Advanced Mathematical Methods for Chemistry
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Module - 05
Lecture - 1
Homogeneous 2nd Order ODE, Basis Functions

Now, we will start module 5 of this course. In this module I will be talking about second order differential equations and the ways to solve them.

Now second order differential equations are almost ubiquitous in all of physical chemistry. So, for example, in quantum mechanics the Schrodinger equation, the time independent Schrodinger equation is typically expressed as a second order differential equation. You have other equations like the diffusion equation in which is used in non equilibrium transport phenomena and which is also written as a second order differential equation and there are various equations that you see in various parts of physical chemistry that involve second order differential equations. So, without wasting much time let me get to the topic of today's lecture that is, in today's lecture we will be talking about homogeneous second order ODEs and basis functions. So, what is the homogeneous second order ODE? So, what is it; look like.

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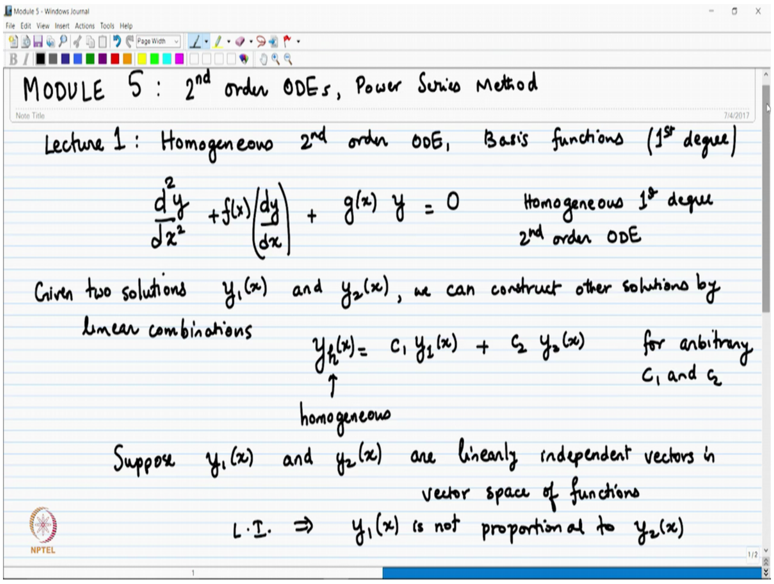

So, essentially if you have a second order ODE you have to have a something like d square y by dx square I am assuming x is the independent variable and y is the dependent variable. So, you have to have a term like this. And let us take first degree equations, for convenience we will just take first degree equations. So, d square y by dx square has power 1. Now if you had a homogeneous second order ODE, then each term will have y or it is powers y or any of it is derivatives to the same power. So, for example, if you have if you have d square y by dx square then you could have a term that has dy by dx times some function of x, then you could have you could have something like g of x times y some another function of x times y and then, so if you did not have anything else. So, this is; this you just set this equal to 0. So, this would be a general homogeneous first degree second order ODE.

So, how much it is each term each term contains either y or a derivative of y or a second derivative y, but to the same, but there is no power of it. So, and you do not have any cross terms. So, therefore, this is the homogeneous first degree second order ODE.

Now we mentioned something in the last class about homogeneous differential equations this is the following. Suppose you have a solution y, so given 2 solutions - y 1 of x and y 2 of x, we can construct other solutions by linear combinations. So, I will just call it y h, h stands for homogenous this is c 1 y 1 of x this is the function of x plus c 2 y 2 of x and you can choose c 1 and c 2 arbitrarily, so for arbitrary c 1 and c 2. So, anytime you have 2 solutions any linear combination of solutions will also be a solution you can easily verify this by putting it in the differential equation and you know you will realize that in order for this to be true each term should have y or it is derivatives to the same power. You can easily substitute this and verify that this is true. So, now, suppose y 1 of x and y 2 of x are linearly independent and then what I mean by linearly independent, what we what you think of as linearly independent vectors in, vector space of functions.

Now, again I would like you to recall what we learnt in when we were learning vectors we said that we can generalize the idea of vectors to 2 functions we can think of functions as vectors in a vector space involving all functions. Now in that vector space of all functions if y 1 and x and y 2 are x are linearly independent and now what does it mean by linearly independent, linearly independent functions. So, linear independence implies y 1 of x is not proportional to y 2 of x; that means, I cannot write y 1 of x as y 2 of x into some constant. So, if these 2 functions are linearly independent. Then any solution any and this is any solution can be expressed as y h of x is equal to c 1 y 1 of x plus c 2 y 2 of x, here c 1 and c 2 are chosen c 1 and c 2 are suitably chosen.

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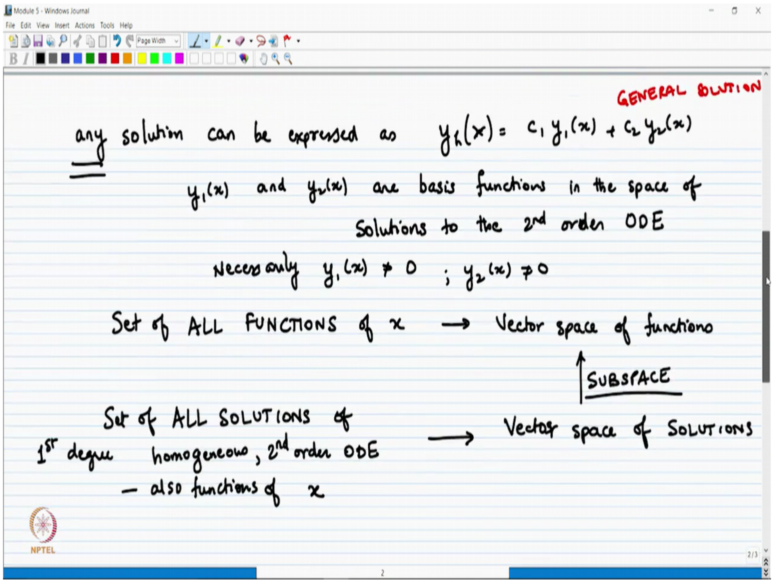

So, you can write any solution as a linear combination of these 2 solutions. this is like writing any arbitrary vector in three d space as a linear combination of the unit vectors I j and k. So, just like that you writing any solution of this differential equation as the linear combination of these solutions.

Now, now in this case y 1 of x and y 2 of x are basis functions, basis functions in now these are basis functions in not the space of all functions, but in the space of solutions to the second order ODE. This is very very interesting concept, that what we think of is that is that you take you take this you take all possible solutions of the second order homogeneous differential equation they if they form a vector space and if and white y 1 I am write you take any 2 independent linearly independent vectors they if they can be if treated as a basis for that space of solutions. So, in order in order for y 1 of x and y 2 of x to be a basis of course, it should be that necessarily y 1 of x not equal to 0 and y 2 of x not equal to 0.

So, these 2 should not be equal to 0 because 0 is also a solution of this homogeneous differential equation. So, you can say that y equal to 0 satisfies this homogeneous differential equation. So, it is necessary that when you are writing this you should have y 1 of x and the non trivial solution is y 1 of x not equal to 0 y 2 of x not equal to 0. And then you can; if you can express any arbitrary solution as the linear combination of those these solutions then you can think of y 1 of x and y 2 of x as basis functions of in the space of solutions.

Now notice that a few things about vector spaces. So, set of all functions of x this is a vector space of functions, now the set of all solutions of homogeneous. So, just to emphasize it is first degree homogeneous, second order ODE this is what we talked about set of all solutions of the first degree homogeneous second order ODE. These are also functions of x, these are also functions of x if x.

Now, what we are doing is this forms the vector space of solutions to the differential equations. So, these are the functions that satisfy the differential equation. So, what you can see is that this is a subspace of this space of all functions. So, this the vector space of all functions will contain the vector space of all the solutions. Now why is this vector space because you take any linear combination of 2 solutions you will get another solution. So, therefore, the set of all solutions is a vector space, 0 is a solution if you have if you have f of x, if you have y 1 of x is the solution than minus y 1 of x is also solution and so on. So, you have a vector space of all solutions to the or to the second order homogeneous differential equation and so now what this means is that that if you have us, so the goal of solving a second order homogeneous ODE is reduced to finding basis solutions basis functions.

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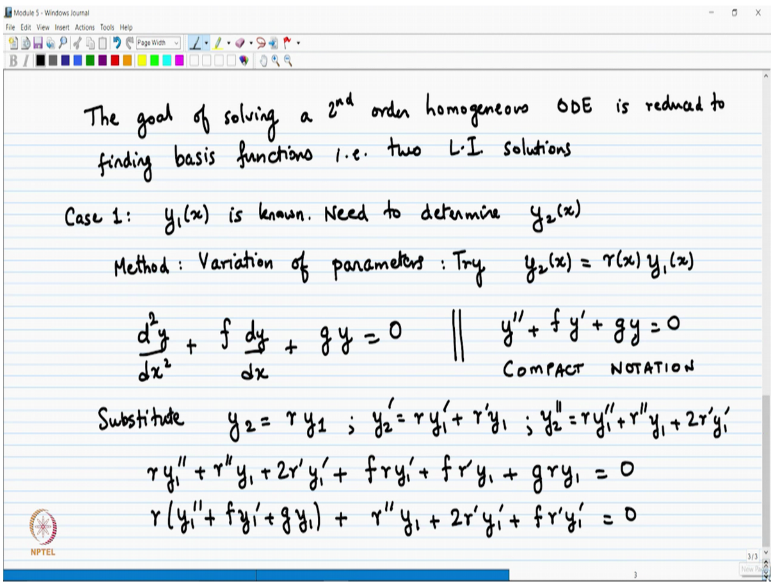

So, what you are supposed to do is to find these basis functions find 2 linearly independent solutions that is 2 linearly independent solutions. So, if you can find 2 linearly independent solutions you are done because general solution can be written as a linear combination of these 2 solutions. So, you can write a general solution in this form. So, this is what we call the general solution where c 1 and c 2 are the arbitrary constants. So, if you know y 1 of x and y 2 of x these are 2 linearly independent solutions then you can write the general solution as the linear combination of these two. So, now, you can, so the goal is to find these 2 basis functions.

So, now, we look at different cases. So, the first case y 1 of x is known need to determine y 2 of x. So, you need to determine y 2 of x. So, how we will you go about doing this? Now there is a method called, this method is called variation of parameters of parameters. So, according to this method what you will say is try y 2 of x equal to r of x times y 1 of x. Remember y 2 r of x cannot be a constant it cannot be a constant because if it is a constant then they are then y 2 of x is proportional to y 1 of x and the solutions are not linearly independent. Now if you try this, so let us start, let us take the differential equation and I will just go back to our original differential equation which had this form second derivative of y plus f of x times dy by dx plus g of x times y equal to 0. So, I will just write it in very compact notation d square by by dx square plus f times dy by dx plus g y equal to 0.

Now alternate notation I will just write this notation here which you will find very common. So, instead of writing the second derivative we just write it as y double prime plus f y prime plus g y equal to 0. So, I will be using both these notations during this course. So, this is compact notation and you will also find it often used in various books.

Now, let us say, now, substitute y to equal to r y 1 then what you get is that y 2 prime equal to r y 1 prime plus r prime y 1, y 2 double prime equal to r y 1 double prime plus r double prime y 1 plus 2 r prime y 1 prime, you can easily work out these things. Now we take this and substitute in the differential equation. So, when you substitute in the differential equation I will be using the compact notation. So, for y 2 double prime has to satisfy this differential equation. So, if I substitute this here what I will get is r y 1 double prime plus r double prime y 1 plus 2 r prime y 1 prime that is the first term, then I have plus f r y 1 prime plus f r prime y 1 plus g r y 1 equal to 0. Now if you take the terms that are proportional to r not derivative of r just r then what you get is r times y 1 double prime plus f y 1 prime plus g y 1 those are the terms that are proportional to r, then the remaining terms look like r double prime y 1 plus 2 r prime y 1 prime plus f r prime y 1 prime equal to 0.

Now, what you notice is that this term that we were, this term that is proportional to that is proportional to r. So, this is y 1 double prime plus f y 1 prime plus g y 1, now since y 1 satisfies the differential equation, so this term is equal to 0.

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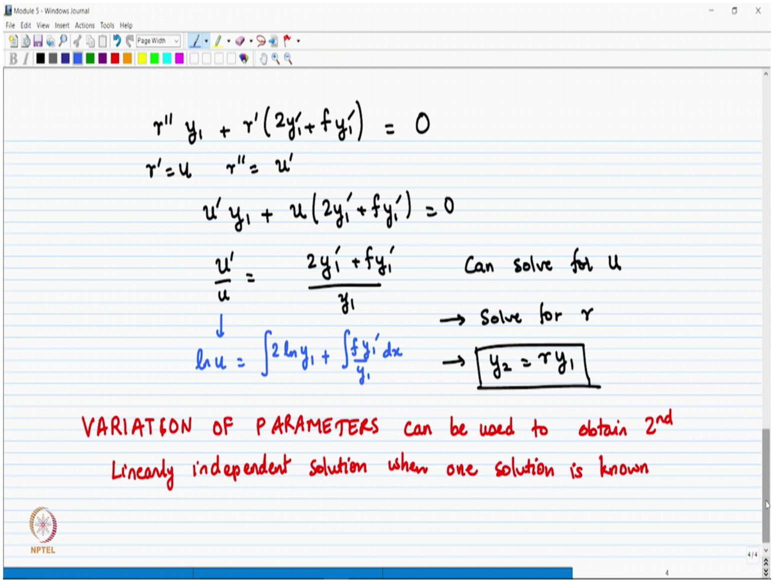

So, now, and the remaining terms I can write as r double prime y 1 plus r prime 2 y 1 prime plus f y 1 prime equal to 0. Now you notice that there is no term involving r. So, this is just, so if I call r prime equal to u, r double prime equal to u prime. Now you can straightaway see that this is just a first order differential equation in u. So, you have u prime y 1 plus u 2 y 1 prime plus f y 1 prime equal to 0. Remember f is a function of x. So, then I can immediately solve for u. So, u prime by u is equal to 2 y 1 prime plus f y 1 prime divided by y 1. So, solving you can get can solve for u and once you have solve for u then you can do from u you can solve for r and y 2 is equal to r y 1.

So, essentially what we are saying is that this the important message that variation of parameters, thus can be used to obtain second linearly independent solution when one solution is known. Incidentally I mean you can just to say a little bit about this, when you integrate this you will get l n of u is equal to integral now you get to y 1 prime by y 1, so that is twice l n y 1 plus now we will get integral f y 1 prime by y 1 d x. So, that is what it will look like. So, this is what this integral we will look like.

Now, if you exponentiate everything then you will get u equal to e to the y 1 square and so on times this, this term. So, I mean we will see, we will work out some of these examples and then we will see how this works in practice. But essentially what we have seen through this is that if you know one solution you can get the second solution. So, if you know y 1 you can get y 2 and once you know them you know the general solution so the problem is solved. So, now, there are there are a few other things. So, at least there are still some concerns that is how do you determine the first solution. So, how do you determine with the first solution, sometimes just by luck or by inspection you can get the first solution, but more formal method to get the first solution would be the power series method.

So, this is one thing that we will be discussing a little later. Now the other case that we will be discussing soon is what to do if your equation is not homogeneous. So, that is the second case that I will take up in the following lecture. So, I will conclude this lecture here. So, in the following lecture we will take up the second case in which the equation is not homogeneous.

Thank you.