Mathematics for Chemistry

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Lecture - 17

We have seen non-homogeneous second order partial differential equations, and what we said is that you can solve them, if you know a homogeneous, if you know the solution of the homogeneous equation and a particular solution.

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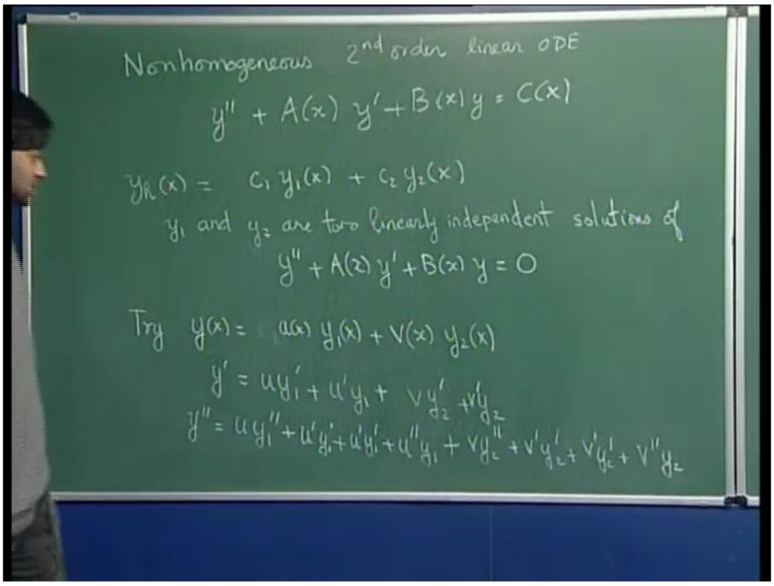

So, suppose we have a non-homogeneous second order differential equations and linear ODE. So, suppose you have this of the form y double prime plus A of x y prime plus B of x y equal to C of x. So if C of x is 0, it becomes a homogenous differential equation. If C of x is not equal to 0, then it becomes a non-homogenous second order linear differential equation. Now, if we had such an ODE, now suppose you knew y h of x is equal to C 1 y 1 of x, in other words y 1 of x and y 2 of x are the basis solution of the homogenous equations; homogenous equation is y double prime plus A x y prime plus B x y equal to 0.

So, for the homogenous equation y 1 and y 2 are two linearly independent solutions of this A x y prime plus B of x y equal to 0. So, y 1 and y 2 are two linearly independent solutions of this homogenous equation, and so the general solution of the homogenous equation can be written in this form. Now, if y 1 and y 2 are known, then you can find the general solution for this equation, and you can use it by a method called variation of parameters.

So, you try y of x u of x y 1 of x plus v of x y 2 of x, where u and v are some functions of x. So, what you can do is in order to find the solution of the non homogenous differential equation, we use the homogenous equation solutions and you assume that there are some functions u and v, which you can multiply y 1 and which can multiply y 2. So, if you have such a form of trial solution, then what you can do is you can show that I will just write for simplicity, I want to show the dependence on x.

So, I will write y prime is equal to u y 1 prime so if I take the derivative with respect to x. So, I take first I take derivative of this, then I take u prime y 1. So, this is the product rule for differentiation here I take v y 2 prime plus u v prime y 2, so this is the first derivative. And then if you take the second derivative u y 1 double prime plus u prime y 1 prime plus u prime y 1 prime plus u double prime y 1 plus v y 2 double prime v prime y 2 prime plus v prime y 2 prime plus v double prime y 2. So, if you take the second derivative we will get this.

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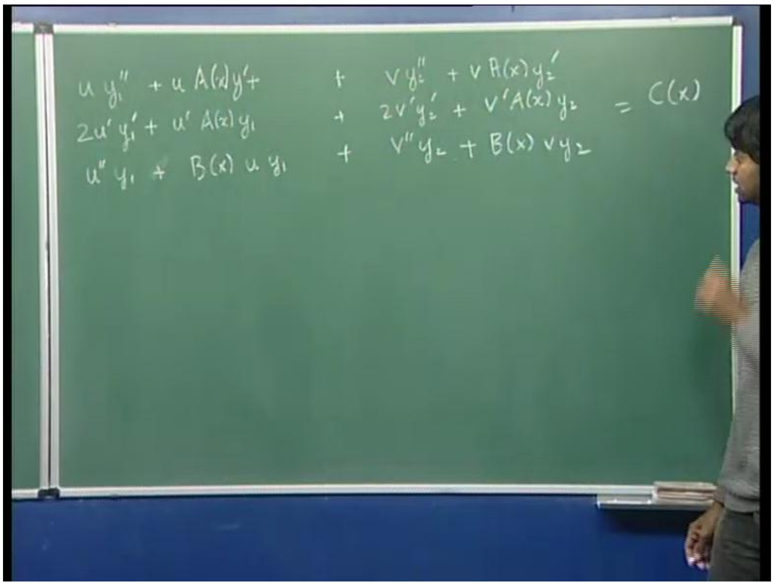

And then what you do is you substitute these two in this equation, then what will happen is that you will get simplification, because y 1 double prime and y 2 double prime satisfy the homogenous differential equation. So, let us go ahead and do that, so when I substitute this form into the non-homogenous equation, what I will get is u y 1 double prime and I will collect the terms that are proportional to u. So, I have u y 1 double prime then all these terms are either all these terms are these two are the same terms. So, you have 2 u prime y 1 prime, so I will write this separately 2 u prime y 1 prime and then I have u double prime y 1.

So, these are the terms that you get here and then what I will have is v y 2 double prime 2 v prime y 2 prime and v double prime y 2. So, these are so I just collected all these terms, I wrote them in this form, it will become clear why I did this. Then I have A of x times y prime, now again what I write is, I collect the terms having u. So, I will get plus u A of x y prime and then the term involving u prime in this case will be this term, plus u prime A of x y 1.

Then I do not have any terms involving u double prime and here I will have v A of x y 2 prime plus v prime A of x y 2. So, that is what I get from A of x y prime and from B of x y, I will get two terms will just be B of x u y 1, x v y 2. So, I will just get two terms from this.

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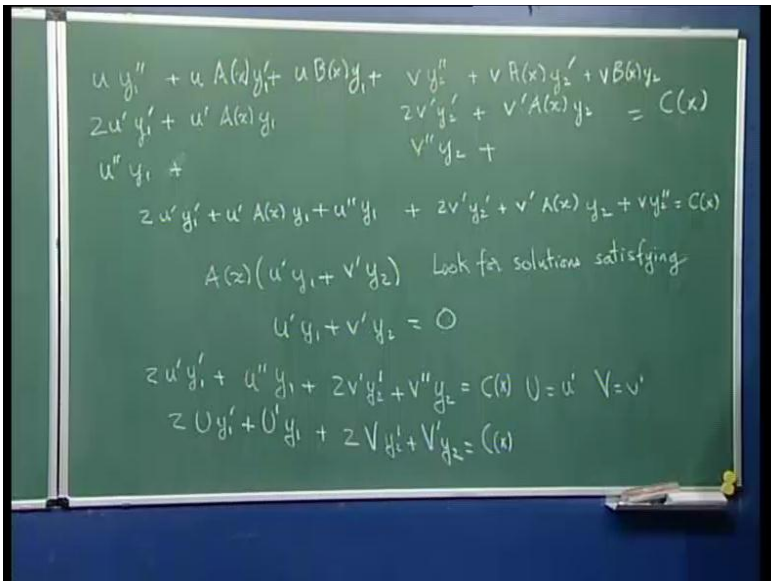

So, it is u y 1 and v y 2. So, I will just get this so this whole thing should be equal to C of x, the sum of all these terms should be equal to C of x. So, I written in this way and then sorry I will put this term up here I just put this term plus u B of x y 1 I will have u B of x y 2 sorry v B of x y 2. Now if you collect the terms in this form what you notice is that u is common to all these and what you have is y 1 double prime plus A of x y 1 prime plus

B of x y 1. And since y 1 satisfies this differential equation that term is exactly equal to 0. Similarly, these three terms have v times y 2 double prime plus A of x y 2 prime plus B of x y 2. And again since y 2 satisfies this differential equation this those terms add up to 0.

So, what you immediately get out of this argument is that these two these six terms just go away and they add up to 0. So, then what you are left with is this sort of equation 2 u prime y 1 prime plus u prime A of x y 1 plus u double prime y 1, and then you have plus y 2 plus v C of x. So, you got it you got your equation in this form, so I can collect the terms containing A of x as, so these are the terms that contain A of x. Now what we will do is we will look for solutions that have this term equal to 0. So, we look for solutions into 0 so we look for solution that that satisfy this condition. And if you satisfy this condition then these two terms will go way.

And what you will be left with is something of this form, plus y 1 2 equal to 0. And now again what you notice is that this is a derivative of u prime and if you call u prime as capital U. So, what you have is y 1 this is what this is the first part plus and if you call capital V as v prime 0 where U equal to u prime v prime and this should sound very similar to you sorry this is not equal to 0, this is equal to C of x. So, you have two equations one is u prime y 1 plus v prime y 2 equal to 0 or in other words u y 1 plus v y 2 is equal to 0. The other equation is this equation, and you can solve these two equations for U and V, and we will write the solution.

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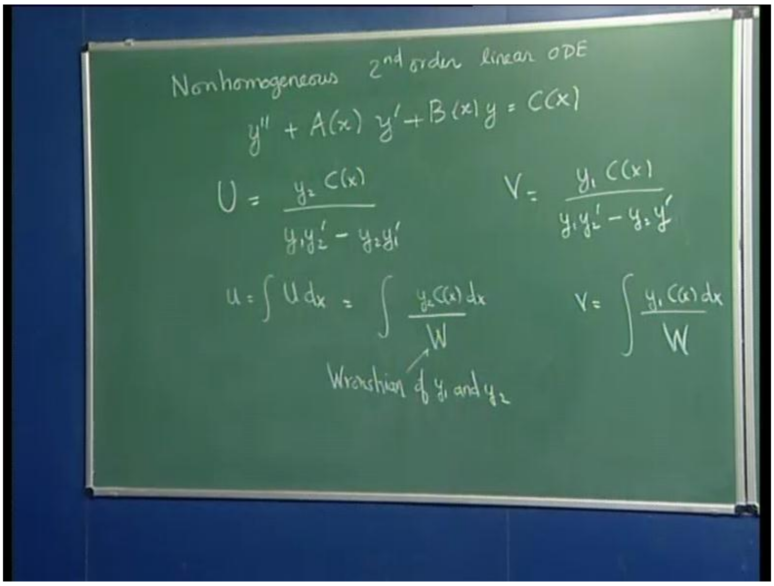

So, once again let me remind you, we started with this non-homogenous differential equation and what we had was the solutions of the corresponding homogenous equation which were y 1 and y 2. And we took a trail solution of the form trail solution of the non-homogenous equation of the form u y 1 plus v y 2. And so , what is left is to determine u and v so now we have these two equations both in terms of u and v. And you can easily solve them and you can write the solution I will just I would not go through the solution, I will just write the final answer. You will get U is equal to y 2 C of x divided by y 1 y 2 prime minus y 2 y 1 prime. And you will get V is equal to y 1 C of x divided by y 1 prime, I will just check and make sure.

So, if you rearrange these equations, then you can easily show that this is the solution of these equations. Now notice that your solution is in terms of capital U and you can easily show that is indeed the case. So the point is what we have is we have solved for capital U and capital V and then you can easily solve you can easily integrate this. So, u is equal to integral U d x and if you integrate this what you will get is integral y 2 C of x d x divided by and this quantity y 1 y 2 prime minus y 2 prime y 1 is called the Wronskian W. So, W is called the Wronskian. Wronskian of y 1 and y 2 and v is equal to integral y 1 C of x d x divided by W.

And y and remember W is also a function of x. So, in this way what we have shown is that if you know the solution of the homogenous differential equation. Then you can solve for the solution of the in-homogenous differential equation using this method of Wronskian's. Now one thing I should mention right here is that this method of Wronskian's is actually quite general, it can be extended to even to higher order differential equation. So, even if you had a third order differential equation which was homogenous and or which is in-homogenous, but you knew the solution of the homogenous equations; then you could use the method of Wronskian's to solve it so.

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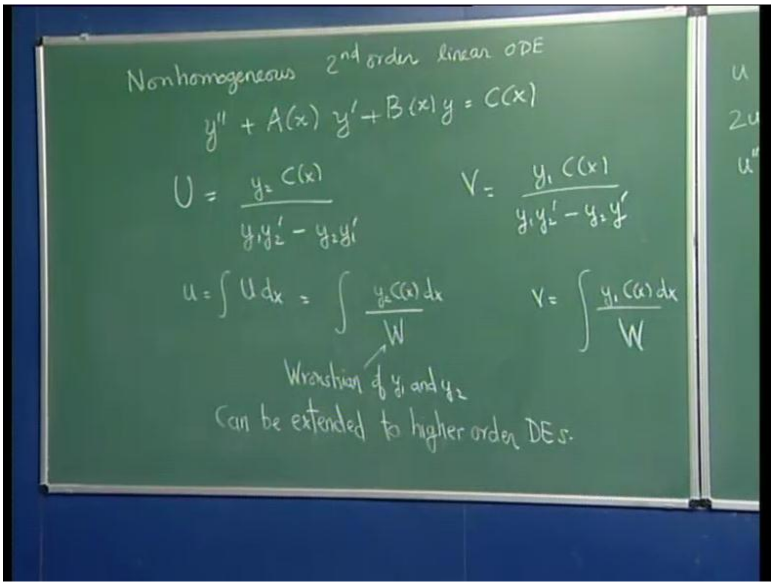

So, you can extend this method to higher differential equations and we just make a mention of that we would not actually see, how to we would not do it explicitly, but you have a form that is very similar to this. In the higher order differential equations typically you will have more than two bases solutions. So, your Wronskian will actually be a determinant of this matrix of involving y and y prime or y 1 and y 1 y 2 and y 1 prime y 2 prime.

So, now the question arises is the following so we know how to go from solution of homogenous differential equation to solutions of non-homogenous differential equations but the question remains how do you solve a homogenous differential equation? Are they are general methods to solve homogenous differential equations. We saw that the method of if we had a homogenous differential equation with constant coefficients, then you could use trial functions like exponentials and then solve it.

Now in case you had equations of the Euler-Cauchy form where, you had x square y double prime plus x y prime some constant times y. then you could use x raise to m as a solution. So, those are very specific cases, but is there a general way to solve second order differential equations. The other thing I should mention right here is that this method of Wronskian's is a very general method of going from a homogenous to an from the solution of homogenous equations to solutions of non-homogenous equations.

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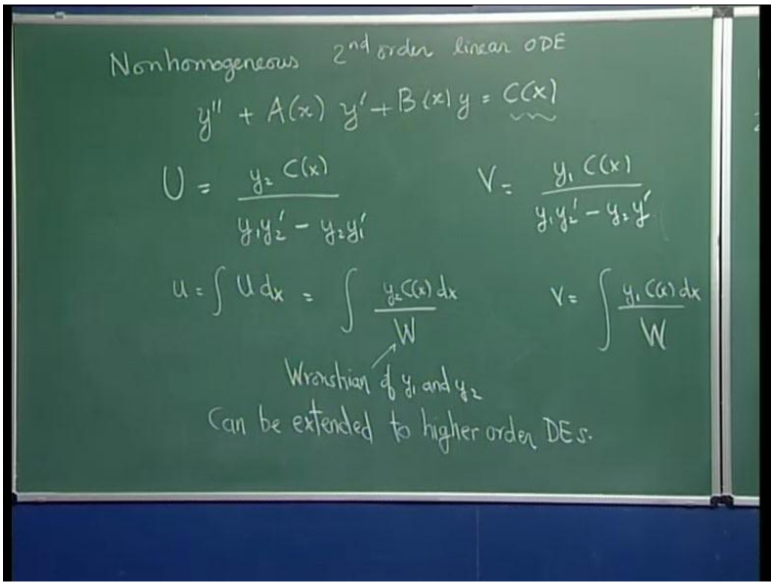

In sometimes since this involves calculating derivatives and doing integrals, it can sometimes become a little tedious, there are other tricks you can use various trail functions. So, depending on the form of C of x you can choose various trail functions. So, for example, if C of x is a polynomial, you can choose the polynomial as a trail function and then determine the coefficients of the polynomial. Similarly, if C of x is a trigonometric function you can choose trial functions that are trigonometric.

So, there are some simple thumb rules where, instead of going through this method of Wronskian's. You can use various trail functions and also solve it, but I would not mention that you can read about them in many standard text books. So, then we will move to trying to solve differential equations using some general methods.

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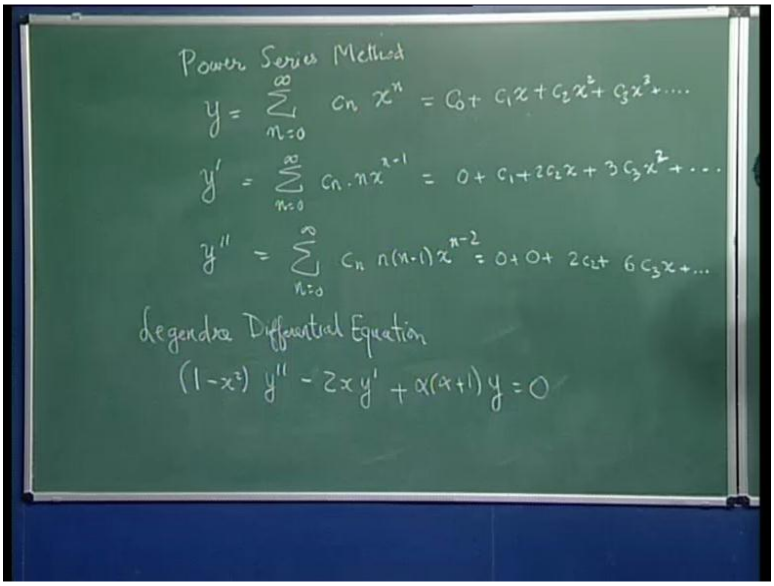

So a general method to solve differential equations is something called the power series method. And I will illustrate this method by taking an example, so before we go to that I will say some general things about what you do in the power series method. So, in the power series methods you use a trail solution, the trail solution that you use is y is equal to sum over n equal to 0 to infinite C n x raise to n, so this is basically C 0 plus C 1 x plus C 2 x square x cube.

So, these are various constants C 1 C 2 C 3 etcetera are various constants. So, you essentially assume that you have a series a power series in x. Now this might be an infinite power series, it might be a finite power series. If it is a finite power series, you call it a polynomial. If it is an infinite power series you just call it as an infinite series. So, but you just try in this power series form so if you have something like these, then y prime or the derivative with respect to x will be nothing like, you have to do term by term differentiation C n times n x to the n minus 1.

And if you do this the first term will give me 0, because n equal to 0 I get 0. So, we have 0 plus C 1 plus 2 C 2 x plus C 3 C 3 x square. So, what you have is a power series that starts with C 1, so here you started with C 0 now you start with C 1. Similarly, if you take y double prime, I can write this as and that will start with first two terms will be 0. Corresponding to n equal to 0 means this term will be 0, n equal to 1 means this term will be 0.

So, the first two terms corresponding to n equal to 0 and n equal to 1 are 0 plus 2 C 2 plus 6 C 3 x plus so on. So, what we are going to do, is to take these we started the trail solution of this form, that implies that the derivative is given by this series. And the second derivative is given by this series and then we will substitute these back in the differential equation and we will see what conditions, we get for these coefficients. And the conditions on the coefficients will determine the nature of the solutions.

So, let us take a specific example so the example will take it is something that you will see in the in quantum mechanics. So, in your quantum mechanics course you will see the example of this sort of equation. The equation is called the Legendre differential equation and it has the form 1 minus x square so let me just check minus 2 x y and just to be consistent I will call the this is minus and this is plus alpha times alpha plus 1. So, the form of the Legendre differential equation is 1 minus x square y double prime minus 2 x y prime plus equal to 0.

So, the interesting cases are when alpha is an integer, but notice that this is a second order differential equation. It is a linear second order differential equation, but you look at it, if you did not have this 1, if this 1 was not there. Then it would look like the Euler Cauchy equation.

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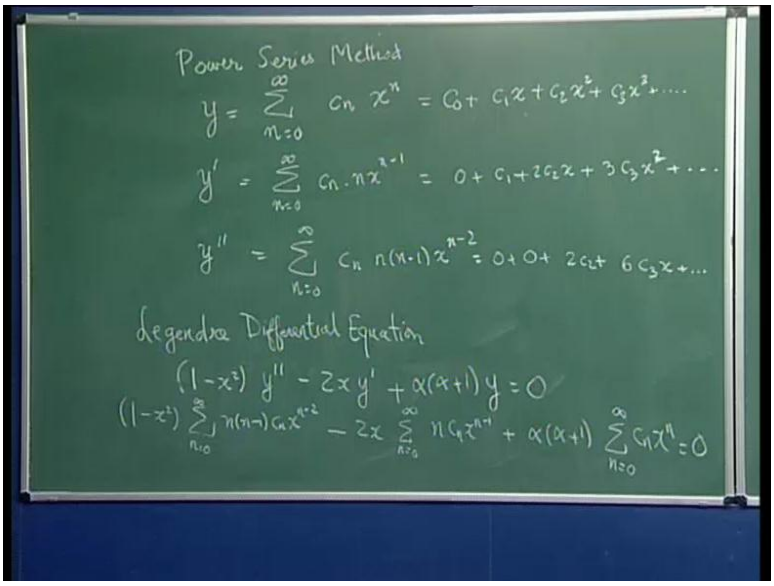

So, the solution would be a form of so x square multiplied y double prime x multiplying y prime constant multiplying y. So, the solution would be x raise to alpha would be a solution, but that is not the case and in this case you really do not know what the solution looks like. So, you try a power series solution, now if I take a trial solution of this form and I substitute in this equation, then the first term will become 1 minus x square sum over n equal to 0 to infinity n n minus 1 C n x raise to n minus 2.

So, that is this term so for y double prime I substituted this minus 2 x sum over n equal to 0 to infinity n C n x raise to n minus 1 plus alpha alpha plus 1 sum over n equal to 0 to infinity C n x raise to n equal to 0. So, all I get was I substituted the form of the second derivative, first derivative and the function and y into this differential equation and I get this result. So, I get this condition and now we can we will expand this out.

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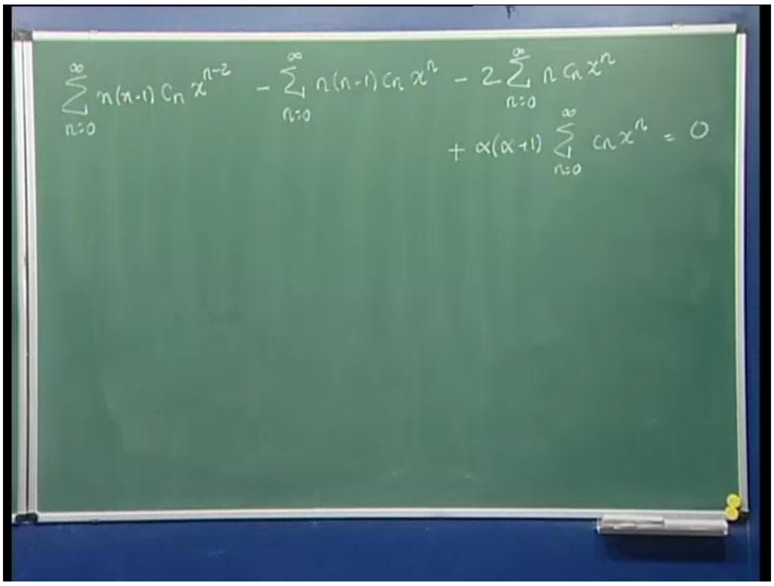

So, when we expand this out you will have we will have something of this form sum over the first term will be n n minus 1 C n x raise to n minus 2, the second term n n minus 1 C n and then you what you had is an x square multiplying x raise to n minus 2. So, x square multiplying x raise to n minus 2 gives x raise to n. Similarly, what you have here is the twice n C n x raise to n and finally, the last term will be equal to 0. So, we have the condition in this form, now each of these terms is a power series in x.

And what I mean is each of these terms has terms of x raise to 0, x raise to 1, x raise to 2, x raise to 3, etcetera. And each of these terms goes all the way up to infinity each of these again this has polynomials of x raise to 0, x raise to 1, x raise to 2 all the way up to x to the power infinity.

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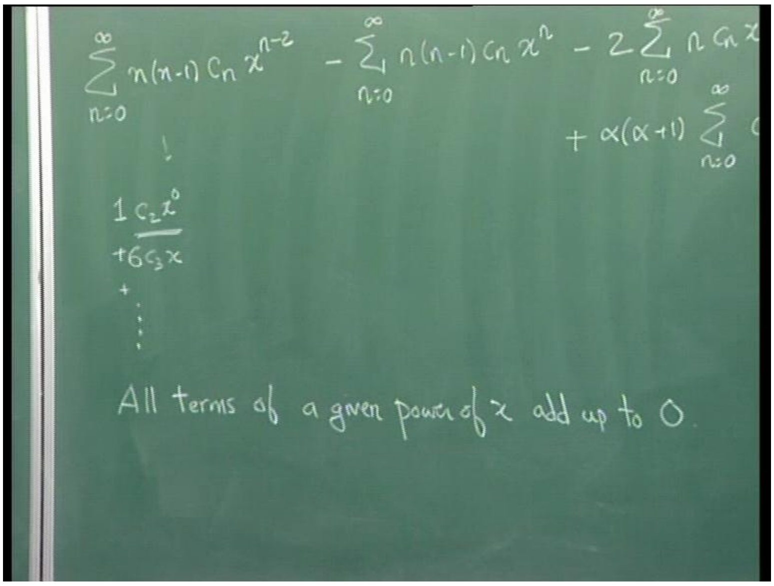

So, each of these are power series, so in other words this will look like, if you if I expand this when n equal to 0 I will get 0, because n equal to 0, n equal to 1 and also get 0, when n is equal to 2 I will get 2 into 2 minus 1 that is 1 into C n equal to 2 C 1 C 2 x raise to 0. Then when n equal to 3 I will get 3 into 2 that is 6 C 3 x and so on. So, I get a power series in x so the powers of x will keep increasing all the way up to infinity similarly, for this also I will get powers of powers I will get terms of various powers of x and for this.

Now, this series this solution is valid for the entire domain of validity of the solution, so it is valid for arbitrary values of x. And therefore, this is where we make the important simplification, so all terms of a given power of x add up to 0. So, in other words the right hand side here is 0, so the right hand side I can write as 0 plus 0 x plus 0 x square plus 0 x cube plus so on. So, then this term now what we do is we do term by term each of these should add up to 0.

So, let us see how that works? So, let us take this and write it term by term. So, if you want to write these term by term what we will say is the following and this I have n equal to 0 to infinity C n x raise to n minus 2. So, let us look at all terms of order x raise to 0.

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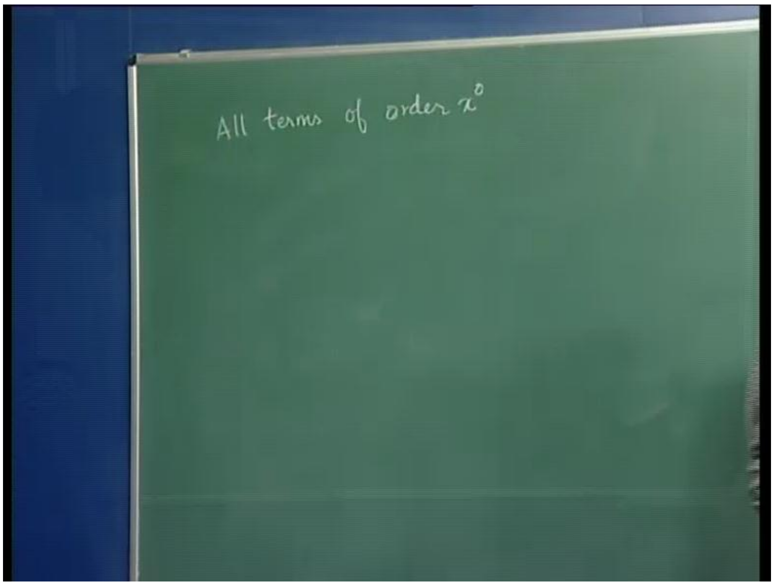

So, all terms where the power of x is 0, here the term with power of x 0 will be C 2, so in this has only one term where, the power of x is 0. Similarly, the power of x will in this case the term with power of x equal to 0 will be n equal to 0 and that term is equal to 0, so this is 0 times x power 0.

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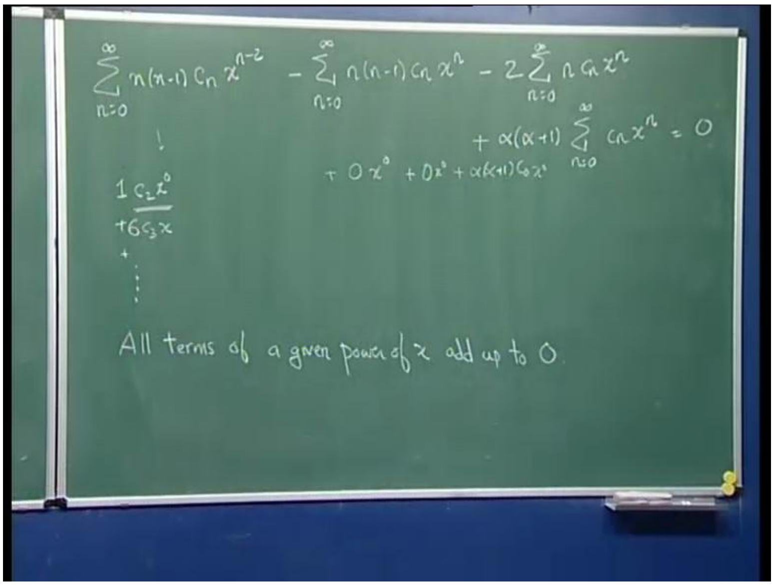

In this case the term with x power 0 will be n equal to 0 n equal to 0 this term is n C n, so n is 0. So, it is 0 and in this case the term with x power 0 is n equal to 0, so you have C 0, so you have plus C 0 x power 0.

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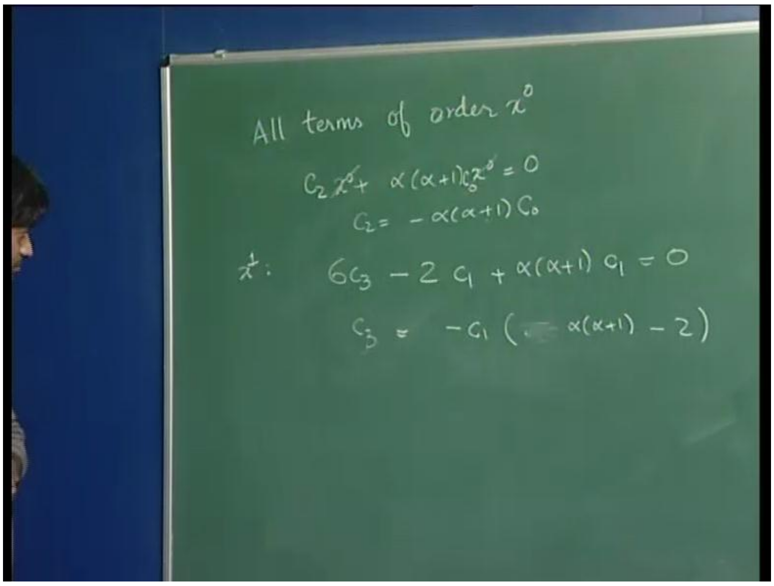

So, if you collect all those terms you will get C 2 times x power 0 plus alpha alpha plus 1 x power 0 equal to 0 and x power 0 is just 1. So, what you will get is that C 2 is equal to minus alpha alpha plus 1, and I have a C 0. So, this is alpha alpha plus 1 C 0, so if I collect this I will have a C 0 here. So, C 2 is equal to minus alpha alpha plus 1 times C 0.

So, notice that by imposing the fact that all terms of x power 0 have to go to 0 or they have to add up to 0. You got a condition between C 2 and C you got a condition for C 2. So, C 2 depends on C 0 and this form, now terms of power x power 1, let us do this for x power 1. And we would not bother writing x raise to 1 in front of each term. So, the term of I have power x power 1 is if x raise if you have to have x raise to 1, then n has to be equal to 3. So, n equal to 3 means you have C 3 3 into 2, so 6 C 3. Then in this case if you have to have x power 1, then n has to be 1. Then n minus 1 is 0. So, this does not contribute in this case n has to be equal to 1, so you get x raise to 1 1 C 1.

So, you have minus 2 C 1 coming from here and finally, in this case you have alpha alpha plus 1 C 1. And this has to be equal to 0, so then you collect this you get C 3 is equal to minus C 1 times 2 minus alpha alpha plus 1 or alpha alpha plus 1 minus 2. So, you have alpha alpha plus 1 minus 2, so C 3 in terms of C 1, so this is the next thing in our so what it gives is the relation between C 3 and C 1.

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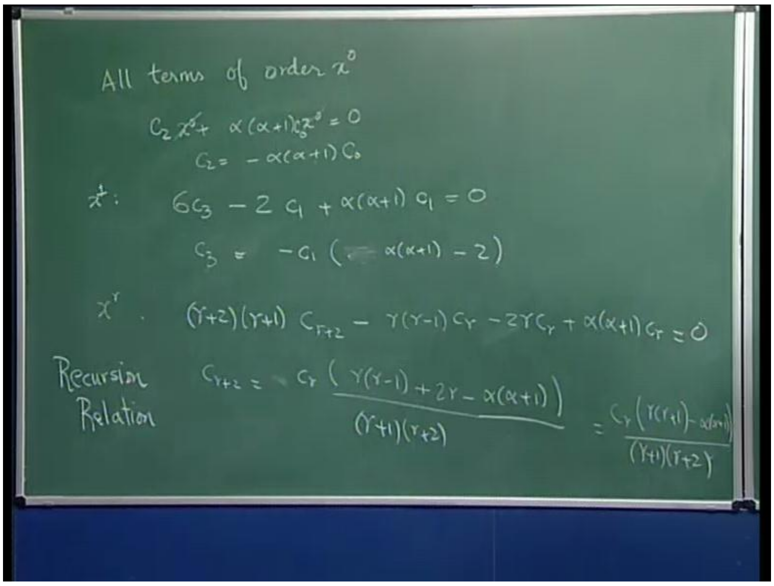

Now if you collect terms of x raise to r where, r is some arbitrary integer greater than 1. So, if I look at terms of terms that are multiples of x raise to r, so I am looking at all terms that that contribute to x raise to r. So, if I wanted the term that has x raise to r here, then n has to be equal to r plus 2, so then n times n minus 1 is r plus 2 n minus 1 is r plus 1. So, this term will be r plus 2 r plus 1 and n, we said is r plus 2 minus, now in this case if I wanted a term of x raise to r. And then n has to be equal to r, so if n is equal to r, this is r, r minus 1 C r.

In this case n is equal to r, because x raise to r you will get when n is equal to r. So, you will get r C r minus 2 r C r. And in this case what you will get is alpha alpha plus 1 C r equal to 0, and we can write this out, we can take we can write C r plus 2 is equal to minus C r times. So, what are left with is r r minus 1 r plus C r into r r minus 1 plus 2 r minus alpha alpha plus 1, this divided by r plus 1 r plus 2. So, what you get is a relation between C r plus 2 and C r.

So, if you know terms of orders if you know the coefficient of expansion of x raise to r, then you can calculate the coefficient of the r plus 2 of x raise to r plus 2, for any r, so this is valid for any r. So, and we can write this is r r minus 1 plus 2 r, so I can write this as r r plus 1 minus alpha alpha plus 1 divided by r plus 1 r plus 2. So, notice that we got a relation between C r and C r plus 2, such a relation is called a recursion relation. So, what we saw is that we looked at terms of power x power 0, we got something like this.

So, notice that 2 is related to C 2 is related to C 0, when we take x power 1 C 3 was related to C 1, when you take x power r C r plus 2 is related to C r.

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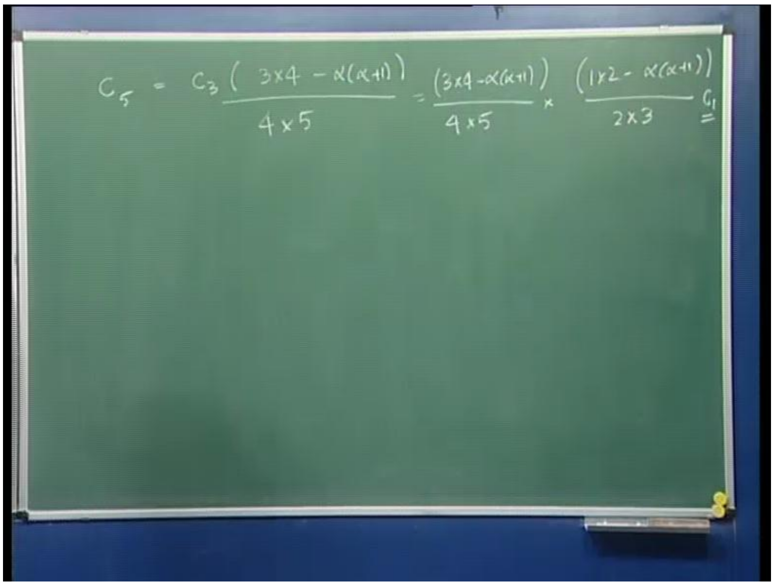

So, this is the general theme of this differential equation solution that C r plus 2 is related to C r. So, what do with all this? So, suppose you take C 5 suppose you want to calculate C 5, what you will do is you will write this recursion relation, you will write it in terms of C 3 times 5 5 plus so C 5, so r plus 2 is 5. So, r is 3. So, C 3, so and r r plus 1 is 3 into 4 minus alpha alpha plus 1 divided by 4 into 5. So, I wrote C 5 in terms of C 3, then what I do is I will write C 3 in terms of C 1. So, then what I will write is I will leave this as it is and then for C 3, I will use this relation this is this divided by 6, 6 which is 2 into 3.

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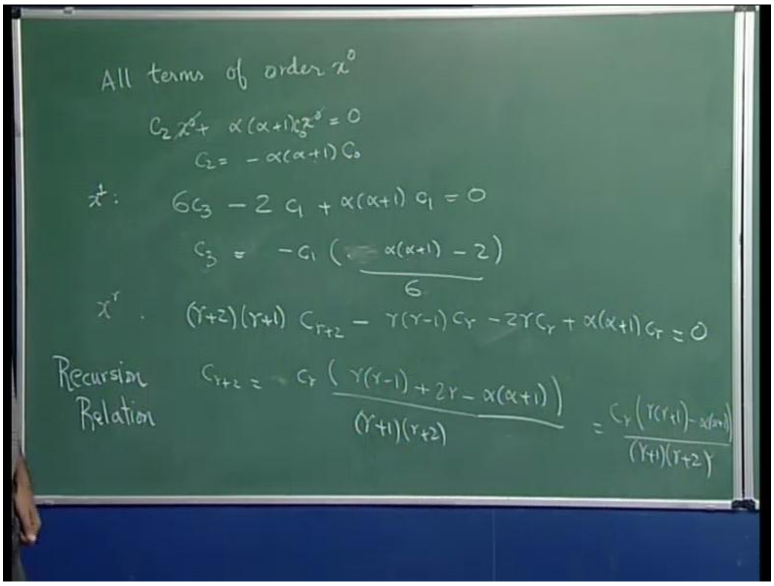

So, what I have here is I can absorb the minus sign inside. So, I get 2 minus alpha plus 1, so 2 is 1 into 2 divided by, it will be 2 into 3. And this whole thing now will multiply C 1, but notice you cannot go from you cannot write C 1 in terms of anything else, so what we wrote is that C 5 is proportional to C 1. Similarly, C 7 you can write in terms of C 5 first and then C 5 to C 3 and then C 3 to C 1, so C 7 is also proportional to C 1.

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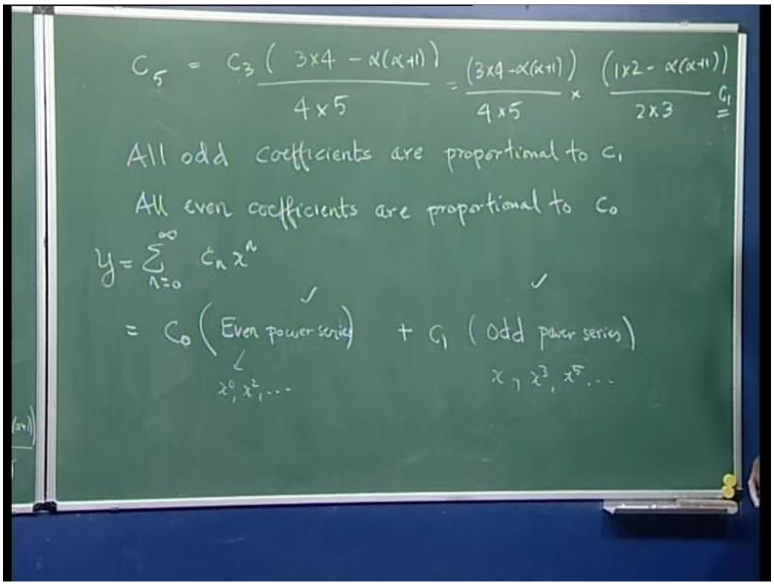

So, in other words all odd coefficients are proportional to C 1, and similarly all even coefficients are to C 0. So, then you can write our y is equal to sum over n equal to 0 to infinity C n x raise to n I can write this in this form. I can collect all the even terms will be proportional to C 0. So, I can write C 0 into polynomial so even polynomial means it will just contain x raise to 0, x raise to 2 and so on. And I can write C 1 times an odd polynomial, so that will contain things like x x cube x 5 etcetera.

So, the general solution can be written in this form, it can be written as C 0 times a polynomial with only even terms. And C 1 times a polynomial with only odd terms, and both these it is I should not call it a polynomial here I should call it a power series. I should really say power series and this will also be a power series. And I am emphasizing this difference, because this can go all the way to infinity. So, the number of terms can go all the way to infinity.

So, what we have shown by this argument is that you can write this as in this form, all the even terms are proportional to C 0, all the odd terms are proportional to C 1. And in terms of C 0, you know these constants exactly, so you know the values of this term, so there is no undetermined terms in this. Similarly, there are no undetermined constants in this, and so you know this only thing is you do not know C 0 and C 1, but then that is not a problem, because these two solutions an odd power series and an even power series are linearly independent.

And so these two solutions are actually bases solutions, so either of these will be a valid solution, so you have found out the two linearly independent solutions. So, next what we want to see is we want to actually look at this even power series and this odd power series, and analyze what these terms look like.