Chemistry Atomic Structure and Chemical Bonding
Prof. K. Mangala Sunder
Department of Chemistry
Indian Institute of Technology, Madras

Lecture – 28
Power Series Method for Differential Equation – I

Yeah, welcome to the lectures in chemistry and the topic on Atomic Structure and Chemical Bonding. My name is Mangala Sunder and I am in the department of Chemistry as a professor in the Indian Institute of Technology Madras Chennai.

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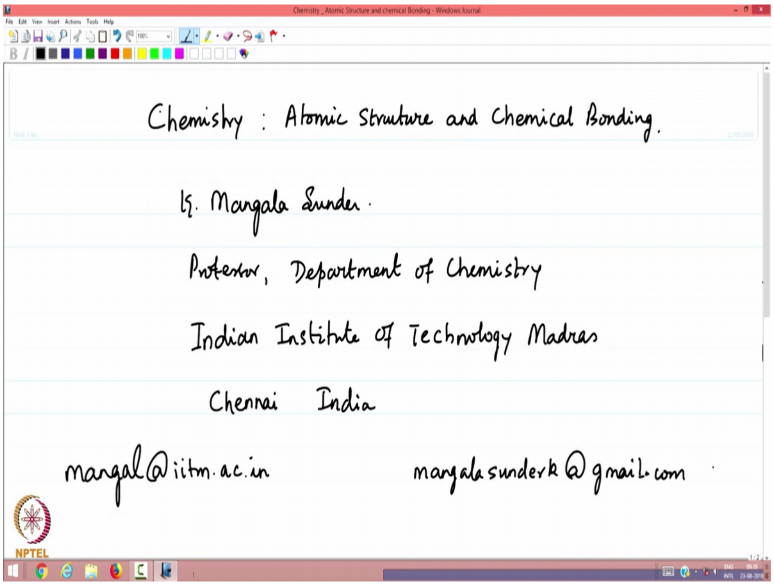

My email addresses are given here for you to correspond or for you to request additional information. This is the first of a number of lectures on solutions to a few important differential equations right.

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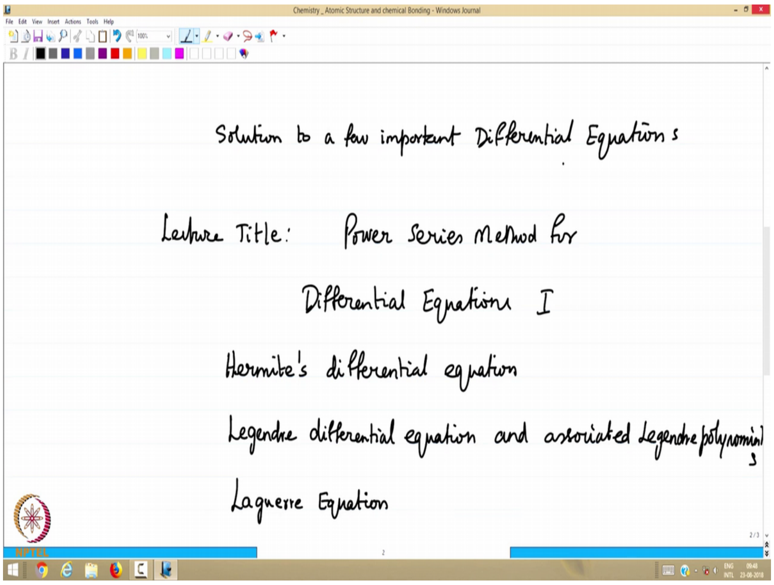

So, the lecture title is power series method. There will be several lectures on this. And this is important for students who would like to understand the mathematics behind and also the solutions behind the problems that we have discussed so far. The harmonic oscillator the hydrogen atom and even particle in the box where the solutions appear to be simple enough for you to write down, but there is a general method.

And the power series method is something that is very well known in the mathematics of the solution of differential equations, second order and partial differential equations, but I shall illustrate what is minimally required for us to understand the method. And will not worry so much about the convergence of the solutions, the uniqueness of these solutions and so on.

That is; obviously, the second level reading, if you are interested in the more abstract mathematical nature of the solutions. Here we are trying to handle the practical problems and try to appreciate why the solutions are the way they are. We will start with the 2 elementary differential equations, for which you already know the solution, but the method of power series will also be shown, to tell you how such methods work for the more complicated equations. The purpose of this series of lectures is to follow up with the 3 equations that you have already encountered, namely the thermite a differential equation for the harmonic oscillator.

The second one is the Legendre differential equation which you have seen now in the form of the solutions to the angular part of the hydrogen atom, namely the spherical harmonics. Legendre and associated, Legendre polynomials and the third equation is the Laguerre equation. The Laguerre equation is the one that you saw as giving you the solutions to the radial part of the hydrogen atom for this whole week or whatever period that, the next few lectures we will contain some details of the mathematics. Let us start with the first simple equation.

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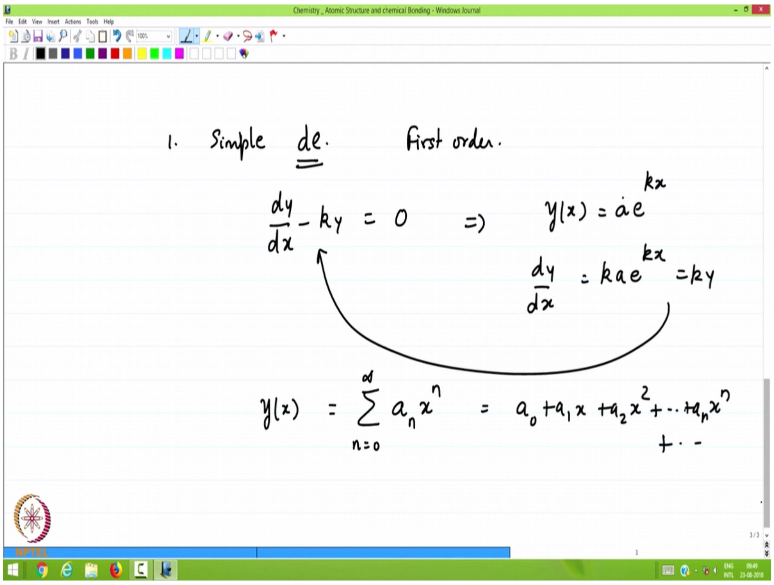

Not even second order, but we will start with the first order, all of you know that the differential equation dy by dx minus ky is equal to 0 has the solution y of x which is a function y is a function of x as some constant a times e, to the kx because that is immediate. Because then you know dy by dx gives you k a e to the kx which is k y and therefore, this is that equation.

Now, let us do illustrate the power series method for this differential equation to begin with. So, let me write propose a solution for y of x as an infant series containing all the terms starting from n equal to 0 to infinity starting from n equal to 0 and going up to infinity, a n x raise to n. This is the short representation for the term a naught plus a 1 x plus a 2 x square plus etcetera plus a n x raise to n plus and so on. It is in infinite series now let us try and understand to this method using this particular form of the solution.

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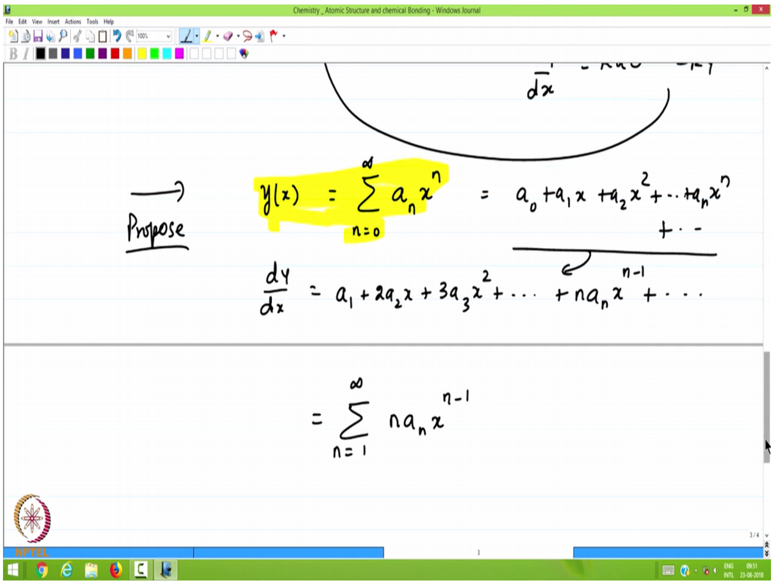

We propose this as a solution and then determine the constants, if we can dy by dx if I take the derivative of this expression. Then you know a naught goes away, and a 1 is the first term that is non zero, then you have 2 a 2 x plus you have 3 a 3 x square plus and so on. And the term that you see here as a general term gives you n a n x raise to n minus 1 plus so on.

And this can be written in the form of a summation as n equal to 1 to infinity n, a n x raise to n minus 1. You can also see that from here. Since n equal to 0 does not contain any powers of x, the derivative of this term will get rid of the a 0, but every other term will have n a n and we will have x raise to n minus 1 and that is what I have written here. Now the differential equation that you are trying to solve is dy by dx minus ky is equal to 0.

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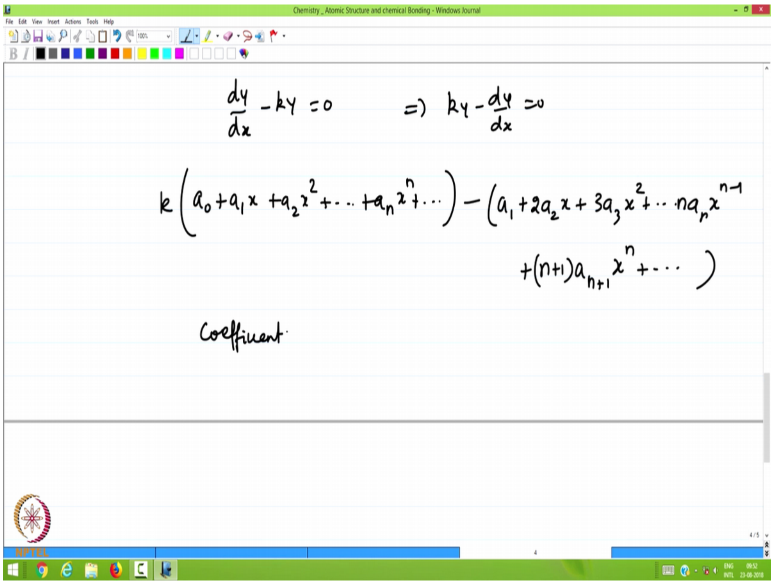

And therefore, let us write this as a naught plus a 1 x plus a 2 x square plus a n x raise to n plus and so on. This is the k y term multiplied by ky. So, let me write this as k y minus dy by dx is equal to 0. And then subtract the derivative namely minus a 1 the x is gone plus 2 a 2 x plus 3 a 3 x square plus etcetera. And the nth order term if you have to write in here.

You will have to write this as n a n x raise to n minus 1 plus n plus 1 a n plus 1 x raise to n plus and so on. So, the general term if you look at it is, if we arrange them in the order of coefficients of various powers of x, if we write down the coefficient of various forms of x.

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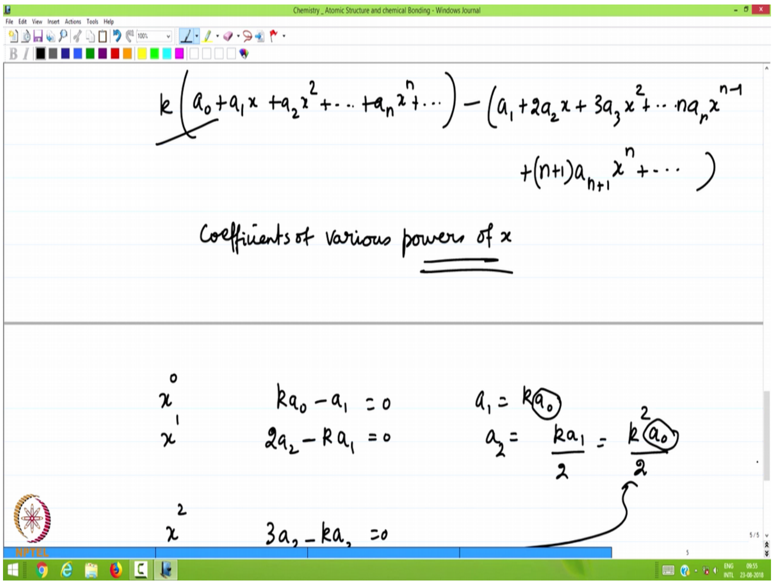

X raise to 0 that is constant if you look at the constant it is k a naught on the first this one and then minus a 1 is equal to 0 or a 1 is equal to k a naught. What is the next term that you see? What you see is 2 a 2 power of x is 2 a 2 plus k minus k y1 is equal to 0 k a 1 yes.

This is the x raise to 1 power. The coefficient has this relation. Therefore, what you have is a 2 is equal to k a 1 by 2, and y a 1 is already there as k a naught. So, you have k square a naught by 2. So, you have a 2.

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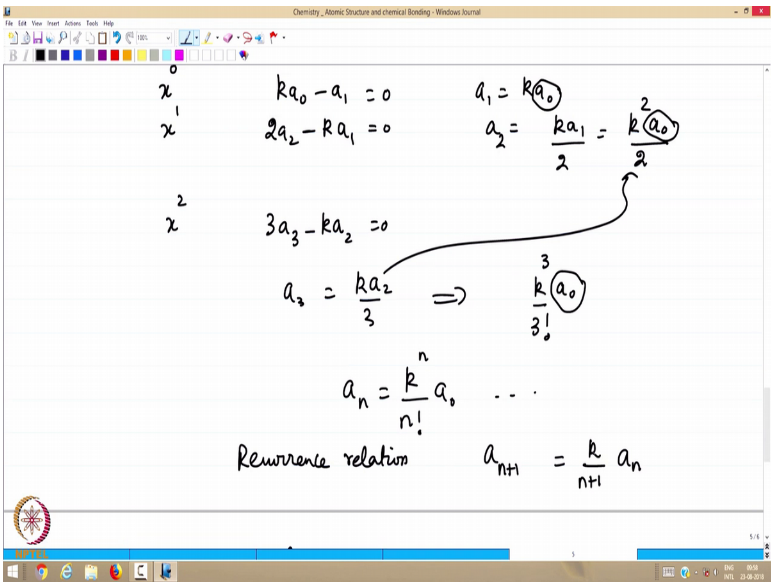

And the third if you write the x raise to 2 x square then the term is 3 a 3 minus k a 2 is equal to 0.

Therefore, you have a 3 is equal to k a 2 by 3 which gives you k a 2 is already given by that. Therefore, it gives you k cube u naught by 3 factorial. Remember now all the constants are expressed in terms of one undetermined constant a naught right. And that is what you should expect anyway because this is a first order differential equation. Therefore, the general solution has only one undetermined constant and now that constant turns out to be v a naught.

So, what is the general term for this? The general term if you do a n following this it will be k raise to n by n factorial a naught and so on. Therefore, now you have found the solution for the differential equation namely.

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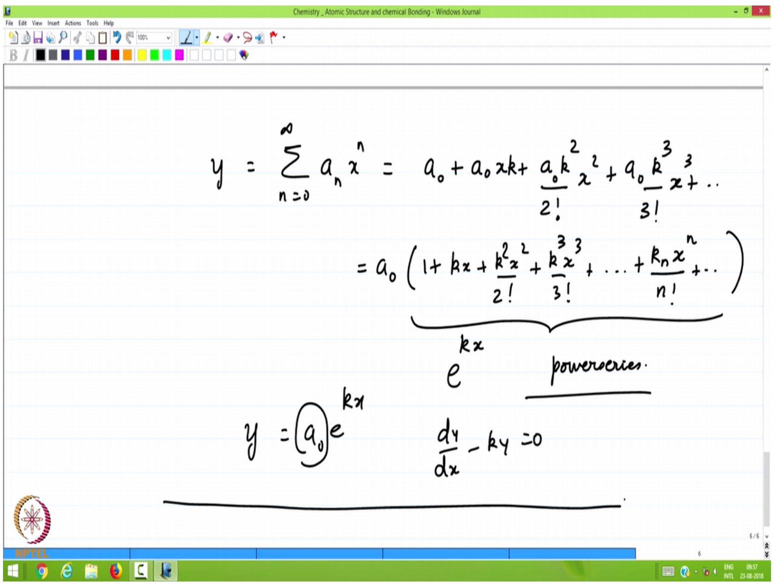

Y is equal to sum over n equal to 0 to infinity a n x raise to n is given by a naught plus a naught x plus kx plus a naught k square by 2 factorial x square plus a naught k cube by 3 factorial x cube and so on here you got all these answers.

A 3 is k cube by 3 factorial a naught a 2 is k square by 2 factorial a naught, a 1 is k a naught and a naught is e naught of course. So, what you have is essentially a naught into 1 plus k x plus k square x square by 2 factorial, plus k cube x cube by 3 factorial plus and so on. Plus, k raise to k n x raise to n by n factorial.

This is nothing but the exponential k x this is the power series for exponential k x inside is therefore, you see y is equal to a naught e to the k x where there is one constant and determined is the solution to the differential equation dy by dx minus k y is equal to 0.

So, this very elementary so, it is easy to see and we have not touch the question of whether this exponential representation and the power series representation whether they the power series converges and so on. You know that the exponential k x keeps on increasing as x increases and is unbounded as x becomes infinite. And so, does the power series. So, therefore, there are questions about the convergence, questions about the uniqueness question we will not discuss in this case of course, it is easy to show that this is a unique solution. And this is one way of looking at to this. The reason for doing this is that one more equation and this will give you the general process by which the 3 equations I indicated earlier. The Hermite's equation, the Legendre equation and the Laguerre equation, how they are solved using the relations.

Now, what I did not specify to you is what is known as that recurrence relation in the whole process. So, let me just indicate that. The recurrence relation is essentially the coefficient a n plus 1, how is it connected to the previous coefficient a n. Now, if you look at that the coefficient a n plus 1 is connected to the coefficient k a n by this relation k by n plus 1. Now, you can see that when n is 0 this is k times a 1 this is a 1 and therefore, it is k times a naught. When n is 2 it is k by 3 a 2 this is a 3, this will be a 2.

So, the recurrence relation tells you the relation between the coefficients in some form such that they can be generalized and the result that you saw here namely this result a n is equal to k raise to n factorial is a repeated substitution of this into a by a n minus 1 and then a n minus 1 by a n minus 2 and a n minus 2 by n minus 3 and so on.

So, finally, you get to this so, this is the recurrence relation and this is the final coefficient that is determined in terms of the undetermined coefficient. Now another equation for which you also know the solution we will discuss that.

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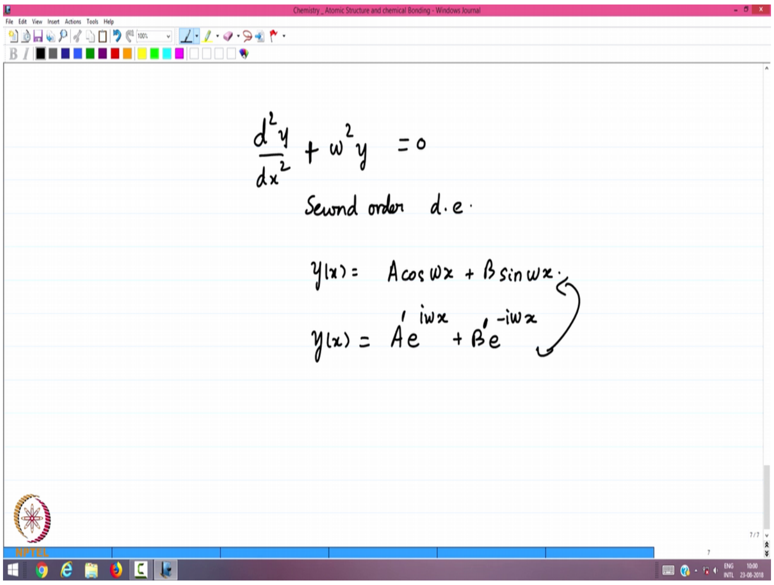

This is d squared y by dx square minus omega squared y is equal to 0. Second order differential equation and all of you know the solution from the particle in the box for this that let us write plus y square. So, that is the one that you have been dealing with, of course, minus y squared will give you exactly the same relation that you already had. So, for d square y plus omega square y we will do that and you know that the solution of y of x is A cos omega x plus B sin omega x. And for a particle in the ring you were using this solution y is equal to A e to the plus i omega x plus B e to the minus i omega x they are both equivalent anyway.

Because if you expand the exponential using cos on sin and the cos on sin and write this many different constants a prime and b prime. And you can relate these constants to each other the general power series method is something that we should look at for this problem. And this will make you familiar with the remaining parts of the lectures on this topic.

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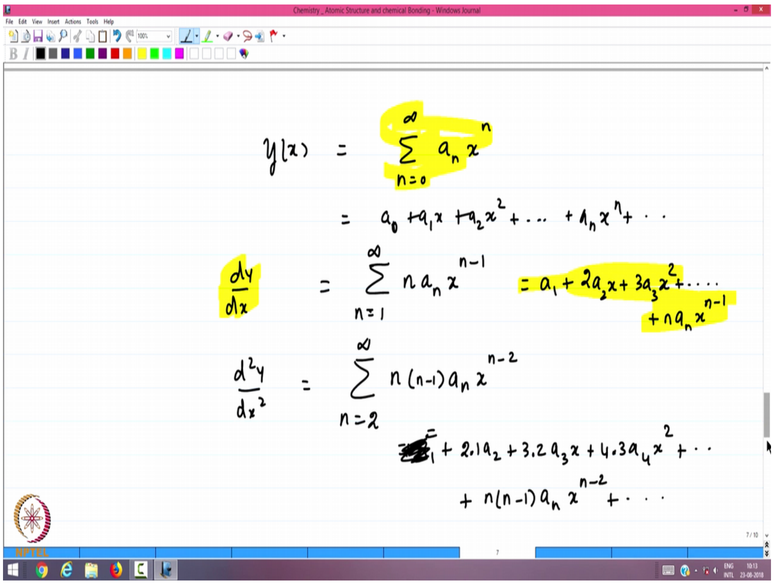

Now, the differential equation that we have to solve is d square y by dx square plus omega square y. So, let me just go back and what I have written.

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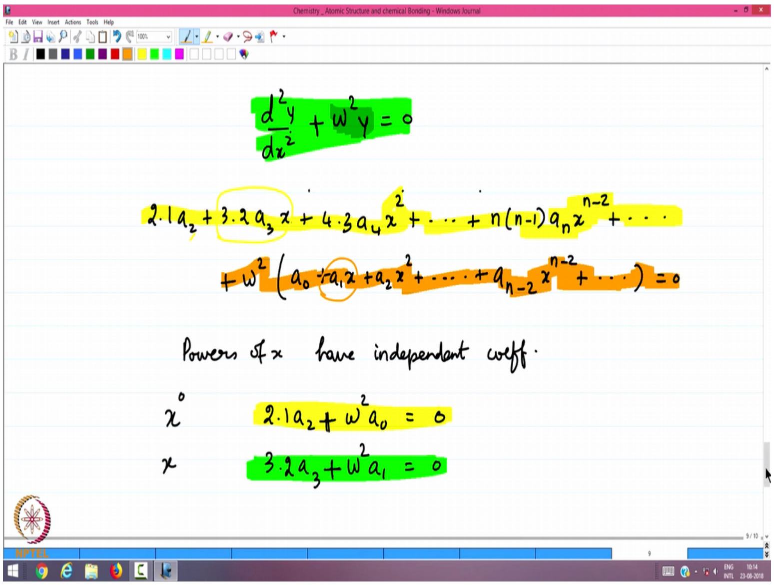

So, if you take the second derivative, the second derivative is the expression that I am just copying here. So, d square y by dx square is given by this term, we highlight all of that. It is given by this term all these things. There is an infinite series and then the differential term namely the omega square y is this term omega square a naught a 1 x a 2 x all these this is the omega square termed.

So, this is the omega square term and this is the d square well. Then you collect the powers of the individual x's namely x raise to 0 which is a constant. And if you look at that you see it is 2.1 times a 2 plus omega squared a naught that is 0. The coefficient of x is 3.2 times a 3 here this term this term and the corresponding the omega square term for the power of x is this term omega square times a 1.

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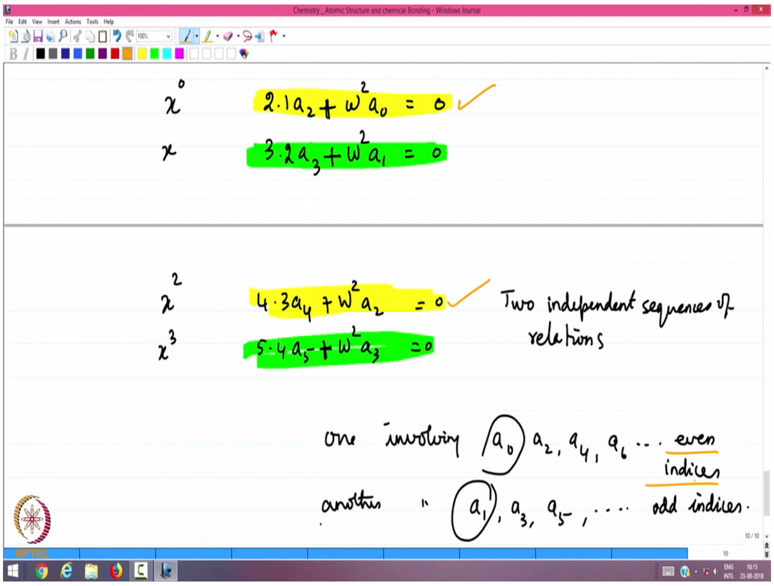

And then you can write down a few more terms namely 4.3, 4 times 3 a 4 plus omega square a 2 is 0 5 times 3 a 5 plus omega square a 3 and equal to 0. So, you see that there are 2 independent sequences of relations. One sequence involves a naught and then 2 a 2 the next that sequence contains the a 2 a 4 and the things that I have not written down a 4 to a 6 a 6 to 8 and so on.

So, that involves only the even indices. The other sequence is the one which is marked in green here it involves a 1 and the relation between a 1 and a 3 and then the relation between a 3 and a 5 and then between a 5 and a 7. So, you can see that the odd index coefficient; odd indexed coefficient a 1 a 3 a 5 they are all connected to a 1. The even indexed coefficient are all connected to a naught.

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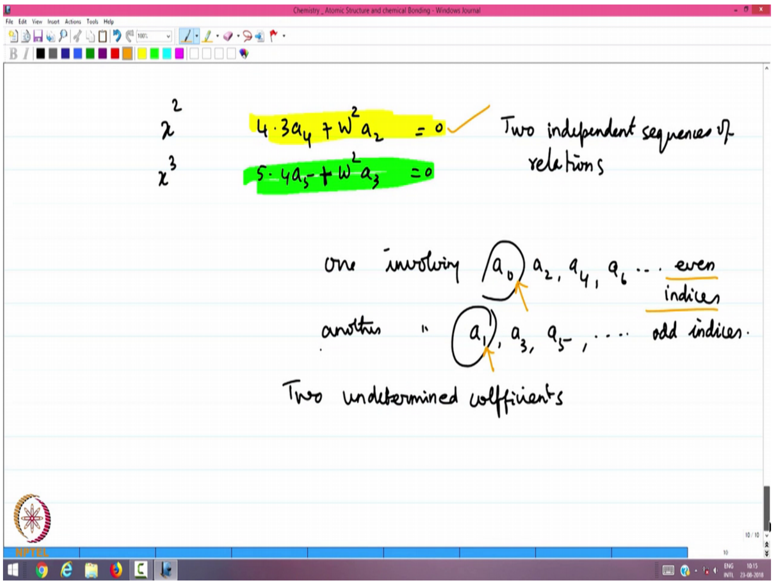

That is not surprising that we have only to undetermined the coefficients. Because it is a second order differential equation. It requires 2 conditions to be fulfilled and for the particle in the box if you recall you did that for the box at one-point psi of x is equal to 0 and psi of x is equal to l 0, you put that in those 2 conditions.

They determined with the other boundary condition they determine both of the a and b. Therefore, we need to undetermined coefficients and everything else can be written in terms of them. So, let me write that therefore, the general relation between these coefficients.

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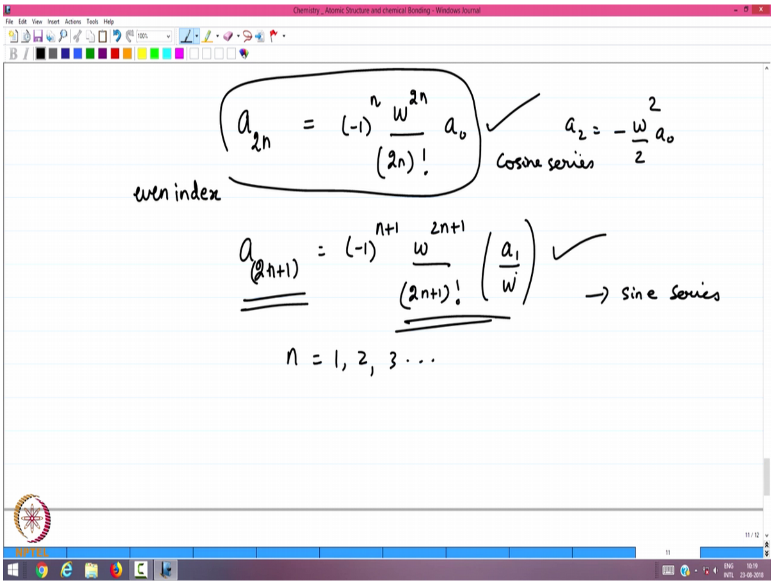

The general relation is a 2 n that is even index a 2 n is minus 1 raise to n omega to the 2 n divided by 2 n factorial a 0, a 2 n plus 1 is minus 1 n plus 1 omega to the 2 n plus 1 divided by 2 n plus 1 factorial, a 1 by omega. Quickly what does this mean, if n is 1 a 2 is minus 1 raise to n. So, it is minus omega 2 n is omega square 2 n factorial is 2, a naught. Now you see the relationship between a 2 and a naught, a 2 is minus omega square by 2 a naught no problem. And a 4 is minus omega square divided by 4 here this one.

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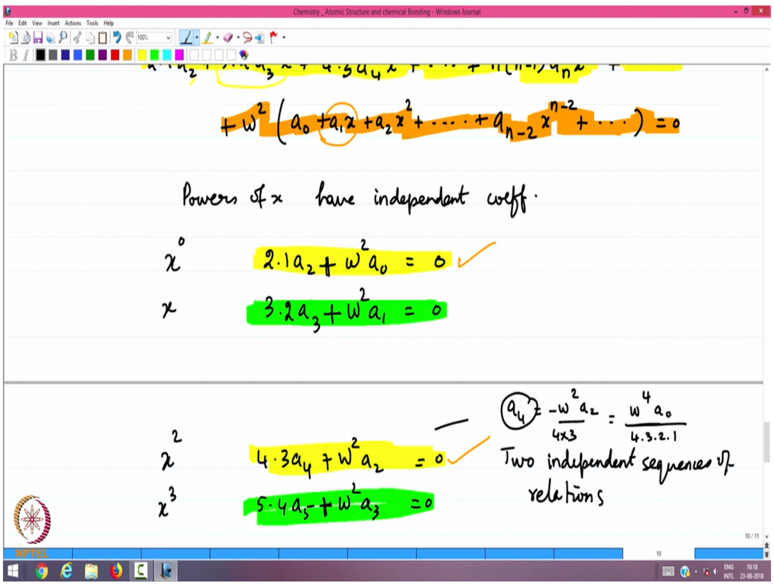

A 4 is minus omega square a 2 divided by 4 into 3, 4 times 3. And a 2 is already a minus therefore, it is plus omega raise to 4 it also contains an omega square. And it is a naught divided by 4 3 2 1 so, it is 4 factorial.

So, a 4 is 4 factorial omega 4 in r. So, it is easy to see that this generality is here, that a 2 n is minus 1 raise to n a 4 is plus a 2 a 6 will be minus a 6 and so on you can see that for this is the recurrence relation between the coefficients in the even n. And this is the recurrence relation likewise between the coefficients in the odd index to n. Now n is equal to 1 2 3 etcetera, the number of the power series for cosine omega x.

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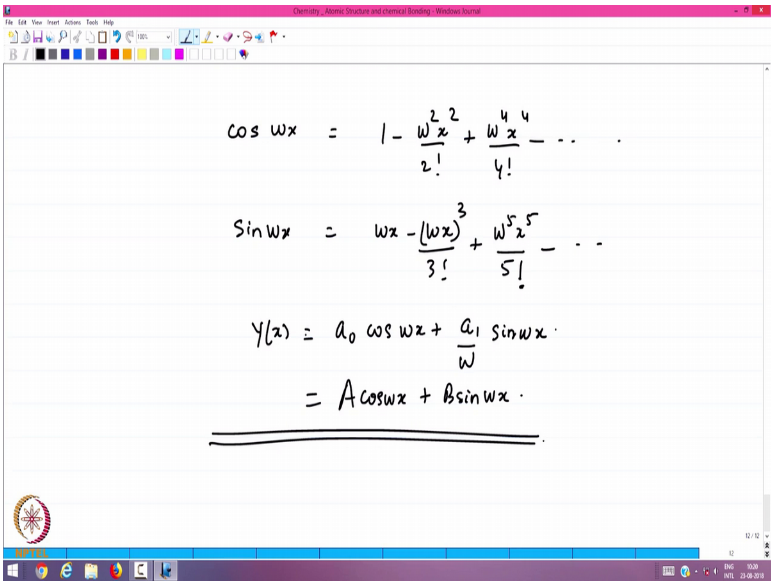

Cosine omega x is 1 minus omega square x square by 2 factorial plus omega 4 x raise to 4 by 4 factorial minus and so on. And the power series for sin omega x is omega x minus omega x whole cube divided by 3 factorial plus omega 5 x raise to 5 by 5 factorial minus and so on. You will see that these 2 coefficients basically lead to exactly those power series starting from a 0 a 2 a 4 a 6 etcetera. They all correspond to the cosine power series.

And the series a 1 a 3 a 5 a 7 etcetera they all correspond to the coefficients of the sin series. With the fact that it is a 1 by omega which is needed because otherwise it will be omega raise to 2 n. So, it is some omega is a constant anyway. So, we have redefined the constant and this is the cosine series. So now, you can therefore, write the final solution as the following namely y of x is equal to A cos omega x, plus A here is our a naught. A naught and then you have a 1 by omega sin omega x, which is the same as what you had earlier written a cos omega x plus b sin omega x.

So, the power series method is something that is the underlying the algebraic tool through which one obtains solutions for complicated differential equations. And the power series method is very well known for a special class of differential equations leading to what are known as special functions. And, some of the examples of these special functions that we will see in physics and mathematics and also sometimes in chemistry or Bessel functions.

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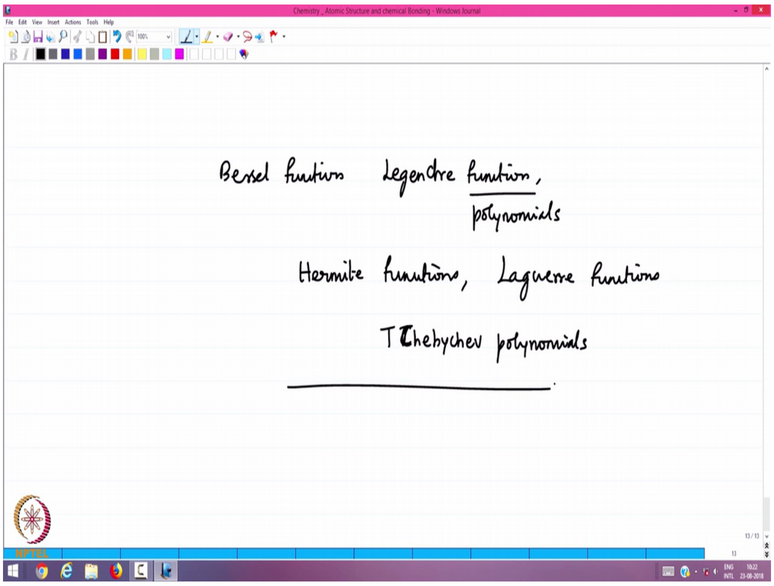

The differential equation is called the Bessel differential equation. Legendre functions and the associated Legendre polynomials coupled with the 5 part they are called the spherical harmonics, Legendre functions. These are called the polynomials, they are all various powers we will see one of them. And then we have the Hermite polynomials or Hermite functions. And then Laguerre functions; functions are Laguerre polynomials and there are others like the Chebychew it is often written in many different ways, Chebychew C. Sometimes people put a T in front of these 2 Chebychew Russian mathematician; Chebychew polynomials and so on.

Therefore, the differential equation method the solution of it using the power series is something that has been well established. And the physicists like Schrodinger and many others her earlier studied the differential equations and then they saw that the mathematics of the hydrogen atom and the mathematics of some of the atomic and the molecular chemistry problems go back to the polynomials and the methods which were discussed in mathematics independently of quantum mechanics. And therefore, they bridge the gap between the non-mathematical results and the unknown the new problem of the quantum mechanics or the problem of quantum mechanics.

And so, you can see that the fusion between the 2 is a very, very well studied mathematical technique. We will see a few examples as part of this course and we will see more of it in the Hermite polynomial in the next lecture until then.

Thank you very much.