Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 06
Special functions

Hello and welcome to the second week of this course on Mathematical Modelling and Simulation of Chemical Engineering Process. In this week we are going to study on various mathematical techniques that is indeed useful and necessary for solving different problems in process modelling and design.

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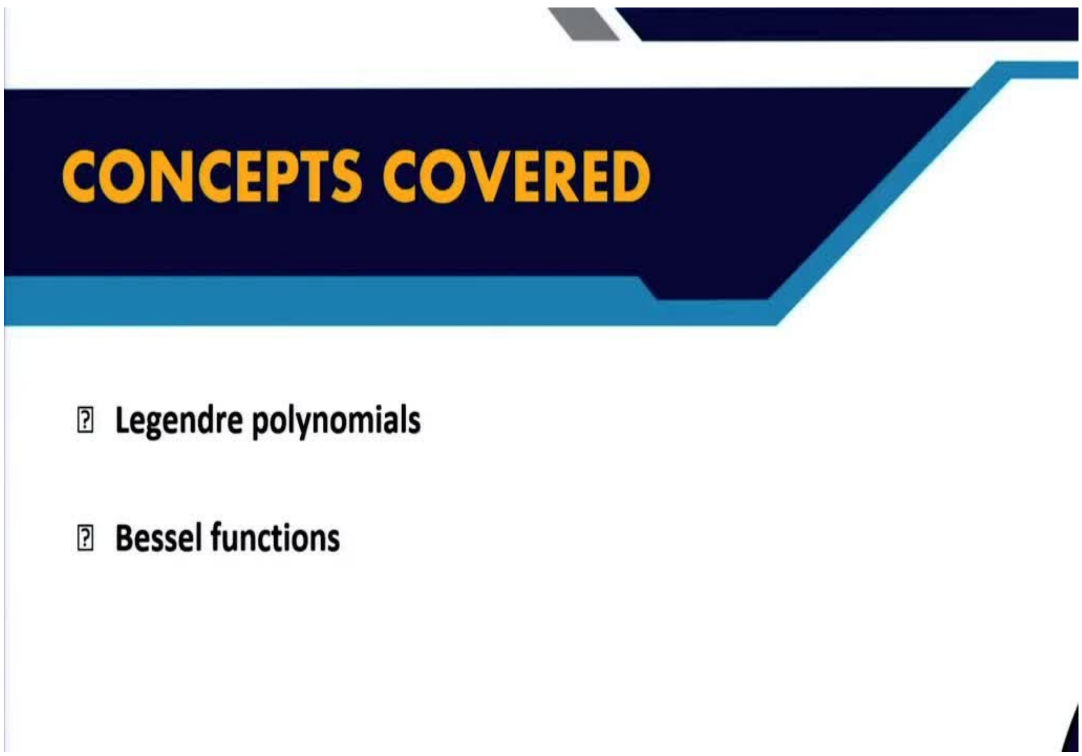

So, first in this class, we will start with the special functions here, we are going to talk about mostly the legendary polynomials and the Bessel functions as these equations are quite commonly obtained in the solution to the ordinary as well as partial differential equations.

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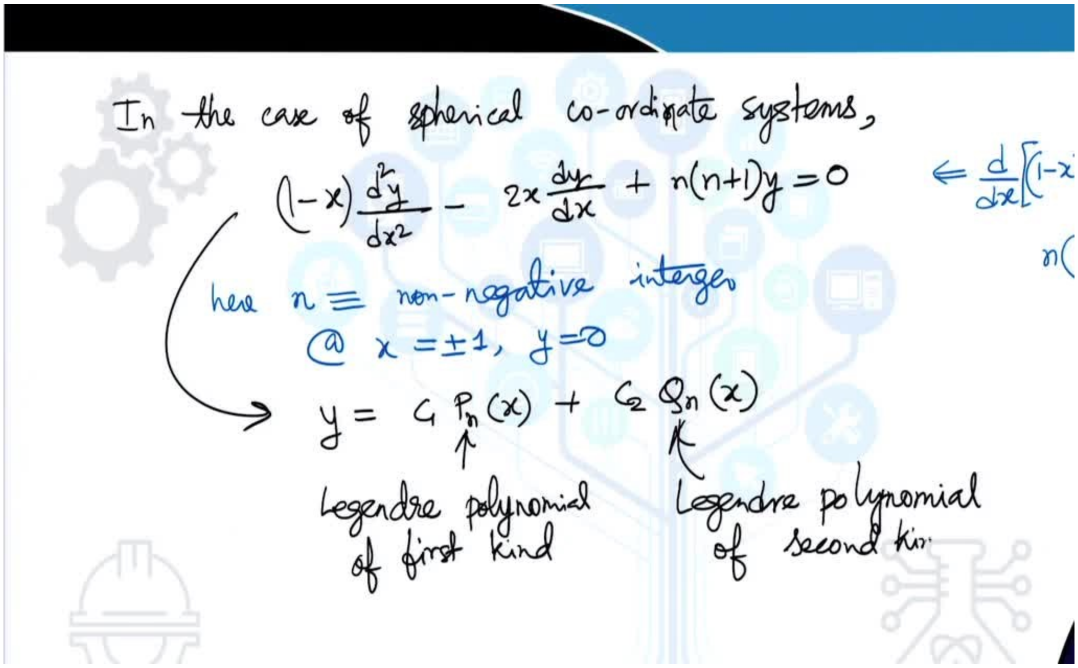

Now, first talking about these legendary polynomials. In the case of spherical coordinate systems, you generally land up with the auxiliary equations, the auxiliary ordinary differential equations for a spherical coordinate partial differential system something like this. So, you can relate this equation to be the theta solution of the spherical Laplace equation. So, the analogue's form of this equation is obtained from something like this. So, here n is a non-negative integer. The boundary condition to this ODE is that x is equal to plus minus 1 you have y is equal to 0. Now, the generic solution to this equation is y equal to C1 Pn(x) plus C2 Qn(x) where this Pn is the legendary polynomial of first kind and Qn is the legendary polynomial of second kind.

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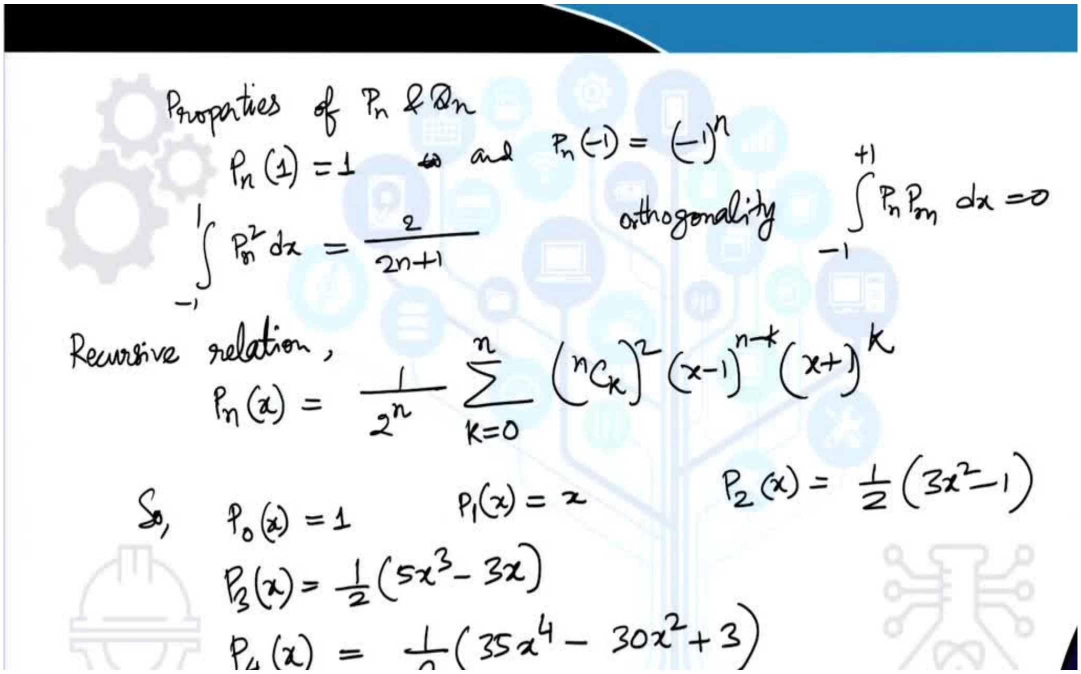

So, now, coming to the properties of Pn and Qn. So, Pn(1) is equal to 1 and Pn (minus 1) is equal to minus 1 to the power n. Integration in properties in the domain of minus 1 to plus 1 if you do the square of integration with this one, it also satisfy the orthogonality condition as Pn Pm dx over the domain of minus 1 plus 1 is equal to 0, for m not equal to n.

The recursive relation Pn(x) is equal to, this is a generating function actually series solution a series in finance series in fact. In C_k square x minus 1 n minus k x plus 1. So, from here you can easily understand that for different values of n, P0 is 1, P1 is equal to x, P2 is a quadratic function, P3 is a cubic function and so on, you can write P4 the fourth order equation.

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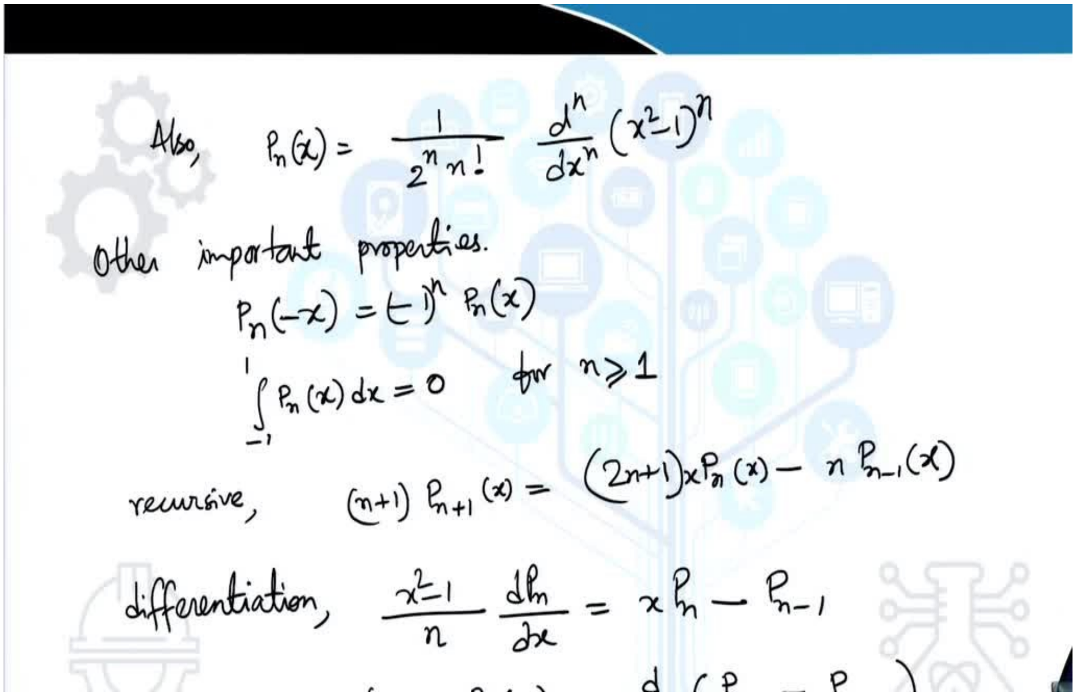

In the form of the differential, you can also write Pn(x) as 1 by 2 power, n factorial and nth derivative. Other important properties of the legendary polynomial of the first kind Pn of minus x is equal to, depending on the order of the polynomial, it takes this form. Integration does gives to 0 for n greater than or equal to 1 because P0 is equal to 1. There is another recursive relation that if the values of n and n minus 1 you can calculate what is n plus 1 and this is one of the most useful relation here, x Pn. Differentiation property, x square minus 1 by n is x Pn minus P of n minus 1. Also, you can write this is another important property I must write it here. So, if you take the derivatives of Pn plus 1 and Pn minus 1 that can give you also Pn.

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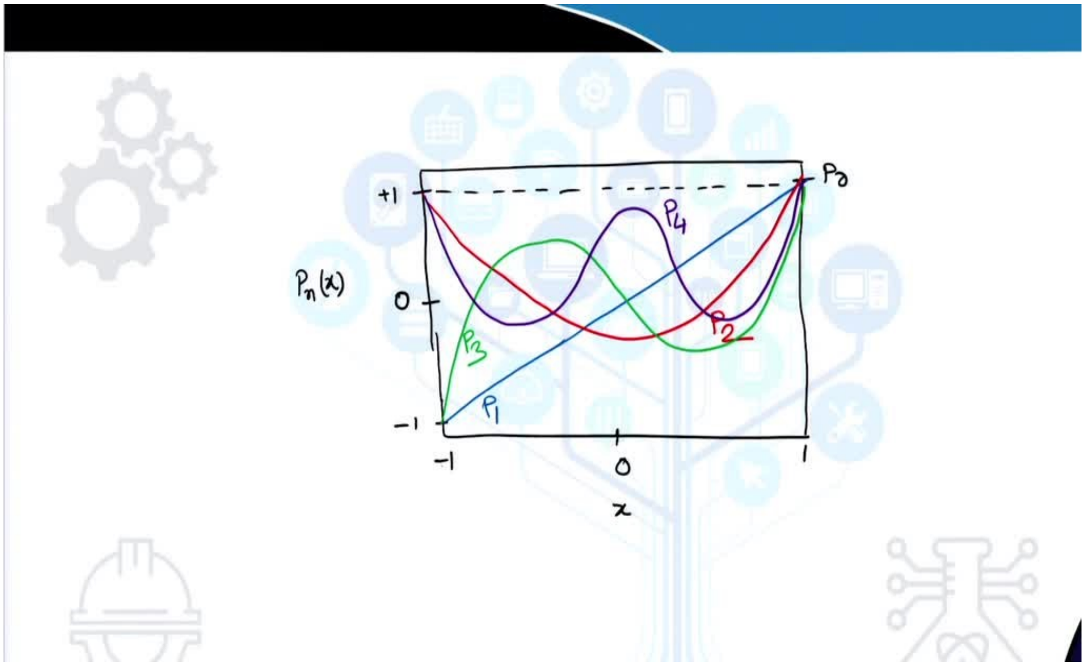

Trying to draw the different curves of P, let us try to draw it, let us say this is the domain of x and here we try to write Pn(x). I will try to make this hand drawing as precise as possible so, please bear with me. So, in the case of P0, it is constant 1. This is P0. Then we have this as P1, then P2 is a quadratic function. So, this is P2. Then P3 is a cubic function so, this is P3 and P4 is the fourth order polynomial. So, this is P4, and you can also draw P5 and all.

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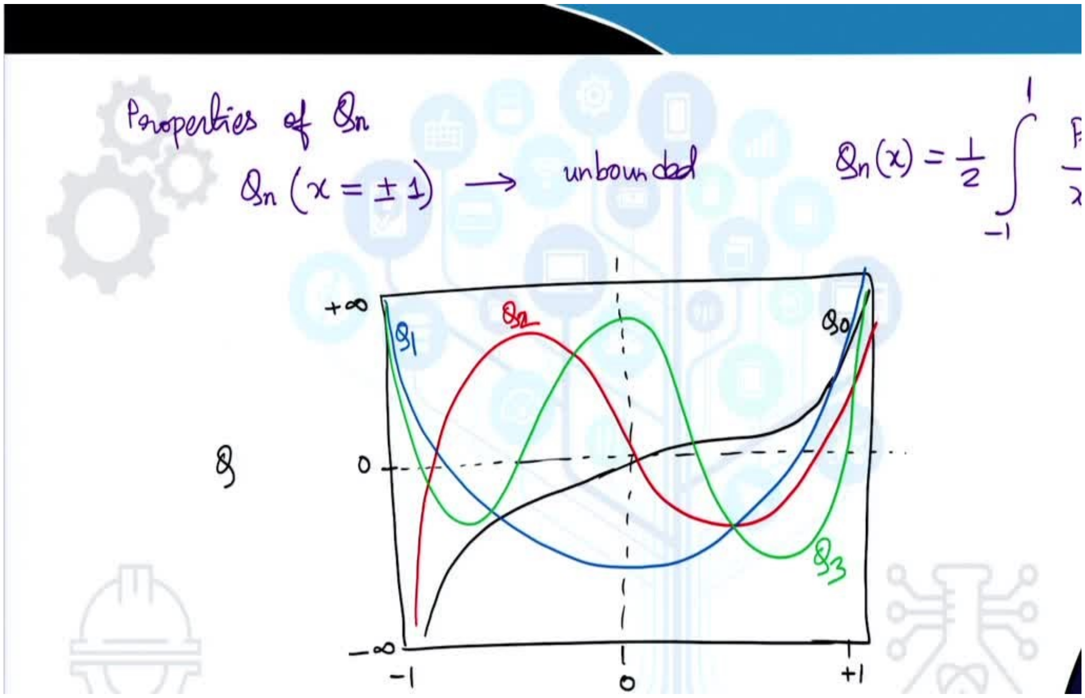

Now, let us try to move into the secondary polynomial that is properties of Qn. So, Qn at the limits plus minus 1 is unbounded, and generally Qn is related to P as in this form. So, if I am trying to draw the different Q curves, it will look something like this, please bear with me once again of my drawing. So, this is minus 1, 0, plus 1 this is x this is Q. So, here we have 0. So, this is almost tending towards minus infinity, and this is tending towards plus infinity. So, in the case of Q0 since it is unbounded let us try to draw it.

So, it is better if I try to make the origin here so, this looks something this. So, this is Q0. Next let us try to draw Q1. So, Q1 is so this is Q1, then sorry this is Q2, I made a mistake here Q2, and let me try to draw Q1 for you. So, Q1 is so this is Q1, Q2 I have already drawn and Q3 is... So, this is Q3 and again simultaneously you can understand what Q4 is. So, Q4 would be leading to minus infinity on the minus side, in the minus one side and plus infinity on the plus side. So, let us try to look into some of the properties of Q.

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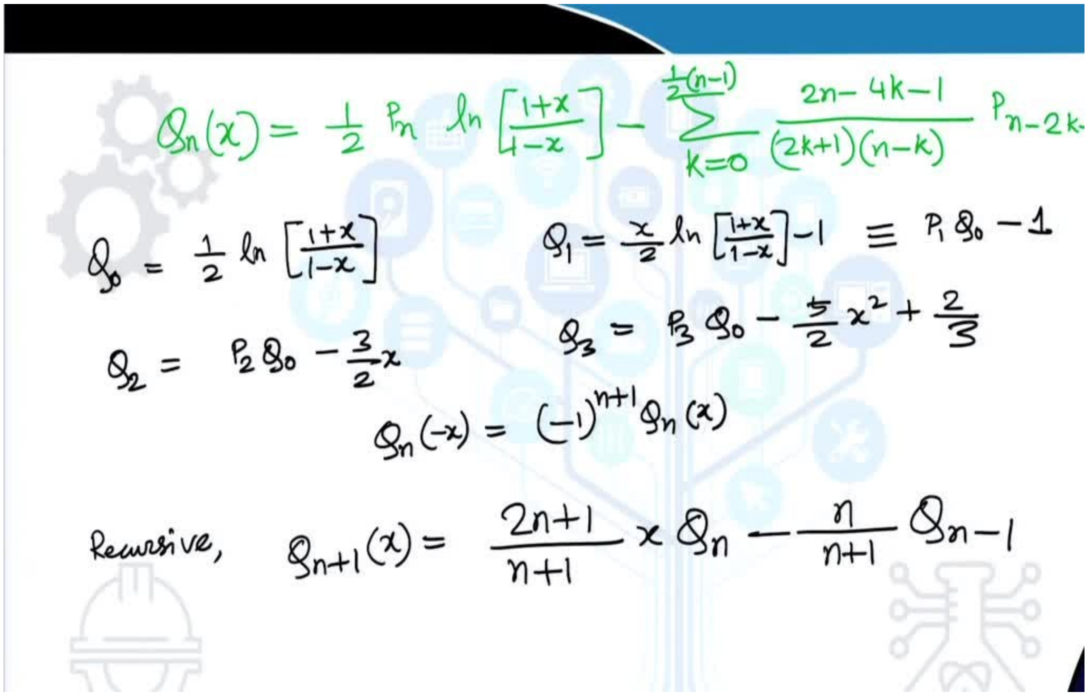

So, Qn is generally written down as an explicit formula provided Pn in this way. So, please bear with me it is the big formula this is the generating function for Q. But please understand that you need to have knowledge of P. So, from here you can easily estimate out what are your Q naught. So, Q naught is half ln 1 plus x by 1 minus x and because of these logarithmic functions it is generally unbounded at plus and minus 1, and from here you can easily spot that this is nothing but equal to P1 Q0 minus 1.

So, similarly Q2 is equal to P2 Q0 minus 3 by 2 x, Q3 is going to P3 Q naught minus 5 by 2 x squared plus 2 by 3 it is all from generating function and Q1 of minus x is in the same way but slight differences there is n plus 1 Qn. Also you have the recursive relation, in this case too that is Q n plus 1 is equal to 2 n plus 1 by n plus 1 x Q n , n by n plus 1 Q n minus 1. So, if you know n and n minus 1 you can also know what the value at n plus 1 is.

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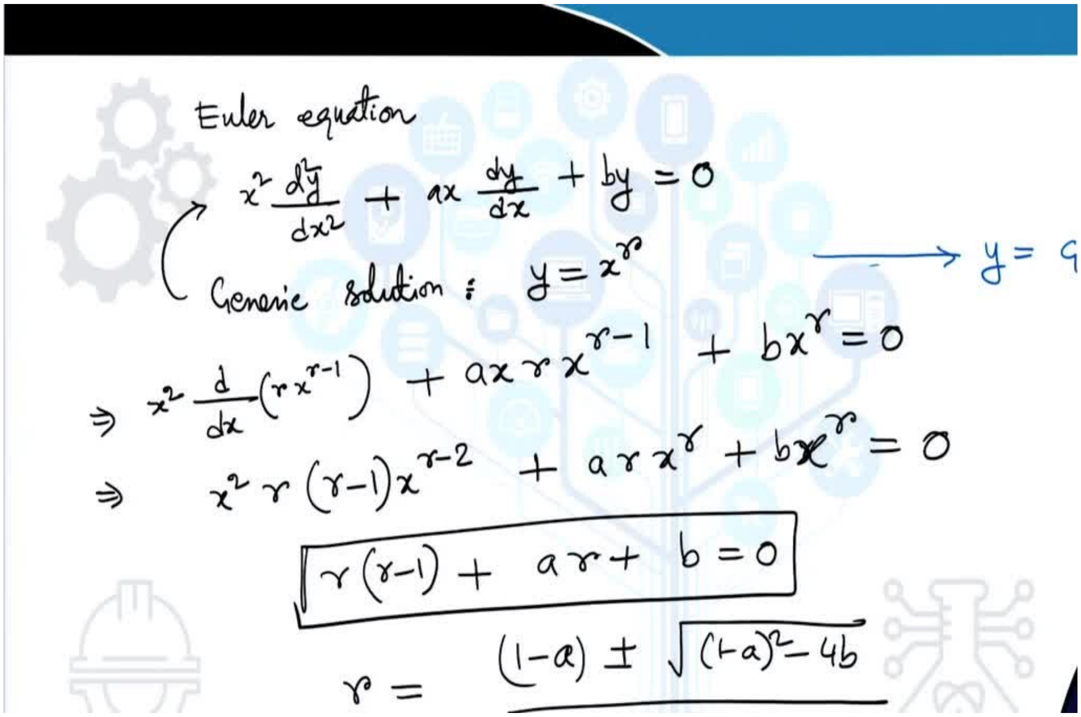

So, now moving to the next case of Euler equation and Euler equation is something which is generally encountered when you try to solve Laplace equation of r coordinate in spherical systems. So, the equation the auxiliary equations in really take this sort of ODEs and general generic solution to this equation is y equal to x to the power r. So, if you put a solution y x to the power r, you will see that it satisfies the Euler equation. How did I say it quickly instead of y i will write it to be x to the power r.

So, I am I have already done one derivation and one derivative that is r x to the power r minus 1 plus ax r x to the power r minus 1 plus b x to the power r is equal to 0. We just do some algebraic steps here. So, if you do simply realize that x r r minus 1, x r minus 2 plus a r x to the power r, plus b sorry x to the power r is always. So, if you divide both sides by x to the power r this is something you are going to get: r r minus 1 from the first time then a r plus b. Now, please understand that this is a quadratic equation in r which has 2 solutions, isn't it.

So, I can write the 2 solutions as r is equal to 1 minus a plus minus root over 1 minus a whole square minus 4 b divided by 2. So, basically what it means is that instead the generic form can be extended to as y is equal to C1 x r1 plus C2 x to the power r2 where r1 and r2 are the solutions to this quadratic equation.

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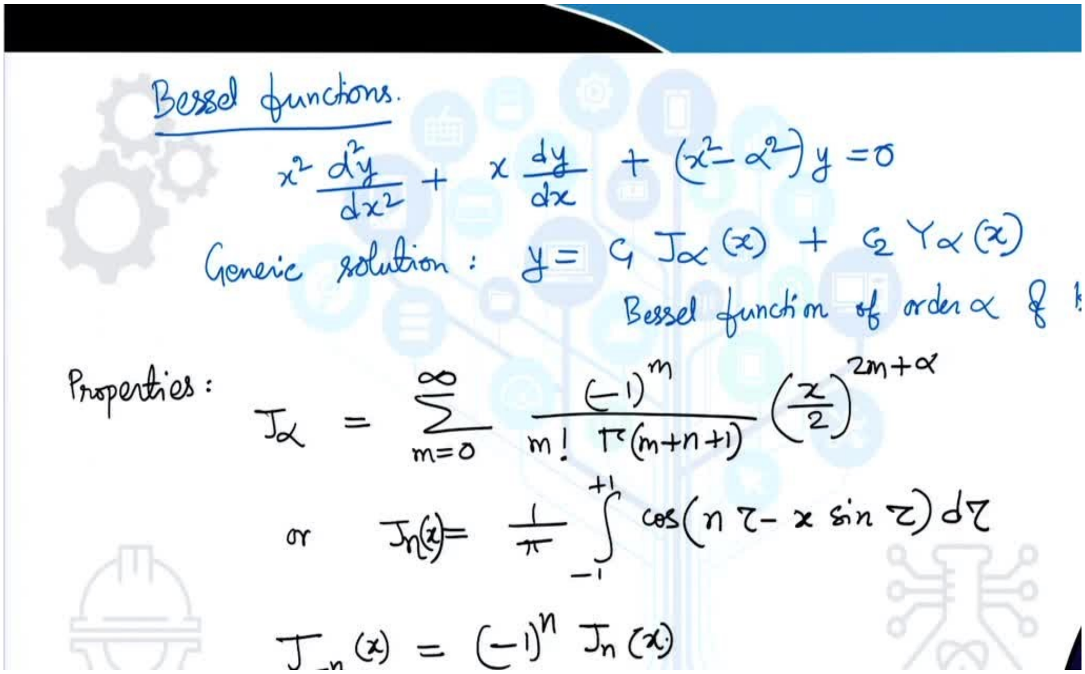

Now, moving towards the Bessel function. So, these Bessel functions are generally encountered in problems related to cylindrical coordinate systems whether you talk about distributed system in 1 dimensional or 2 dimensional, whatever in the case of multi-dimensional problem these are the auxiliary partial differential equations that you get from separation of variables otherwise, we will be getting them in the form of ODEs. So, how does the equation looks like x squared d2y/dx2 plus… So generic solution to this ODEs is y is equal C1 J alpha, this is the these are the Bessel functions and please note that these are the Bessel functions of order alpha of first kind.

So, this is Bessel function of order alpha of first kind. So, let us write some of the properties of J and Y. So, generally J alpha is given down as an infinite series, this is the generating function. The gamma function and here you have 2 m plus alpha. Alternatively, you can write this way as 1 by pi, some of the important properties J of minus n x is equal to minus 1 and J n x.

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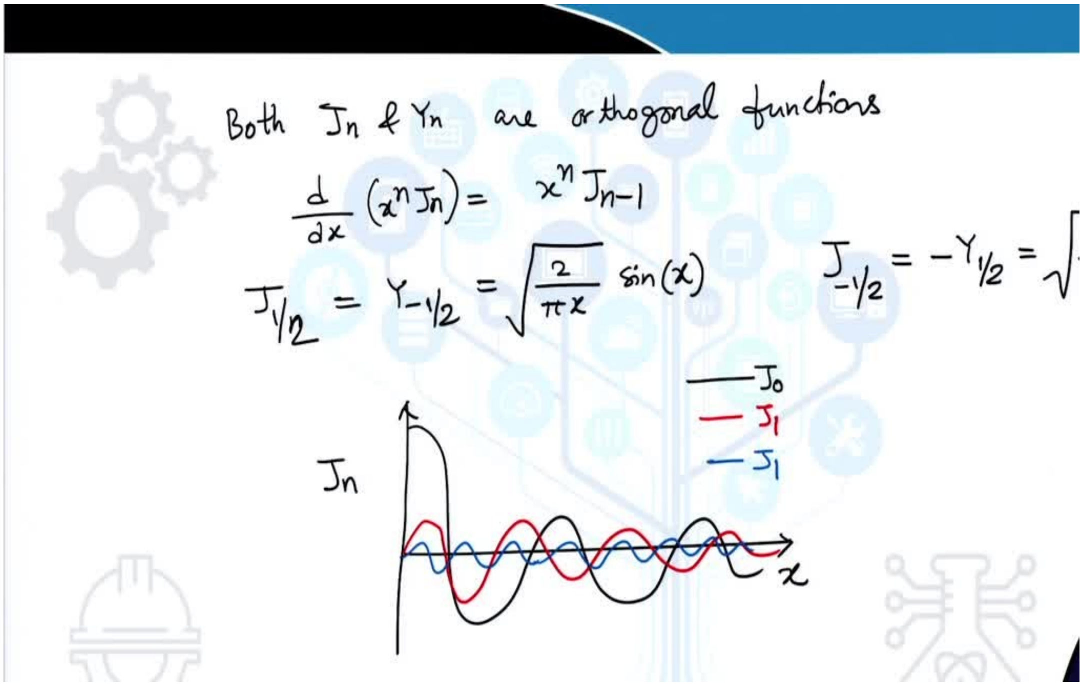

Both Jn and Yn are orthogonal functions. I leave it to you as an exercise to find out or to prove that these are orthogonal functions. In terms of derivatives this d dx to the power Jn would give you x to the power n J n minus 1. Two important points about J half order n is the order. So, if I write J half and that is equal to y of minus half and that is equal to 2 by 2 over pi x sin x. Similarly, J of minus half is equal to minus Y half and that is again equal to the cosine function.

Now, trying to write down the situation for J, J versus x, so, this is J0 then so, apart from J0 all starts from 0, so, this is J1, so, this is J1, J2 and the magnitudes of these derivative I mean this Bessel functions reduces. There are other integration and derivative properties of this J which you can look into any standard reference textbooks.

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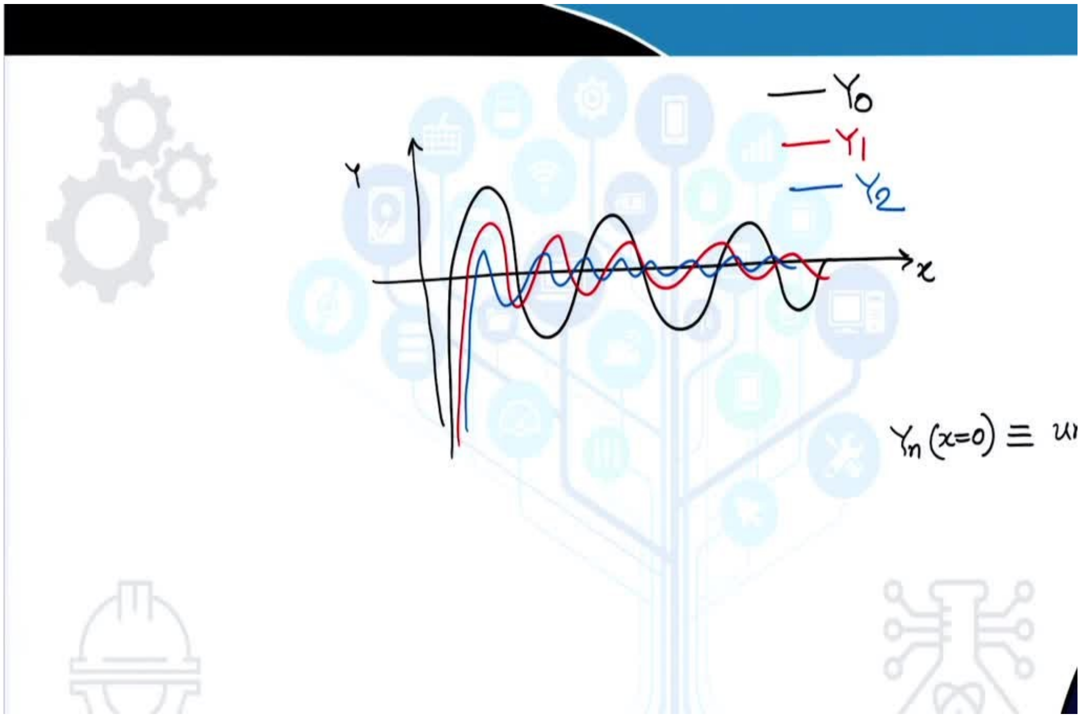

For the case of Y let us try to draw the case of I mean the plots for Y. Y let me just write this before we draw the curves. At x is equal to 0 it is unbounded. So, please keep this in mind. So, this is Y0. This is Y1, and this is Y 2.

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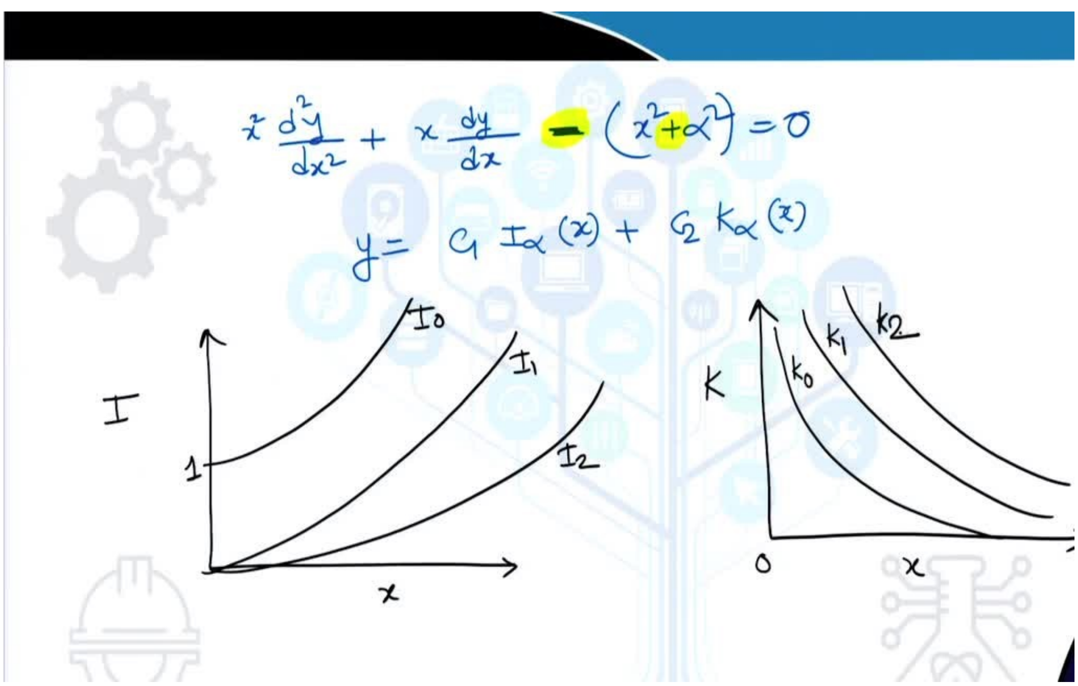

Then moving next there is also possibility that you can have an equation where there is a minus sign in the last term, this is the minus sign. So, this is known as the modified Bessel function or Bessel this gives you the generic solution where they are of second kind. So, this is C1 I. So, the second kinds are given as I and K.

So, the previous one where the Bessel functions of first kind, this one we are getting here as the Bessel functions of second kind. So, please do not get confused because in many places we will see that this nomenclature is different. But essentially you will get the I and K functions when there is a negative sign in front of the third, I mean this is the important sign. Let me use a highlighter here.

So, this is the important part. So, if you get a negative sign here, then you are expected so, if there is a negative sign before the, this x square term the last x square term then you are getting the second kind equations, but if there is a positive term then you are going to get the first kind equation and let me show you the nature of the I and K functions. So, this is I0. It starts from 1 then all the remaining I actually starts from 0. K as you can easily interpret here from this plot that these are sort of hyperbolic in nature, but all are unbounded at x is equal to 0.

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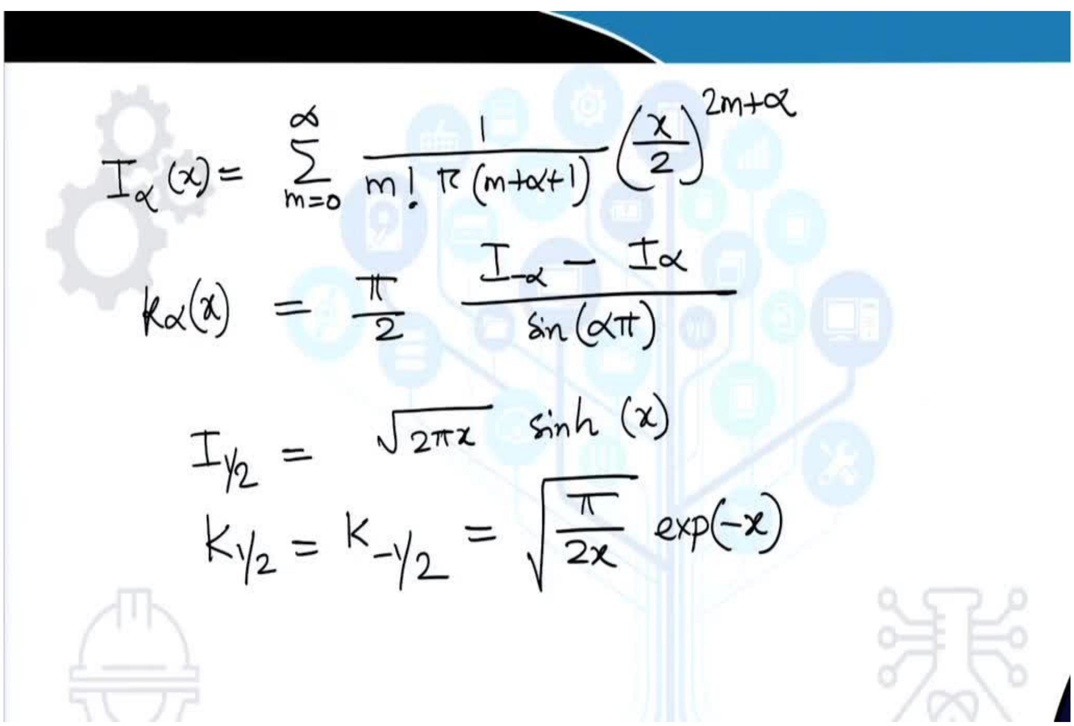

The generating function for I is very similar to J but with slight difference of course. These are all in finite series. I hope you can spot the difference. The only difference is without the minus 1 to the power m factor. Similarly, for K this is related to again the I function Fractional orders of the second kind functions like I half is given by the sin hyperbolic and the cos hyperbolic functions. I think one question I should pose here for you to find out whether these Bessel functions, I and K are orthogonal or not? Okay.

So, with this will close this lecture session in the next class we are going to talk about partial differential equations, it's classifications with different types, the technique of separation variables and so on. I hope you enjoyed the lecture today. Thank you.