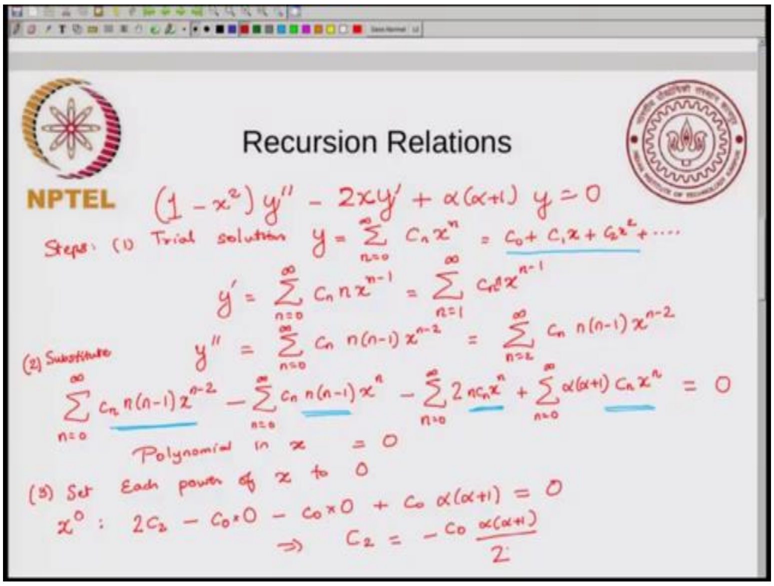

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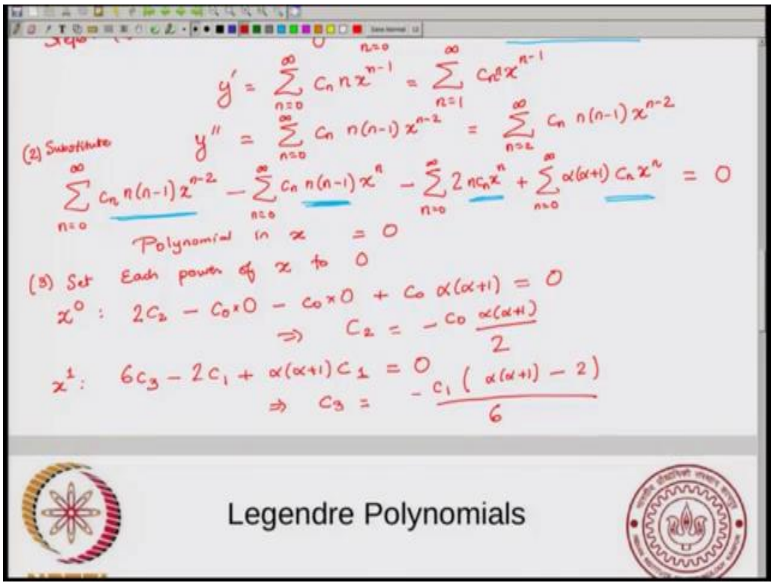

So, I will just list the various steps. So, the first step, I will write the equation again 1 minus x square put 0. So, the steps are; so the first one use a trial solution. So, you try a solution of the form y is equal to sum over n equal to 0 to infinity, C n x raise to n. So, C n is a coefficient and you have x to the n th power. So, basically this is called the power series. So, this looks like C 0 plus C 1 x, plus C 2 x square plus so on it goes up to infinity. So, this is a trial solution and the basic idea of the method is to use this as a trial solution in the differential equation. So, if you use this as a trial solution then you can immediately write y prime is equal to; now what you can do is you can you will have a sum over z n equal to 0 to infinity, and then you have to take a derivative term by term derivative. If you take a derivative C n is a constant. So, you will C n will be left as it is derivative of x raise to n is n times x raised to n minus 1.

Now, when you do this you will notice that the n equal to 0 term is actually 0. So, this actually starts from this sum even though you can write it from 0 to infinity, the n equal to 0 term is 0, so you can also write this as 1 to infinity. C n n x raise to n minus 1. So, this is the derivative and then you can write the second derivative similarly, and this will be sum over n equal to 0 to infinity; now you have C n n, n minus 1 x raise to n minus 2 and again now in this case the n equal to 0 term is 0, n equal to 1 term is also 0. So, actually you can write this sum as starting from n equal to 2 to infinity, and if you look at the form of y, y has this form and now when you take the derivative; obviously, the constant term will give you 0 derivatives. So, therefore, you would not have a constant term. So, the C 0 term n equal to 0 term will not contribute to the derivative; when you take a second derivative both these the first 2 terms will actually go out they would not contribute to the derivative. So, therefore, the derivative contribution start from C 2 onwards.

So, now once you have this trial form we substitute in the differential equation, and when you substitute this in the differential equation what will happen is you will have. So, I will write each term I will write this as 2 terms. So, the 1 minus x square I will write each of the term multiplies y double prime. So, the term is just y double prime. So, that I will write as sum over n equal to 0 to infinity, C n n, n minus 1 x raise to n minus 2. The second term is minus x square y double prime. So, now, if I multiply this by minus x square, so I have a minus and I have some over n equal to 0 to infinity, now I have C n n n minus 1, now I have x raise to n x square into x raise to n minus 2 is x raise to n. So, that is what you will get from the first term on the left, the second term the minus 2 x y you can see that it gives you minus sum over n equal to 0 to infinity; now you have a 2 and you have n x raise to n. So, that is the that is what you get from this minus 2 x y minus 2, x y prime minus 2 x y prime gives you that.

Now, the next, so and the last term will give me plus sum over n equal to 0 to infinity, alpha, alpha plus 1 look I missed a C n here there should be a C n x raise to n, and alpha alpha plus 1 now you just have y, y is just C n x raise to n equal to 0. So, you can verify that these are the terms that you will get, when you substitute this form of y in the in the differential equation; now what can you do with this. So, this is a polynomial in x. So, what you have this whole left hand side is a polynomial in x, in x and the right hand side is 0. So, if a polynomial in x is 0 then each power of x should equal 0. So, each power of x on the left hand side should equal 0.

So, this I will say is the second step. So, the second step was to substitute; now the third step in this in this method is to set each power of x to 0. So, for example, if you take if you look at the power of x raised to 0. So, it is a polynomial, so the constant or x raise to 0 term. So, how can you get an x raise to 0? So, in the first term here in this term you can get an x raise to 0 if n equal to 2. So, if n equal to 2 then you will get something that looks like C 2 and then you have 2 into 2 minus 1, 2 into 1.

So, that is 2. So, you have 2 C 2 and then you have x raised to 0, then here in this case you will get x raised to power 0 if n equal to 0. So, in the second term in this term you should have n equal to 0. So, that will give me. So, minus C 0; now if n equal to 0 then actually n equal to 0 this becomes 0. So, you have into 0, this will actually not contribute the contribution will be 0. Similarly here also you have to have x raised to 0 in the third term, the third term x raise to 0 comes from n equal to 0 and again that will also contribute 0.

So, you will have minus C 0 into 0, in the fourth term you will have x raised to 0 contribution from n equal to 0. So, when n equal to 0 you will have C 0 alpha, alpha plus 1. So, you have plus C 0 alpha, alpha plus 1 equal to 0. So, what we did is we equated the coefficient of x raise to power 0 to 0 it gives you the ray of very nice relation, it gives you C 2 equal to minus C 0 alpha, alpha plus 1 divided by 2. So, this is a relation between C 2 and C 0. Now next we can set the power of x raised to 1 to 0. So, what is the coefficient of x raise to 1? So, if you want to have x raised to 1 then here n has to be equal to 3. So, you will have a 3 into 2 that is 6 C 3 from this term, here if you have to have x raised to 1 then they then n has to be equal to 1, but if n equal to 1 then you have n into n minus 1. So, this is the second term. So, the second term will again be 0 and I would not write at this time.

In the third term you can have n equal to 1. So, if n equal to 1 then you will get minus 2 into 1 into C 1. So, minus 2 C 1 and then again in the last term you can have n equal to 1 and in this case we will get plus alpha, alpha plus 1 C 1. This is the coefficient of x to the power 1 and this has to be equal to 0. So, what that gives you is that you will get the relation C 3 equal to equal to. So, now, I will write it in this form, I will write it as minus C 1 times alpha, alpha plus 1 minus 2 divided by 6. So, C 3 is related to C 1. So, C 3 is proportional to C 1, C 2 was proportional to C 0. Now you can go on you can do this and let me do it right here.

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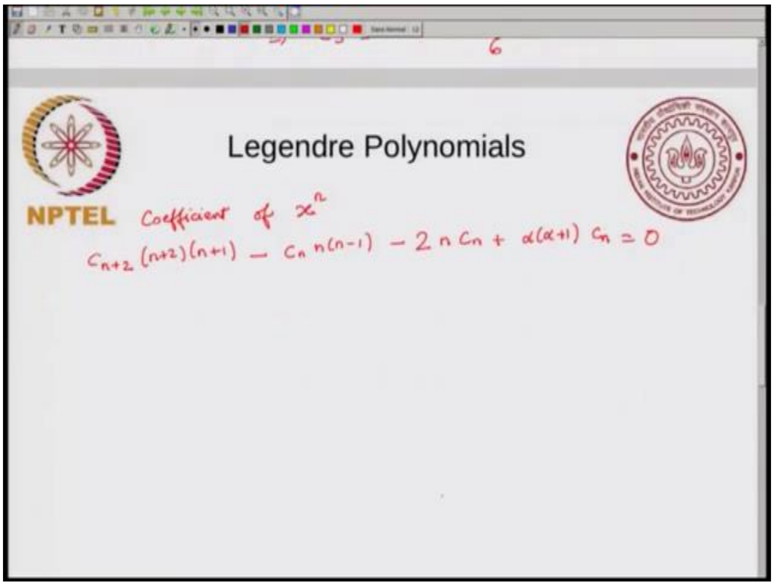

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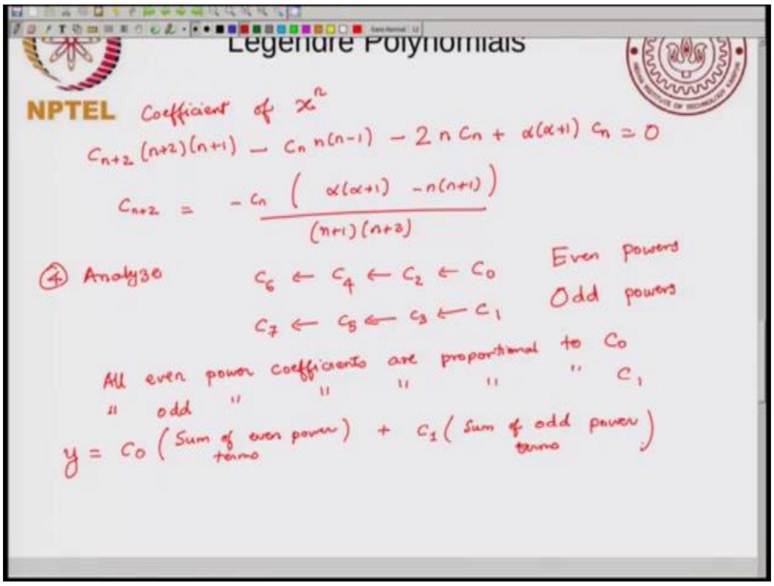

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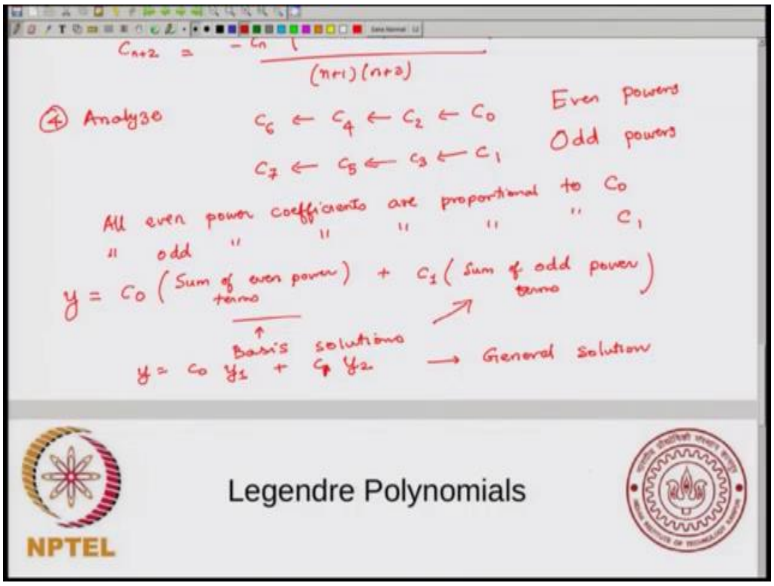

Let me now look at the coefficient of x raise to power n, x raised to power n. So, if you have to have any power of x raised to n then I will show it in green. So, in this term you should have n equal to n plus 2. So, what you will get the term that had that has the power of x raise to n will actually contain C n plus 2, into now you have n plus 2 into n plus 2 minus 1. So, n plus 2 into n plus 1, this is the coefficient of x to the power n. The second term will have x to the power n. So, we will have C n, n, n minus 1. The third term you will have minus 2 n C n, and the fourth term you will have plus alpha, alpha plus 1, C n is equal to 0. So, this is what you get from the coefficient of x raise to n, and you can rewrite this I will let you work it out so, but I will just write the final results. So, you have C n plus 2 is equal to and I will write it in minus C n times alpha, alpha plus 1 minus n, n plus 1 divided by n plus 1, n plus 2. So, this is what you will get.

What you will get is that C n plus 2 is related only to C n. So, now, now the fourth step is to analyze. So, what do we mean by analyze. So, what we notice is that from C 0 you can calculate C 2; C 2 you can express in terms of C 0, and C 4 can be expressed in terms of in terms of C 2. So, you can write C 4 in terms of C 2, using this general relation that we have and you can writes C 6 in terms of C 4, C 4 in terms of C 2, C 2 in terms of C 0. So, in similarly you can go other side, so you can write C 7 in from C 5, you can write C 5 from C 3, you can write C 3 from C 1.

So, what this means is that any these are the even terms, even powers of x these are odd these are terms these are coefficients of odd powers of x. So, you can write the coefficient of any even power of x in terms of C 0. So, basically you can write my you can say that all even power coefficients are proportional to C 0. Now this is again very specific for the Legendre differential equation, it is not generally true in this particular case you found that all even power coefficients are proportional to C 0, and you also find that you can similarly see that all odd power coefficients are proportional to C 1. So, basically what you can say is that I can write y, I can collect all the even power coefficients and they will. So, what I will get is C 0 times sum of even power terms, plus C 1 times sum of odd power terms.

So, I can write my solution in this form. So, all I did was I took my original trial solution which has this form C n, x raise to n. So, what I did is I take this C and x raised to n and what I see is that all the even terms C 0, C 2, C 4 etcetera they are all proportional to C 0. So, I collect them together similarly all the odd terms C 1, C 3 etcetera they are proportional to C 1. So, I collect those together and I can write it in this form.

Now, this is a very nice form because you can think of these as basis solutions. So, this and this I can think of basis solutions, and then what you have is you can you have the form y equal to C 0 times y 1, plus C 2 C 1 times y 2. So, you are writing a general solution with these 2 basis solutions and so, C 0 and C 1 are arbitrary. So, this looks like a general solution. So, this is the crux of the power series method, and this is how you find a general solution of a differential equation. Now what we will do is we will just analyze this little more. So, in terms of the method this is how you use the power series method and C 0 and C 1 or 2 arbitrary constants and essentially you are done, now what we will do is we will just look at the properties of these general solutions and this is where we is come across something called Legendre polynomials.

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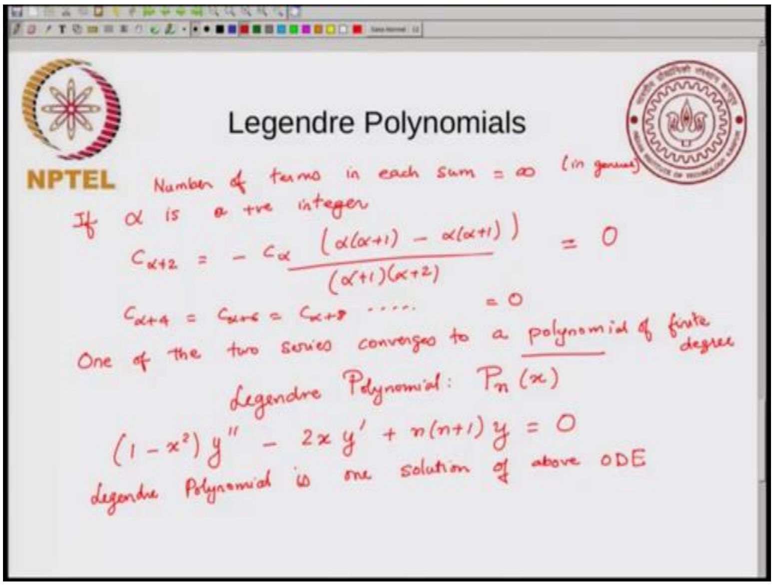

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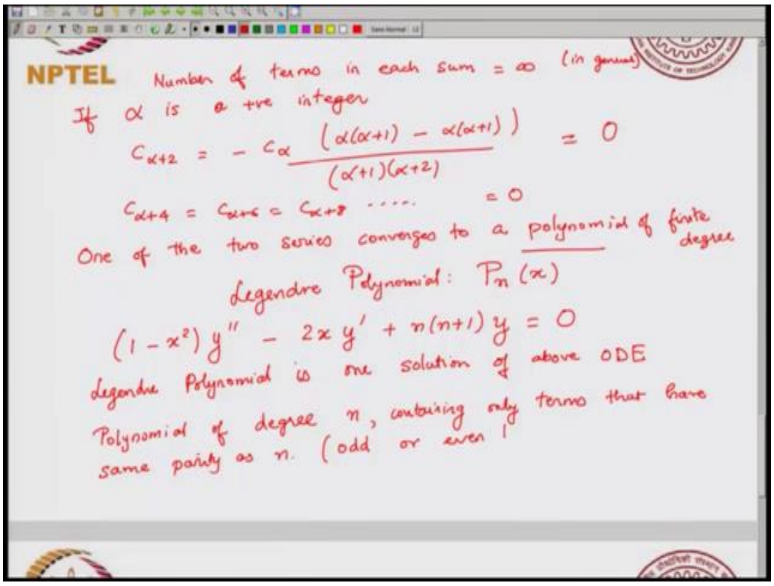

In order to motivate them what I see is that in this sum of even terms, even power terms and some of odd power terms. So, the number of terms in each sum in general equal to infinity so, in general. So, in general there are infinite many terms in each of these because the series keeps on going.

Now; however, if alpha is an integer is a let us say positive integer. So, if alpha is a positive integer then we notice that C of alpha plus 2. So, if you look at C of alpha plus 2, so I can write it as minus C alpha times alpha, alpha plus 1 and then I had minus n, n plus 1 which is nothing, but alpha, alpha plus 1 divided by alpha plus 1, alpha plus 2 and this is equal to 0. C of alpha plus 2 equal to 0, and what you notice is that lets just go back to our relation by the way I did not mention this, but this is called a recursion relation. So, the recursion relation relates C n to C n plus 2 there are many other kinds of recursion relation, but this is one form of the recursion relation that you always encounter whenever you are doing the power series method.

So, what happens is that when alpha equal to n, when n is equal to alpha then the numerator goes to 0 in the recursion relation and so you get 0, and what does this mean? This means that also C of alpha plus 4 equal to C of alpha plus 6 equal to C of alpha plus 8 all of them is equal to 0. So, all those any term that is of the same parity as alpha, but has the value greater than alpha. So, like alpha plus 2, alpha plus 4, alpha plus 6 all of them all those sums go to 0 so; that means, if alpha is a positive integers then one of the 2 series converges to a polynomial to a polynomial; that means, a polynomial of finite degree, and this polynomial of finite degree is referred to as the Legendre polynomial.

So, what is the Legendre polynomial the symbol used is P n of x. So, P n is this is a symbol for the Legendre polynomial, n is the degree of the polynomial. So, that means, your P n Legendre polynomial, P n is a solution of the differential equation 1 minus x square,, y double prime minus 2 x y prime plus n, n plus 1 y equal to 0. So, the solution of this differential equation, so it is one solution, so Legendre polynomial is one solution of above ODE. So, it is one of the solutions. So, the other solution will be an infinite series. So, if you look at your sum of even power. So, you have these 2 basis solutions sum of odd powers, now one of them if alpha is even then this term then the sum of even powers will go to 0 at when n is equal to alpha, if alpha is odd then the sum of all power terms will go to 0 beyond sum alpha.

So, one of these will become a polynomial and that polynomial is called the Legendre polynomial. So, what can you say about Legendre polynomial. So, I will just mention this. So, it is a polynomial of degree n containing only terms that have same parity as n. So, what I mean is that it contains only odd or even or even terms.

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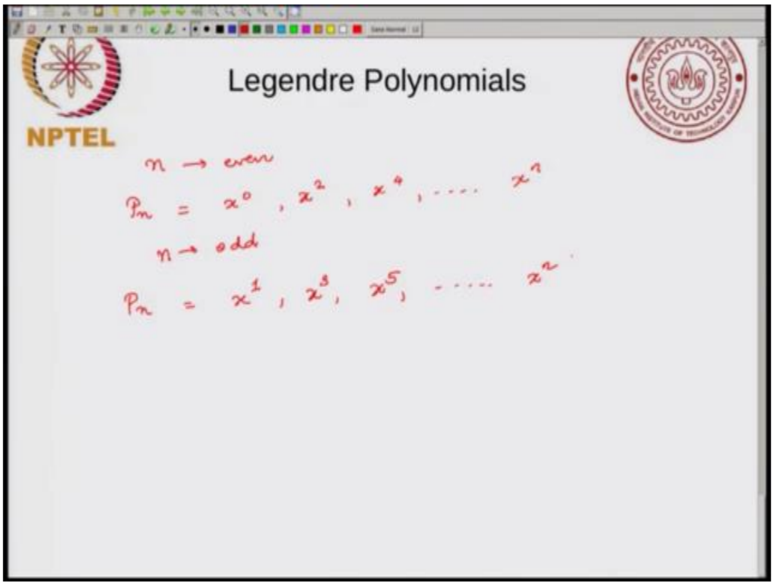

So, for example, if you have n even, then P n will have terms that that contain x to the power 0, x to the power 2, x power 4 and so on up to x power n. If n is odd then the P n will contain terms that look like will have terms of x power 1, x power 3, x power 5 and so on up to x power n. So, it will be a polynomial that contains only one type of terms. So, in the next class we look at some of the properties of these polynomials, we look at what the forms of these polynomials are we will investigate some of their properties.

Thank you.