Mathematics for Chemistry

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Lecture - 19

In the last 2 lectures, we have see how to use the power series method to solve certain second order differential equations. The power series method is a fairly general method, but turns out that in some cases it does not work out as well as you would expect.

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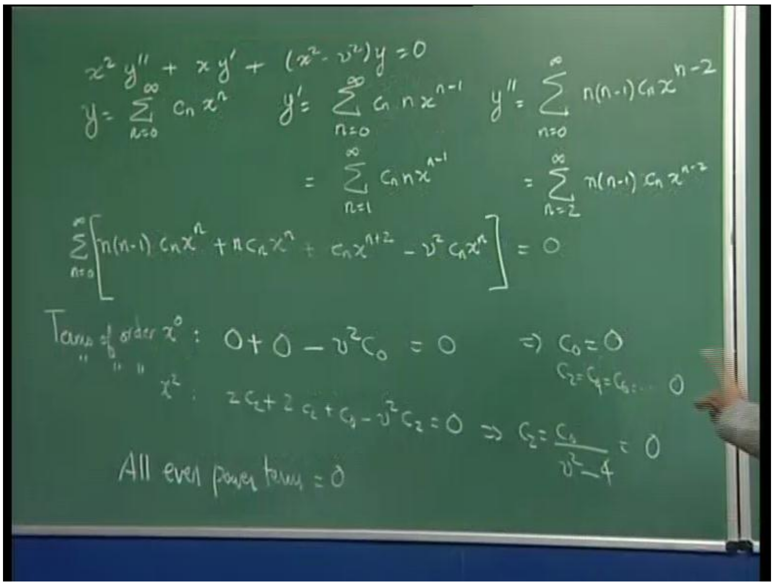

Let us take the example of the differential equation x square minus y square equal to 0. So, suppose you have this differential equation, then if you just use the power series method you will say n equal to 0 to infinity c n x raise to n and then you will say y prime and y double prime. Now, before I substitute this I want to mention one thing is this n equal to 0 to n equal to infinity, the lower limit n equal to 0, when n is equal to 0, this term is 0, because it is multiplied by n. So, sometimes this is the non zero terms start from n equal to 1.

So, it is identically equal to this, so this is equal to this, similarly in this case the term with n equal to 0 is 0 n equal to 1, then n minus 1 is 0. So, the first two terms are 0, so this is identically equal to n equal to 2 to infinity minus 2. So, sometimes in some books they will write this from n equal to 1 to infinity and they will write this from n equal to two to infinity; but even if you write n equal to 0 to infinity there is no harm done. So, now you take this and you substitute in these equations.

And what you will get immediately is that the first term x square y double prime, so that will give me x raise to n, I will just the second term, I will just take n equal to infinity common. The second term will give me x y prime, so that is n c n x raise to n, the third term will give me x square minus nu square into y, so that is I can write it as two terms, one is x square into y n c n. So, that is c n x raise to n plus 2 and the other term is minus nu square c n x raise to n and this is equal to 0.

Now, let us look at terms of order x raise to 0, so if you look at the term of order x raise to 0, in this case n has to be 0, n has to be 0 here, n has to be here there is no term of x power 0 and here there is one term of x power 0. So, if you write that here you will get 0 plus from this againn equal to 0. So, you get 0 here there is no term, because this even when n equal to 0 this starts with x square and you have minus nu square c 0 equal to 0. So, nu square is some general number and if nu is not equal to 0, then you have c 0 equal to 0, so you get c 0 equal to 0 and you can immediately show that this implies that c 2 equal to 0 all are 0.

So, c 2 will be related to c 0, because if you look at the terms of order x square, then you will get terms of order x square, then this will get 2 into 1 into 2 c 2 plus here will get x square, so n is equal to 2. So, 2 c 2 plus here you will get a term at n equal to 0, so c 0 minus nu square c 2 equal to 0. So, that implies that c 2 equal to c 0 divided by nu square minus 4 so c 2 is equal to nu, so 4 c 2 minus nu square. So, c 2 is c 0 divided by nu square minus 4 equal to 0 and similarly, you can show all the even terms go to 0.

So, basically all the even terms go to 0. Now, we can look at the odd terms, so when you look at terms of x of x raise to 1, so all even power terms equal to zero.

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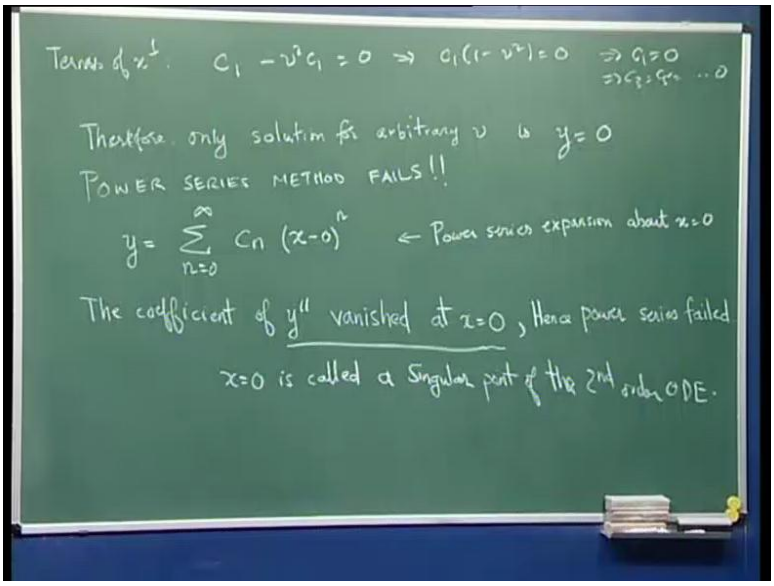

And next you look at termsof x raise to 1, so if you x raise to 1 then in this case n has to be equal to 1, but if n equal to 1 this term gives 0 in this case n equal to 1 implies you have 1 c 1 so you have c 1. In this case you can never have x raise to 1 because even if n equal to 0 you get x square and in this case you have nu square c 1 equal to 0 and this implies c 1 times 1 minus nu square equal to 0. In general nu square is not equal to 1 so, if you take a value of nu square, which is not is equal to 1.

So, this implies c 1 equal to 0 and this implies c 3 equal to c 5 equal to 0. So, therefore only solution for arbitrary nu is y equal to 0, so from these two what you will conclude is that the only possible solution for an arbitrary value of nu where nu is not equal to 0, nu is not equal to 1 is when y equal to 0. So, what you realize is that if you apply the power series method for this differential equation you end up with a trivial solution that is y equal to 0.

So, any homogenous equation always has a solution y equal to 0 but that is not the solution that you are interested in, so therefore, the power series method fails, so you conclude that the method fails. Now, what we will do is we will modify the power series method, so that you can use it for this problem but before that we want to understand why this failed or we want to look at some reasons why this failed.

In this case your power series infinity c n x minus 0 raise to n, so I am writing my power series as an expansion about x equal to 0. So, just as you write a Taylor expansion about x equal to 0, so I am just writing it this way. So, this is the same as this, but I just write it this way just to highlight that this is power series expansion about x equal to 0. So, what we used when we wrote the power series method is that we did a power series expansion about x equal to 0, you can also do power series about x equal to 1 x equal to 3 any number x equal to 0.5 anything. But, in this case we used about x equal to 0 and it failed in this particular case, because the coefficient of y double prime vanished at x equal to 0.

So, the coefficient of y double prime is x square and when x equal to 0 x square is equal to 0. So, the coefficient of y double prime vanished at x equal to 0 therefore, the power series failed. So, hence failed, now in order to actually see why such a statement is true you have to go through some exercise you have to actually take a general power series and it is possible to show that such a statement is true; we would not go into that detail. What we will do is, we will do a small analysis here of how the coefficient of y double prime of x the nature of the solutions.

So in this case whenever the coefficient vanishes at x equal to 0, then x equal to 0 is called a singular point of the second order ODE. So, whenever the coefficient of y double prime vanishes at some value of x then that point is called a singular point of the second order ODE. So, let us look at these singular points in a little bit more detail and what I will do in the next 15 or 20 minutes is to tell you what methods you can use whenever you have singular points in a differential equation.

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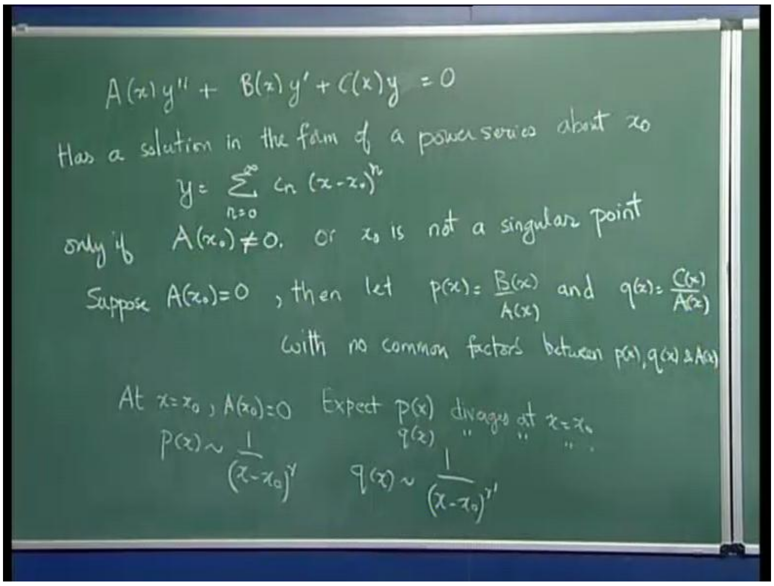

So, suppose you had a differential equation of the form A of x y double prime plus B of x y prime plus C of x y equal to 0, then this such a differential equation has a solution in the form of a power series about x 0. And that solution will have the formy is equal to sum over n equal to 0 to infinity c n x minus x 0 raise to n. So, this differential equation it has a solution only if A of x 0 not equal to 0, this has a solution only if A of x 0 not equal to 0 or x 0 is not a singular point.

So, such a differential equation has a solution in the form of a power series. So, you can use the power series method only if a of x 0 is not equal to 0 or x 0 is not a singular point, so this is a statement we would not actually prove it, but you just take it as a given. Now, suppose A of x 0 equal to 0, then let p of x is equal to B of x by A of x and q of x equal to C of x and A of x.

So, you let this be this and we also ensure that also with no common factors between p of x, q of x and A of x. So, we basically make sure that any common factors between p of x, q of x and u of x are divided out. Now, remember that at x equal to x 0 this goes to 0, so this goes to 0 at x equal to x 0 therefore, at A of x 0 equal to 0, so therefore you would expect if p of x diverges at x equal to x 0. So, unless B of x has some other factors of you know which also goes to 0 you would expect that p of x will go to infinity, when x equal to x 0.

So, in other words p of x goes as 1 over x minus x 0 to some power I will call it r similarly, q of x similarly, you can write the same thing q of x diverges at x equal to x 0. So, q of x will go as 1 over base to prime where r prime is some positive number. So, then when x equal to x 0 p of x goes to infinity q of x goes to infinity if r is a positive number then it diverges in that form.

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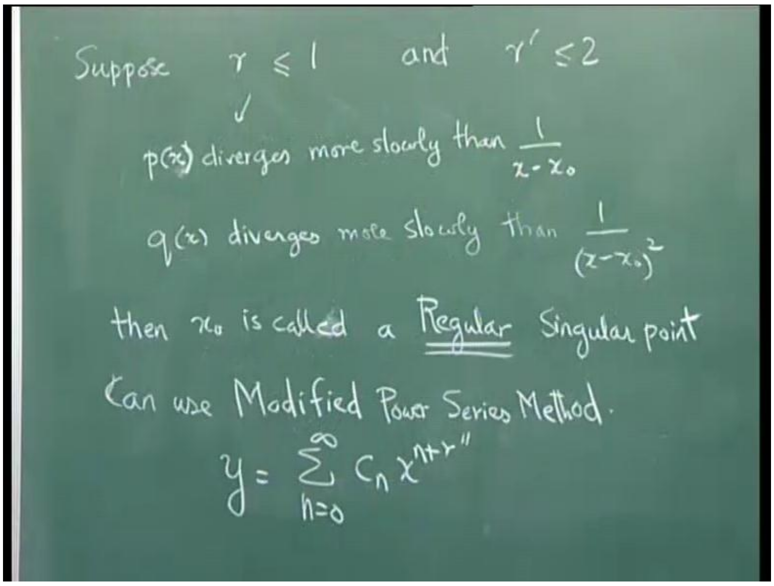

So, now suppose r is equal to 1 and r prime less than equal to 2, so suppose r is less than equal to 1. So, the divergence of p of x is slower than or equal to x minus x 0 1 over x minus x 0. So, in other words p of x p of x 0 diverges p of x diverges more slowly than 1 over x minus x 0 and q of x diverges more slowly than x minus x 0 square. That means the q of x divergence is more slow than this; that means, r is r prime was less than or equal to 2.

So, then x 0 is called a regular singular point, if this condition is satisfied then x 0 is called a regular singular point and for a regular singular point you can use power series. So, now can use modified power series method and in the modified power series method we use y is equal to 0 to infinity c n x raise to n plus r n plus some number r this r is not the same as this r, this is some other r or if you want you call itr double prime. And we will see how to use this method shortly, but just to remind you once again what we have done is we started with the differential equation.

Now this differential equation has x equal to x 0 as a singular point. So, it has a singular point at x 0, so you could not use a power series of this form if x 0 was not a singular point you would have just used this as the power series method. But, since you are not able to use this what you said is, we will look at the nature of the singular point in order to see the nature of the singular point you have to see what is the divergence of p of x what is the divergence of q of x.

So, how do you see how p of x diverges how q of x diverges, and if this divergence is slower than 1 over x minus x 0. And similarly this divergence is slower than 1 over x minus x 0 square then x equal to x zero is called a regular singular point, and we can use the modified power series method. I will before I go into using the modified power series method I will try to show you some examples where how you will check whether some point is a regular singular point or it is not a regular singular point.

And if you have a singular point how do you find out this r and r prime. So, I will just show you an example of that, let us go back to the to the differential equation that we had.

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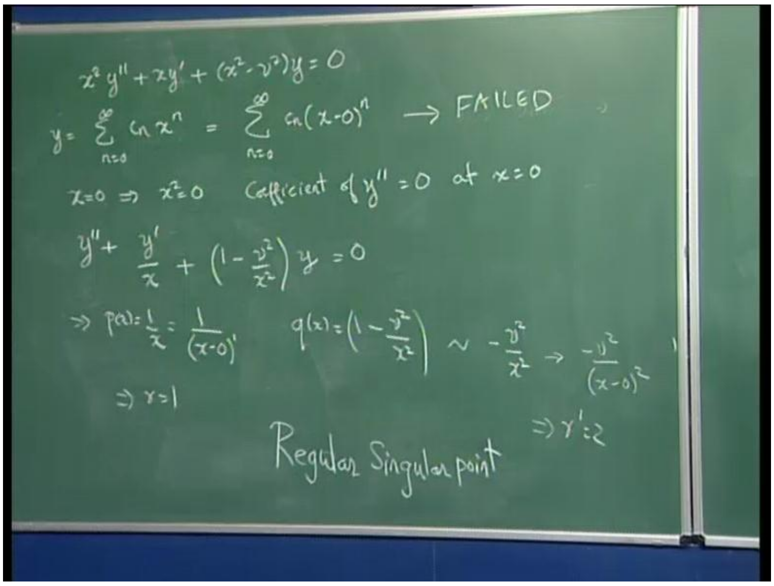

So, let us consider the case where you had x square y double prime plus x y prime plus x square minus nu square y equal to 0, so let us consider this case. Now, we said that we wanted to try y is equal to sum over n equal to 0 to infinity c n x raise to n, so this is same as sum over n equal to 0 to infinity c n x minus 0 raise to n. And this method failed, the reason it failed was x equal to 0 implies x square equal to 0, so the coefficient of coefficient of y double prime equal to 0 at x equal to 0.

So, therefore, this power series method failed, now we have to find out whether this is a regular singular point or it is not a regular singular point. So, what we do is we divide this plus y prime by x plus 1 minus nu square by x square y equal to 0 so I just divided by x square, so this implies p of x equal to 1 by x and q of x. Now, we have to find out whether this diverges faster than 1 over x minus 0 and this diverges faster than 1 over x minus x 0 square.

So, you have to find out how this diverges and clearly this is equal to 1 over x minus 0 raise to 1, so this implies r equal to 1, so r equal to 1 here, what about this case how do we write this in terms of this expression.

So, we have to look at what happens when x tends to 0, so when x goes every close to zero this term becomes very large so when x becomes arbitrarily close to 0 this term becomes very large this compared to this. So, this goes as minus nu square over x squareas x tends to 0, so this diverges as implies r prime equal to 2, so r equal to 1 r prime equal to 2, so this is a regular singular point.

So, this is the regular singular point so, you have to analyze what is the term that is largest when x tends to 0 and x tends 0 and that term turns out to be this, because this becomes much smaller than that and this is proportional to 1 over x square. And so r prime equal to 2 so since r equal to 1 r prime equal to 2 this is a regular singular point.

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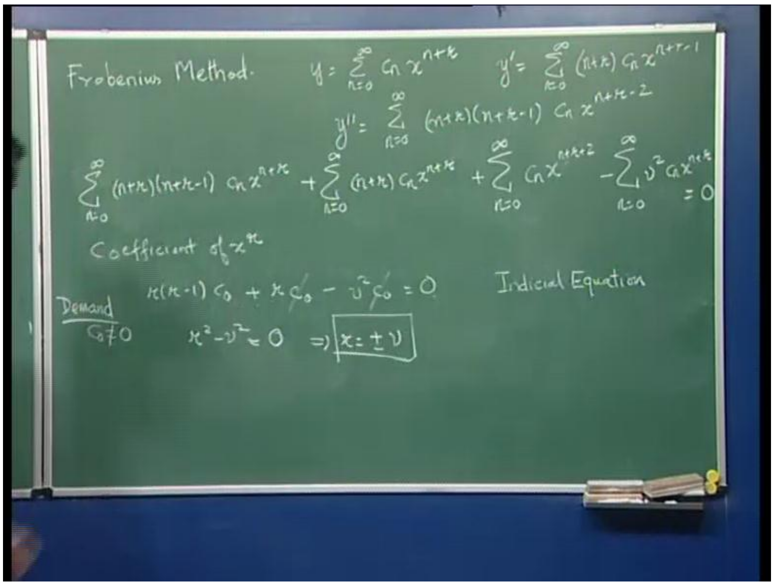

And now that means you can use the modified power series method which is also called the Frobenius method, so what we will do is we will apply the Frobenius method and try to solve that differential equation. This differential equation is called Bessel’s equation and it is one of the most famous equations in applied mathematics. So, the Frobenius method what you say is y n plus r and again this r should not be confused with this r so y equal to c n x raise to n plus r. Now, what we will do is, we will apply the we will start with this series and then we will applied and see what happens.

So, this implies y prime is equal to sum over n equal to 0 to infinity n plus r c n x raise to n plus r minus 1 and y double prime. So, this is the first step of the Frobenius method and then what you will do is you will substitute it in this equation. So, when you substitute this in this equation what you get is first term is sum over for n equal to 0 to infinity c n x raise to n plus r. The second term is x times y prime and that is and the third term I will write it as sum of two terms the first terms is c n x raise to minus nu square this whole thing equal to 0, so I wrote it as four terms.

So, now we need to determine the value of r, so you need to determine r and in order to determine r we look at the coefficient of x raise to r. So, if you want to x raise to r in this expression n has to be equal to 0, so if n equal to 0 this is r minus 1 and n equal to 0, so c 0. In this case what will get isn equal to 0 again, so we will get plus r c 0 in this case if you want if you wantx raise to r then n has to be n has to be minus 2, so it is not possible, so you cannot have a coefficient of x raise to r. In this case if you want x raise to r n has to be equal to 0, so minus nu square c 0 equal to 0.

So the coefficient of x raise to r and this is called the indicial equation and you can immediately see if c 0 is not equal to 0, so we demand c 0 not equal to 0. So, we choose a value of r such that c 0 is not equal to 0 and you can do that and what you have is r square minus r plus r minus nu square. So, r square minus nu square equal to 0 implies r equal to plus or minus nu, so what we did is we started with this under the, we demanded that c 0 is not equal to 0 and when you substitute this in the differential equation the coefficient of x raise to r gives you a condition for r.

So, what you got is r r equal to plus minus nu, now r has to be equal to plus minus nu and now you will have different cases and in each case we look at the nature of the solutions so I will just mention a few things about the nature of the solutions using the Frobenius method. In the particular case of the differential equation the Bessel’s equation, we saw that r has to be equal to plus minus nu.

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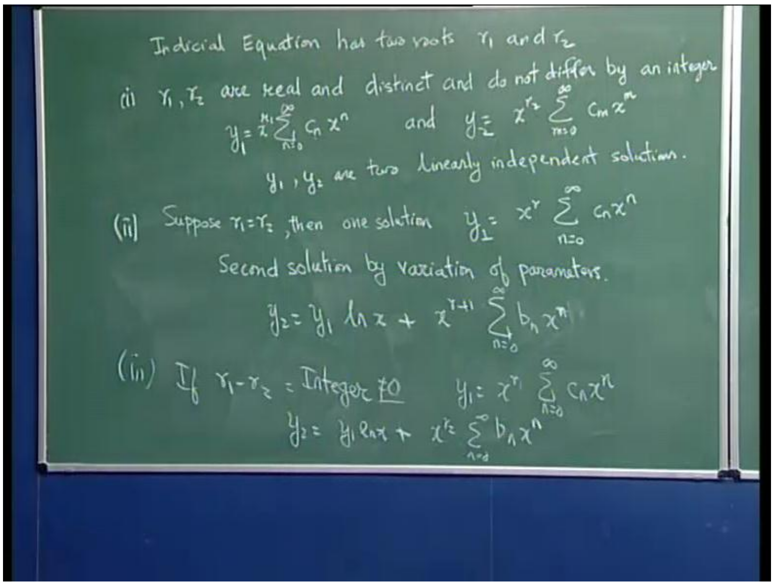

In general the indicial equation has 2 roots r 1 and r 2 in the case of Bessel's equation r 1 was equal to nu r 2 was equal to minus nu. And there are 3 case, first case r 1 r 2 are real and distinct, so if these two are real and distinct then you can have 2 possibilities y is equal to sum over x 2 to the r 1 c n x raise to n. So, I wrote c n x raise to n plus r 1, so I just took x raise to r 1 outside and y is equal to x raise to r 2 sum over, I will just say m equal to 0 to infinity c m x raise to m, I can call this n also.

So, basically these are the two linearly independent solutions, so I call this y 1 y 2, so y 1 y 2 are 2. So, if these two are distinct, then these two become two linearly independent solutions there is one more condition real distinct and do not differ by an integer. This is the condition for you to be able to write this as linearly independent, if r 1 and r 2 differ by an integer. If r 1 and r 2 differ by an integer then it turns out that these two series become very close related you can write one series in terms of the other then you lose the fact that they should be linearly independent. Now, suppose r 1 equal to r 2 then one solution y is equal to x raise to r x raise to n and we can determine the second solution by variation of parameters.

So, suppose you have one solution in this differential equation if you have one solution you can determine the second solution by variation of parameters. And I leave this as an exercise to you but you can show that the second solution looks to be of the following form. So, y 1 is this y 2 is equal to y 1 and y 1 times nature log of x plus x raise to r plus

1 sum over n equal to 0 to infinity d n x raise to n plus r b n x raise to n sorry x raise to n. So, where the coefficients of b n can also be found out so this is a second solution we would not go into details of this, but essentially you can always calculate one solution using the Frobenius method the second solution you can calculate by variation of parameters.

Now, the interesting case is if r 1 minus r 2 equal to integer not equal to 0 and in this case two you can do exactly the same thing you can calculate the first solution y 1 is equal to x raise to r r 1 x raise to n. And y 2 you can determine by a variation of parameters and y 2 turns out to be y 1 and n of x plus x raise to r 2 sum over n is equal to 0 to infinity b n x raise to n. So, the interesting case is we have to check whether these two roots are they real distinct and do not differ by an integer or whether they are the same or if they differ by an integer. So, let us now get back to the Bessel's equation and see what we get.

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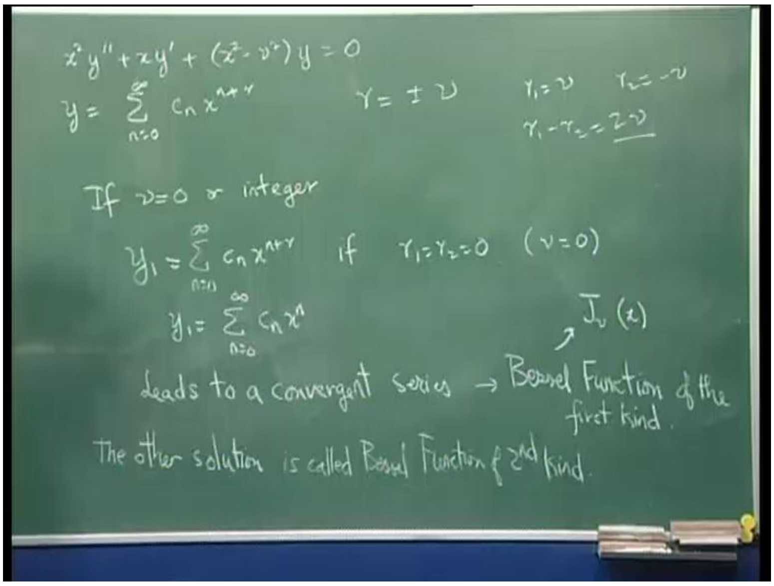

So, remember in the Bessel's equation was x square y double prime plus x y prime plus x square minus nu square y is equal to 0 and we put y equal to a sum over n equal to 0 c n x raise to n plus r and what we got was r is equal to plus minus nu. So therefore, r 1 minus r 2 equal to 2 nu or absolute value of r 1 minus r 2 is 2 nu. So, actually I should write it slightly differently I will say if r 1 equal to nu r 2 equal to minus nu r 1 minus r 2 equal to 2 nu. Now so, depending on if nu is a nu can be an integer it can be or it can be zero or it can be some fraction or it can be rational number which is not an integer.

So, if nu equal to 0 or integer, then we have to look at one of these two cases depending on if nu is 0 or an integer if nu is 0 then both the roots are the same r 1 equal to r 2 equal to 0. And then you can write in this case the solution y 1 is equal to sum over infinity c n x raise to n plus r now or in this case, if r 1 equal to r 2 equal to 0 then y one is equal to sum over n equal to zero to infinity c n x raise to n, so this is the case when nu equal to 0.

So, one solution you can do this in the form of this power series and what you can show is that you, now you use this power series method in the usual way. So, we already started with the modified power series method and then we saw that r equal to plus minus nu but nu was equal to 0.

So, one solution can be written in terms of a power series and this series turns out to nu when you substitute this and you work it out you will find that it leads to a convergent series and remember what we said is that the convergence series is some series that truncates somewhere. So, instead of going from 0 to infinity it stops at some points andthat that is that series is called Bessel function this series is called Bessel function so this is called Bessel function of the first kind.

I would not go into the details because the way you find the Bessel function the first kind is exactly similar to the way we found the Legendre polynomials. Just as we did the Legendre polynomials you can show that this leads to the Bessel function of the first kind; the other solution is called Bessel function of second kind.

So, the other solution that you get by variation of parameters is called Bessel function of second kind the symbol used for Bessel function of first kind is j nu of x. So, if nu equal to 0 then this function as called j 0 Bessel function of degree 0 if nu equal to 1 it is called Bessel function of degree 1 and so on. So, this is about what how much I want to talk about the power series method, now in the in the next class we will see an application of this power series method.

The application will lead to a problem that you will encounter in your quantum mechanics courses or you have already seen it in quantum mechanics courses. This is calculating the angular part of the wave function for a hydrogen atom problem, so we will look at that in the next class.