Mathematics for Chemistry
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Module - 07
Lecture - 32
Properties of Legendre DE

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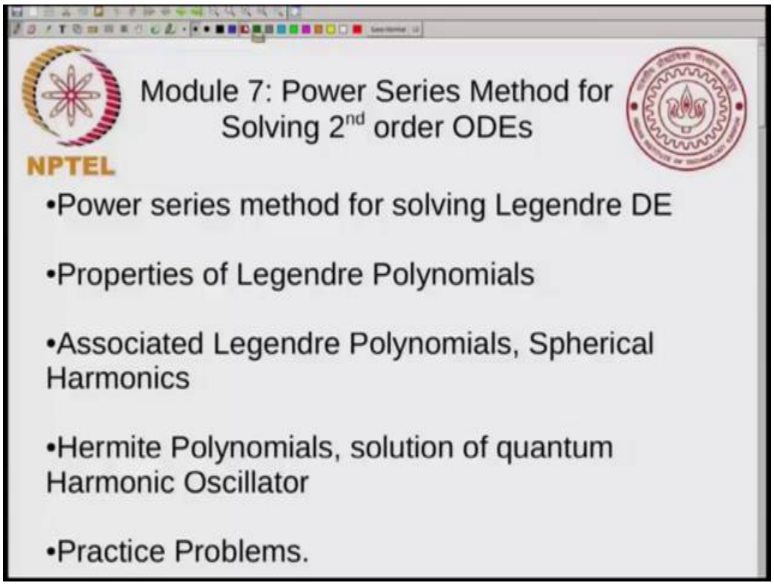

So we just saw how to use the power series method and we took the example of the Legendre differential equation, we briefly mentioned what Legendre polynomials are. So, in today's class I am going to be talking about the properties of these Legendre polynomials.

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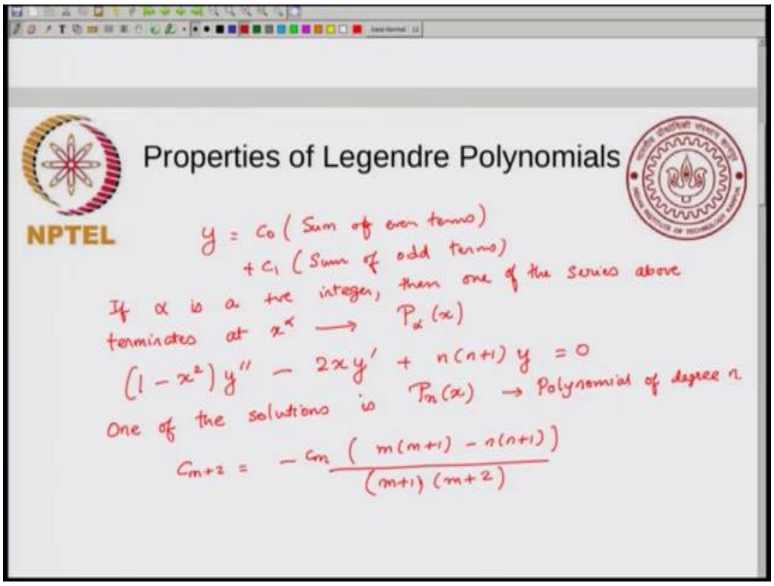

So, from the last class we saw that Legendre polynomials they are solutions of a differential equation, and do is that a differential equation has the solution y is equal to c 0 times sum of even terms, plus c 1 times sum of odd terms, this is the general solution of the Legendre differential equation for any value of alpha and one of these terms if alpha is a positive integer, if alpha is a positive integer then one of the series above terminates at x bar alpha. So, this series is what we called P alpha of x. So, in other words if you had a differential equation 1 minus x square y double prime, minus 2 x y prime plus n n plus 1 y equal to 0, then one of the solutions is P n of x. So, one of the solutions and this is a polynomial, this is a polynomial of degree of degree n and what we said is that if n is even then there will be only terms of even powers of x, if n is odd there will be only terms of odd powers of x.

So, now we can ask what are these polynomials. So, you can actually use this since we know how to calculate the individual coefficients. So, we had the recursion relation C n plus 2 equal to minus c n times we had this (Refer Time: 02:47) I should write a slightly differently I will use c m plus 2 is minus c m times, now you had m m plus 1 minus n n plus 1. So, I am using n to because n is what the degree of the Legendre polynomial is. So, my differential equation has an n. So, earlier I had an alpha now I am using n here because when alpha because what we said is alpha is a positive integer. So, n is a positive integer, and now I am writing the recursion relation that relates the m plus 2 th term to the c m term, and what I have in the denominator is m plus 1 m plus 2. So that means, I can calculate each of the polynomials; now we will write down some of the polynomials.

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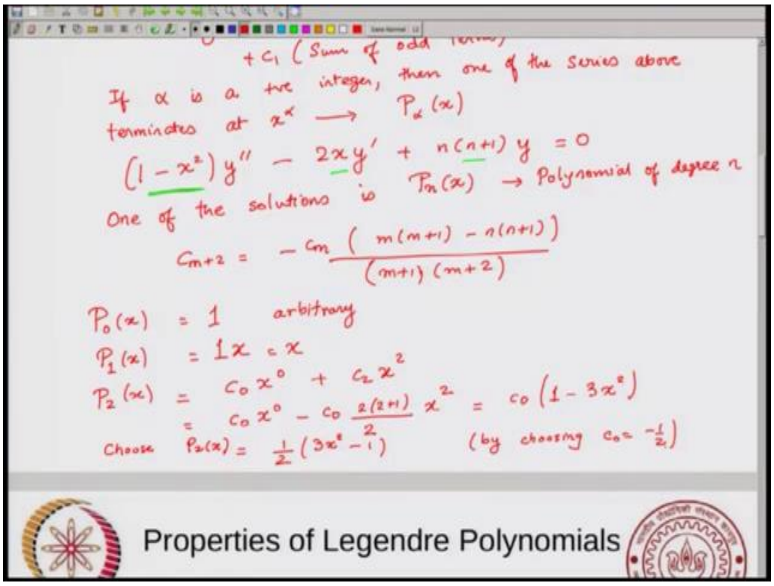

So, your P 0 of x this is chosen to be 1. So, this is arbitrary you can choose P 0 in anyway P 0 is just a constant, and any constant will satisfy this differential equation and we just set that constant to be equal to 1. If you take P 0 then n equal to 0, so then this last term drops off and you can see that any constant will satisfy the remaining differential equation. So, your P 0 is arbitrary we choose it to be 1; similarly P 1 of x this is also chosen to be 1, if you set n equal to 1 then your differential equation this should be 1 into x, x equal to x. So, if you set P 1 of x equal to x, now for n equal to 1 this is 1 into 2 that is 2 y. So, you have minus 2 x y prime plus 2 y equal to 0, and anyway y double prime. The second derivative of x is 0, the first term in the differential equation will go away this term will not contribute for when you set y equal to x, this term when you set y equal to x y prime is 1 so we will get minus 2 x, and this is plus 2 into x. So, you can clearly see that x satisfies this differential equation. So, P 1 of x is taken as x. In fact, x is the correct solution for this ok.

Now, P 2 of x, if you want to calculate P 2 of x, P 2 of x will have two coefficients will have a c 0 and a c 2, but c 2 and c 0 are related to each other through this recursion relation, and when you use that relation and relate c 0 and c 2 you can finally, write an expression for P 2, now remember it has both a constant and a and a second power term.

So, I will just write the final expression for P 2, and you can work this out it is not very hard. So, you have c 0, x power 0 plus c 2 x square, and c 2 we already saw that c 2 is equal to from. So, we already saw that c 2 is related to c 0 through. So, for we have c 0 x power 0 now c 2, I can write as minus c 0 into alpha, alpha plus 1 by 2.

Now what alpha is nothing, but n and n is equal to 2, so I have 2 into 2 plus 1 divided by 2, and this multiplies x square. So, finally, I can write this as. So, this is 2 into 3 6 by 2 that is 3. So, I can write this as c 0 times and I can write this as 1 minus 3 x square. So, now, so, I can choose any value of c 0; so the choice that we make for c 0. So, we choose P 2 of x again I emphasize that this is a choice because you can choose any value of c 0. So, we choose c 0 and this is for a this choice actually ensures certain properties of the Legendre polynomials which we will see soon.

So, you choose your c 0 such that, you choose c 0 equal to minus half. So, this becomes half 3 x square minus 1. So, you choose your c 0 to be minus half. So, then P 2 of x becomes half 3 x square minus 1. So, this is by choosing I should emphasize that your choice of c 0 is completely arbitrary, it has no relation to what you chose for another for another polynomial and so on.

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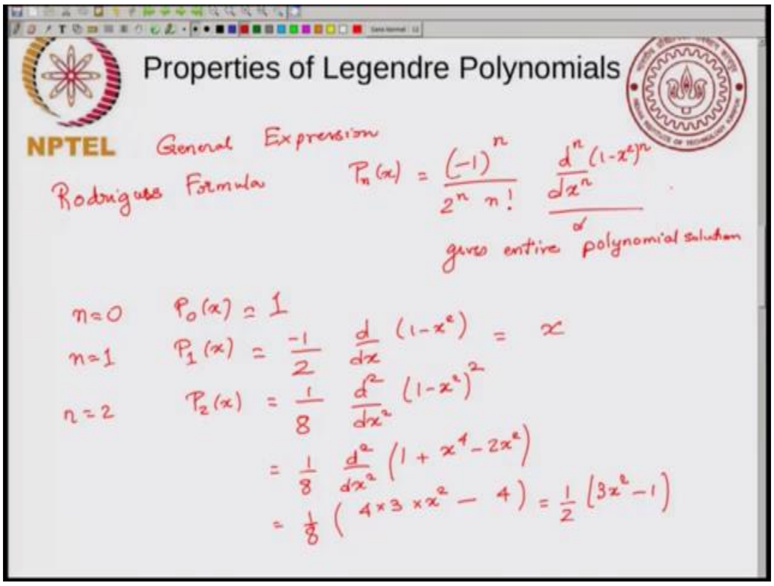

Now, you can go on and you can write the other polynomials also, but basically there is a certain choice of polynomials I will come to the general expression. So, the general expression this is called the Rodriguez formula. So, your P n of x is chosen as minus 1 to the power n divided by 2 raised to n into n factorial, and this is d n by d x raised to n 1 minus x square raised to n. So, this factor the last factor the n th derivative with respect to x of 1 minus x square raised to n, this will give you the polynomial then you multiply the this by this constant. Now this constant is chosen, so that you know you satisfy certain properties of the certain relations between various polynomials. So, even if you did not have this constant you would still satisfy the differential equation, because it is a homogeneous equation multiplying it by a constant will still give you a solution.

So, what is important is that this particular choice will preserve certain relations and we will see that in a minute. Now what is interesting is that this d square by d x raised to n this gives entire polynomial not just one of the coefficients, gives the entire polynomial solution this is very important and we can just try a few just to be just to make sure that you are consistent with what we had. So, if n equal to 0, then P 0 of x is equal to. So, now, all these constants will just become 1, now the 0 th power of this 0 th derivative is just nothing you do not take any derivative, and 1 minus x square is to 0 is also 1. So, this is just 1. So, it matches what we had earlier, then n equal to 1 then you have P 1 of x. So, this now what is P 1 of x? So, we have minus 1 raised to 1, 2 raised to 1 that is 2 and 1 factorial is 1. So, you have 1 over 2, now what you have is d by d x of 1 minus x square. Now what is d by d x of 1 minus x square? It is just you have a minus 1; d by d x of 1 minus x square is just minus 2 x.

So, minus 2 x times minus half, that is equal to x. So, P 1 of x is equal to x; n equal to 2, P 2 of x now you have minus 1 square which is 1, 2 square that is 4, 2 factorial that is 2. So, 1 over 8, now you have d square by d x square of 1 minus x square whole square, and you are taking the second derivative of this, now again you can work out the second derivative. So, this will have 3 terms will have an x power 4. So, I will just write this directly. So, 1 over 8, d square by d x square of 1 plus x raised to 4 minus 2 x square, and when you take 2 derivatives of x raised to 4, you will get 4 into 3 into x power 2. So, and when you take 2 derivatives of 1 you will get 0, when you take 2 derivatives of 2 x square you will get 4 minus 4.

So, this gives me 1 by 8, 4 into 3 into x square minus 4. So, this is nothing, but half 3 x square minus 1 which is exactly what we had earlier. So, now, this formula that Rhodri is give it is a very nice formula it tells you how to generate.

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Each of those each of the Legendre polynomials. So, I mean it is not something that you can derive directly, I mean this is something that is I mean there is a certain reason for this choice which will be clear soon, but the point is that you can have this formula and you can this simple formula can generate each of the Legendre polynomials, and I emphasize that you know we are not going to derive the Rodriguez formula, you can try to derive it is actually a lot of work, but we just notice these formulas because these are very interesting ways to generate the Legendre polynomials; and once you have the Rodriguez formula you can get lot of other interesting properties of Legendre polynomials.

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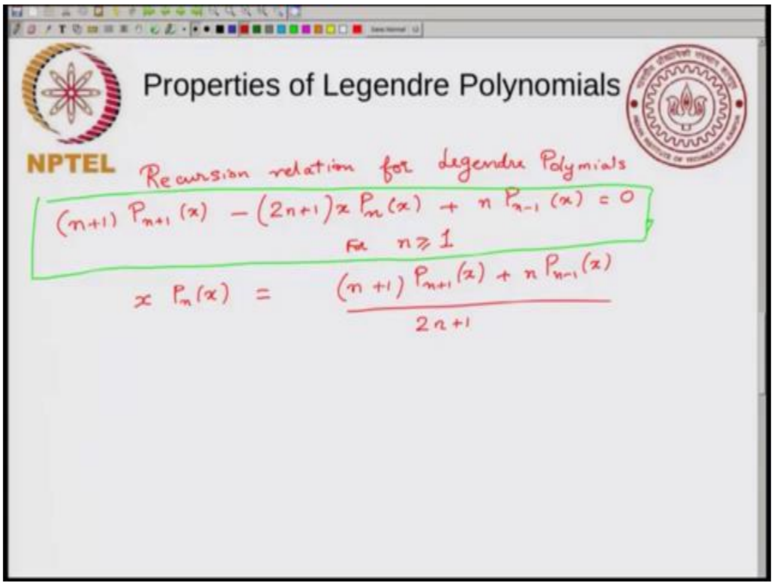

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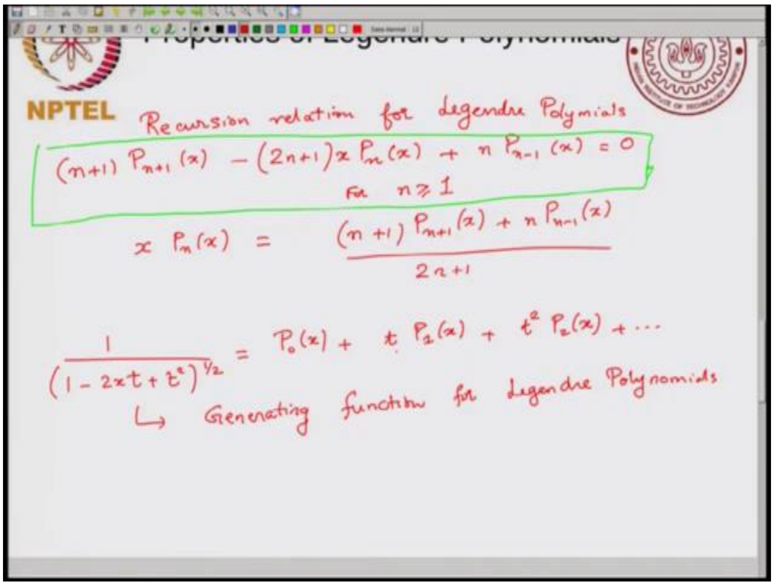

So, one interesting formula is what is also called a recursion relation for Legendre polynomials. This is different from the recursion relation between the coefficients that we got in when we were doing the power series. So, this recursion relation says at n plus 1 times P of n plus 1 x, minus 2 n plus 1 into x P n of x, plus n times P n minus 1 of x equal to 0, this is for n greater than equal to 1. Obviously, when n equal to 0 then such a relation is not valid, because you do not have P minus 1 ok.

So, now this is a very interesting relation, it relates a Legendre polynomial of degree n plus 1 to a Legendre polynomial of degree n multiplied by x, and a Legendre polynomial of degree n minus 1. And you know another form in which this relation is often written is the following. So, it is written as x times P n of x is equal to n plus 1 times P n plus 1 of x, plus n times P n minus 1 of x divided by 2 n plus 1. So, what that means is if we take a Legendre polynomial multiply it by x, you can write it as a combination of the n plus 1 th Legendre polynomial, and the n minus 1 th Legendre polynomial with some factors. This is again a very nice relation and it actually turns out to be fairly powerful; another interesting relation I am just going to mention these now I do not expect you to remember all these relations, but you should have the sense that that you know you can I mean I actually I take that back. So, this recursion relation is something that you should try to remember. So, this is a relation that you that you should try to remember, there are some factors n plus 1 and n and you know, but the important content of the equation should also be very clear to you, the content of the equation is that you relate the n plus 1 th polynomial to the n th polynomial with a multiplication factor of x, and the n minus 1 th polynomial.

So, this is a recursion relation and you know it is it is good to remember the recursion relation for the Legendre polynomials, it is also good to I mean I do not expect you to remember the Rodriguez formula, but at least you should have you should know what the first few Legendre polynomials are. Now what about what are some of the other interesting things? And these I do not expect you to remember. So, there is a relation this is suppose I take 1 over 1 minus 2 x t, t is a variable plus t square raised to half. So, I take this function of t, it is a function of t and x and I do a Taylor expansion, I write it as a pole I do a Taylor expansion about t equal to 0. So, the first term will turn out to be equal to P 0 of x, second term will be t times P 1 of x, third term will be t square times P 2 of x, and you can show this you can show that whatever you get will exactly be equal to the Legendre polynomial of degree n. So, the n th term will be the will be related to P n of x. So, this is called a generating function for Legendre polynomials.

So, this function generates all the Legendre polynomials just by Taylor expansion. So, you can do a simple Taylor expansion about t equal to 0, and you will get all the Legendre polynomials. Again it is a very nice relation I do not expect you to remember this generating function, but what we will we will see when we do other power series that each of these power series methods that we do will generate polynomials and each time you have a polynomial you will have some sort of generating function.

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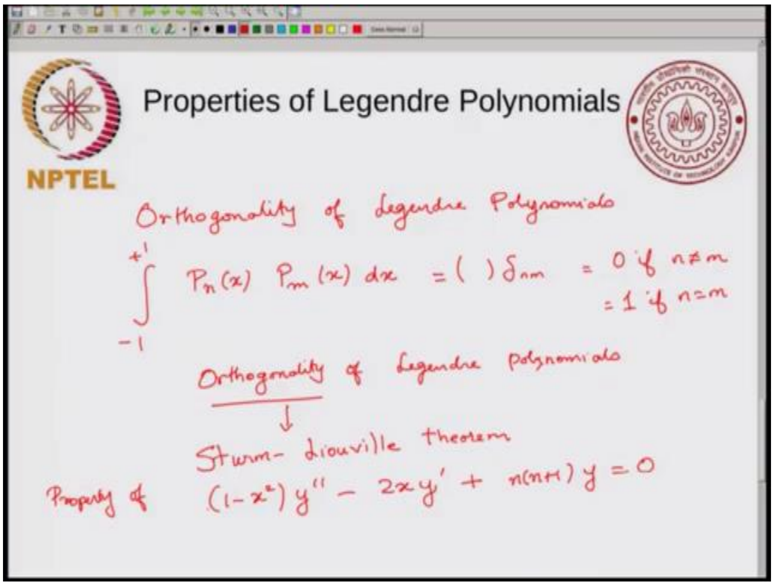

Now, the next important point and this is a point that I think is really important and really useful. So, this is the property of the Legendre polynomial that is called orthogonality. So, the orthogonality of Legendre polynomials, so what this means is that if you take integral minus 1 to plus 1 of P n of x, P m of x, d x. So, what you are doing is you are taking the n th Legendre polynomial and the m th Legendre polynomial both these are functions of x.

So, you multiply them and integrate them from minus 1 to 1, then this is equal to delta n m; that means, this is equal to equal to 0 if n is not equal to m and equal to 1, if n equal to m. Now this is a very it is an extremely powerful relation. So, this orthogonality of Legendre polynomials I should actually there is a factor of two. So, I would not if you take I would not write this as a delta function yet. So, it is actually a delta n m multiplied by some factor ok. Multiplied by some factor I would not mention that factor right now, but the point is that it is equal to 0 if n is not equal to m, and this delta n m is equal to 1 if n equal to m. So, it is some factor multiplied multiplying the delta function; it is not just a delta function.

Now, what we say is that this is orthogonality of Legendre polynomials, we will see later on that you know lay you know in advanced classes you might learn that this orthogonality of Legendre polynomials is related to something called Sturm Liouville theorem, which we would not be doing in this course. So, it is related to something called a Sturm Liouville theorem. So, you are, it comes directly from the differential equation. So, this is a property 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, it is a property of the differential equation. So, the property of this differential equation is that the polynomial solutions are orthogonal, that comes from the Sturm Liouville theorem.

Now, also I just want to point out one thing we will come back to this later that the range of range of x is minus 1 to 1, now notice that when x equal to minus 1 or 1 then this goes to 0. So, this goes to 0. So, the second derivative term goes off when x equal to minus 1 or 1, and we later on see that these are what are called singular points, and we will see how to deal with differential equations that have singular points, but nevertheless in this range from minus 1 to 1 you never have this term go to 0.

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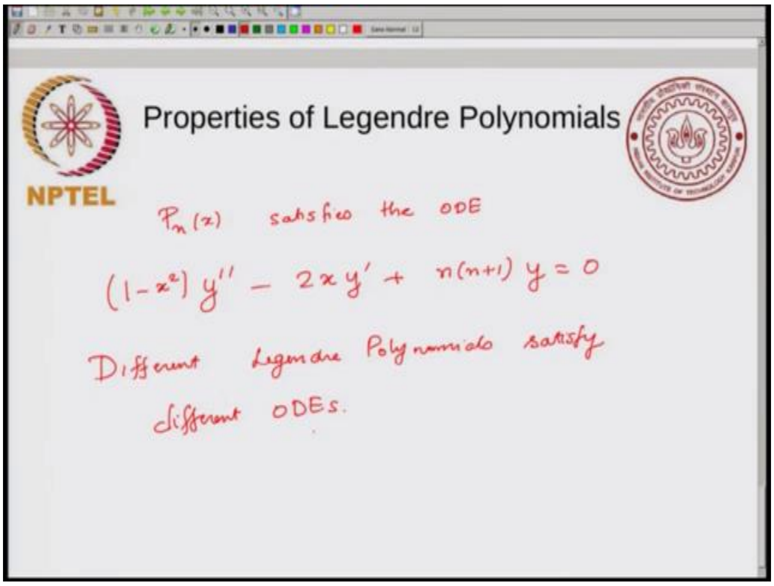

Now, these are some of the properties I just want to mention one more thing right here is that, I will just say it right here that P n of x satisfies the ODE 1 minus x square y double prime, minus 2 x y prime plus n, n plus 1 y equal to 0. So, a point that I should emphasize here is that different Legendre polynomials satisfy different ODE’s. So, what it means is that if I take P 1 then P 1 will satisfy an ODE with n equal to 1, if I take P 2 I will get a different ODE if n is equal to 2 then the o my ODE is different. So, different

Legendre polynomials satisfy different ODE's. So, they do not satisfy the same differential equation it is a same form, but they satisfy different differential equations, and this is a very important idea when you are dealing with these power series methods you have to keep in mind that they are not solutions the different polynomials are not solutions of the same differential equation, they are solutions of different differential equation nevertheless they are related to each other, and they also are orthogonal to each other.

So, in the next class I want to go to the connection with spherical harmonics, and what is called the rigid rotor in quantum mechanics. So, we will try to connect these Legendre polynomials with the rigid rotor problems in quantum mechanics.

Thank you.