Advanced Mathematical Methods for Chemistry

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Module – 05
Lecture – 04
Frobenius Method / Power Series Method

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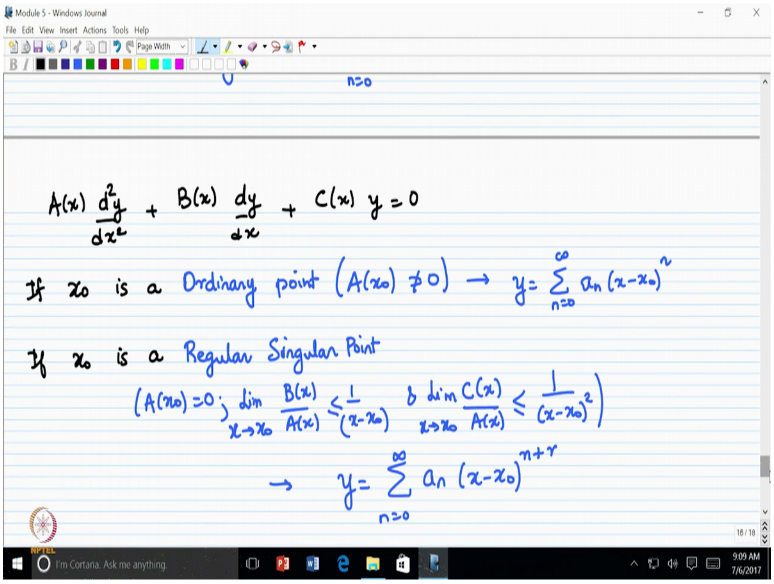

Let us look at how the power series method works in practice. In the last class we talked about the 2 kinds of alternate ways you can use it. So, for an ordinary point you can write it as just a power series, but if you have a regular singular point then you need to then you have to have this x raise to r an additional factor of that. Let us see this method in action and what all try to do in this lecture is to briefly give you the overview and when you actually apply this method to see how it works more clearly.

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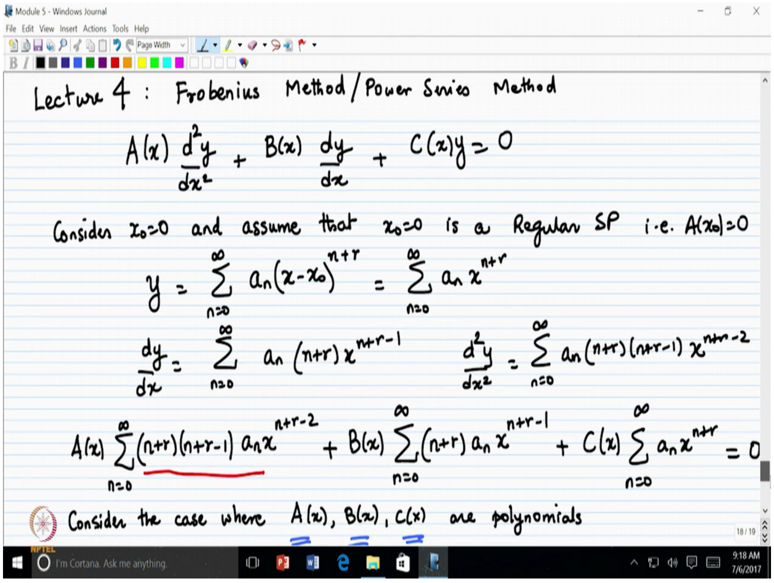

So, let us get back to our equation and A of x d square y by dx square plus B of x d y by d x plus C of x equal to 0.

So, the basic idea of the power series method is that you substitute. So, let us consider, for simplicity let me take consider x 0 equal to 0 and assume that x 0 equal to 0 is a regular singular point. You can do for other cases also, but let me take the case where x 0 equal to 0 is a regular singular point. So, that is A of x 0 equal to 0 and you have the other conditions for the derivative. So, now, what is the basic idea of the power series method? You are going to write y as sum over n equal to 0 to infinity a n x minus x 0 now x 0 equal to 0 so raise to n plus r the advantage of taking x 0 equal to 0. So, I do not have to write this x minus x 0 every time. So, I will just write this as n equal to 0 to infinity a n x raise to n plus r. So, it just makes my notation easier. You can do this with x 0 not equal to 0 and it will not change anything, it just writing will be easier if I take x 0 equal to 0.

So, you have this and then you know that we have to take d y by d x because that appears in the differential equation and this is sum over n equal to 0 to infinity a n n plus r x raise to n plus r minus 1 and you have d square y by d x square, I can write as sum over n equal to 0 to infinity a n n plus r n plus r minus 1 x raise to n plus r minus 2. So, now, if you put all these in the differential equation what you will get is you will get A of x times sum over n equal to 0 to infinity, n plus r n plus r minus 1 a n x raise to n plus r minus 2.

Now I have b of x sum over n equal to 0 to infinity, n plus r a n x raise to n plus r minus 1 plus C of x times y if why I have missed the y in the original equation. So, if you have C of x times sum over n equal to 0 to infinity a n x raise to n plus r and this equal to 0.

Now the basic idea of the power series method is to realize that each of this whole thing on the left hand side looks like terms that have different powers of. So, it looks like terms with different powers of x. In order to do this we have to have, so we will consider the case where A of x, B of x, C of x are polynomials.

So, these are polynomials. So, it could be like x x square 1 minus x square x cube and so on or x square plus x plus 1 or some such thing. So, just for simplicity let us consider the case where these are polynomials, I should emphasize that if they are not polynomials it is not a problem.

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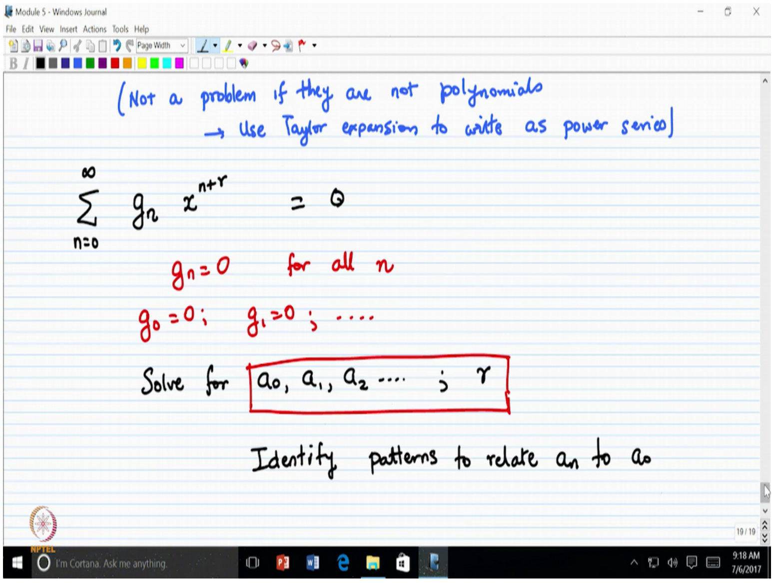

So, let me emphasize that it is not a problem if they are not polynomials, not a problem if they are not polynomials. All you need to do is to use Taylor expansion to write as infinite as power series. So, if your A of x, B of x and C of x are not polynomials then what you can do is you can use Taylor expansion and write each of them as an infinite series.

So, what you will get finally, what you will get finally is you will get something like you know I will just write this in the following form. So, A of x is a polynomial. So, it will have terms of x of constant x x square and so on. Now when you multiply this then what you will get is you will get a left hand side, if you collect all the terms with the same power you will get left hand side that has something like this I will just write from n equal to 0 to infinity n plus and you will get some I will just write it as sum g of n and then you have x raise to n plus r. So, if you collect everything you will get something like this equal to 0.

Now, g of n is will be it involves not only all these factors of n plus r n plus r plus r minus 1 a n, but also whatever terms you get from a x. Similarly or it involves n plus n plus r times a, a n plus whatever terms you get from b x and so on, a n and whatever terms you get from c x and you sum all of these and you write it in this form then what you do is once you have this form you are going to set g n equal to 0 for all n because the right hand side is 0 and, so each term will be 0. So, so you start with g 0 equal to 0 g 1 equal to 0 and so on.

Now, when you do this, so once you do this you solve for a 0 a 1 a 2 you also have to solve for r. So, these are the things, these are the unknowns. So, these are all the things that you need to solve for and basically all these equations will give you ways to solve for them and usually typically we identify patterns, patterns to relate a n to a 0. We will see we will see how this works in practice in some differential equations, but this is the basic crux on which the power series method is based. So, what you will be doing is we will be applying this to some specific equations.

Now I will just list the places where you see the power series method, what are the cases in which you see the power series method?

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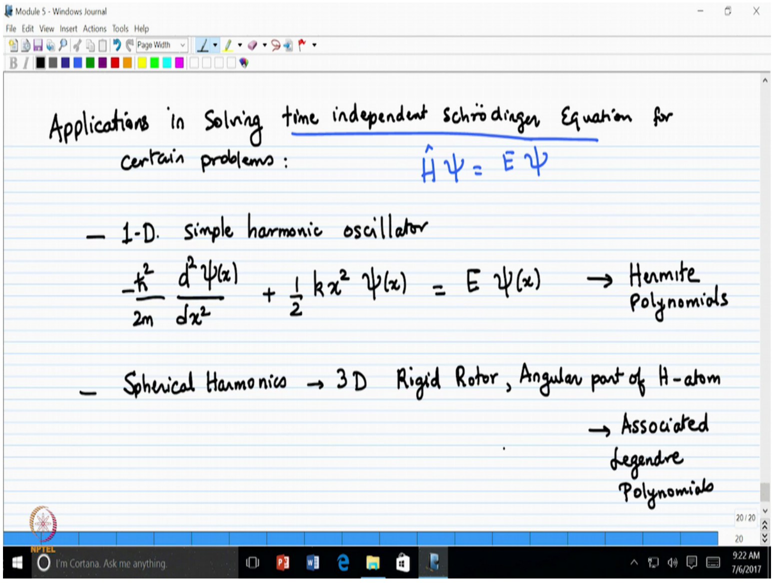

So, I will just write applications and this is in particular in solving the time independent Schrodinger equation for certain problems. So, there are certain problems which we will see in your quantum mechanics course where the time independent Schrodinger equation, remember the time independent Schrodinger equation is basically given by H the Hamiltonian operator, operator on psi gives E times psi.

Now, psi can be a function of various of different coordinates, but this particular where you see the power series method appearing, so you will study in the one dimensional simple harmonic oscillator. So, the quantum mechanical simple harmonic oscillator I will just write differential equation this is the differential equation looks like d square psi of x by d x square times minus h bar square by 2 m plus half k x square psi of x is equal to E times psi of x. So, what you want to solve you want to solve for both psi of x and E and E. So, this is the solution involves Hermite polynomials. So, you can solve this using the power series method and you get something called Hermite polynomials.

So, the power series method will converge to give these Hermite polynomials the second example is what are called as spherical harmonics. So, this appears in the 3 D rigid rotor or the angular part of hydrogen atom and this spherical harmonics are given by what are called as Associated Legendre Polynomials. I will not write the differential equation for this, but we will see this when you actually apply it. So, this is usually written in terms of spherical polar coordinates.

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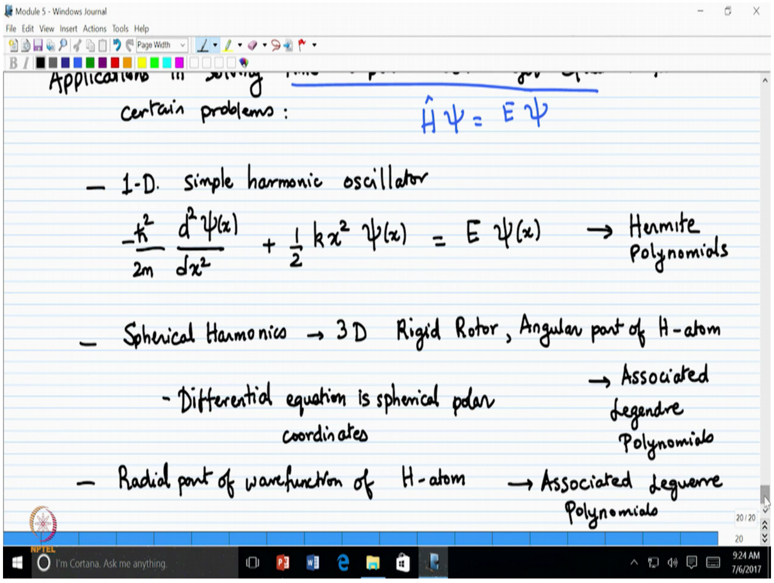

So, I will just emphasize that you have a differential equation and equation in spherical polar coordinates.

The third very common place where you see, where you see these power series method is in the radial part of wave function of hydrogen atom. Just the radial part of the wave function you see what are called as Laguerre polynomials or rather these are the associated Laguerre polynomials. I should emphasize that in each of these cases when you get the Hermite polynomials or the Legendre polynomials or the Associated Laguerre Polynomials you have to use some sort of intuition or some sort of clever tricks in to actually get the differential equation in these forms.

I will conclude this lecture here. In the over the next 2 lectures I want to look at applications of the power series method over the, actually over the next lectures I will look at how this power series method is applied and I will take the particular case of the hydrogen atom, I will show the solution of both the angular part of the wave function and the radial part of the wave function. So, I look at the Schrodinger equation for the hydrogen atom and then as we solve it we will see how the solution appears in terms of polynomials.

Thank you.