Mathematics for Chemistry

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Lecture - 16

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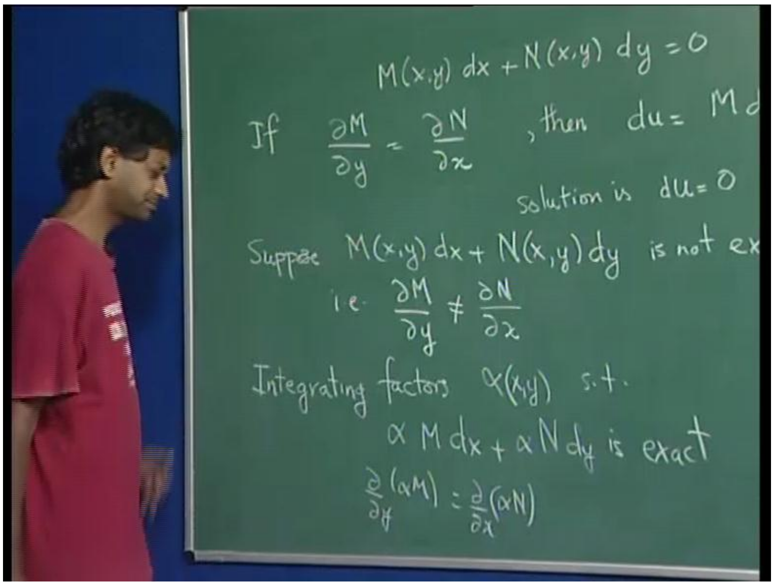

So, we have seen so far that if you have a differential equation of the form M x y d x plus N of x y d y equal to 0. So, this is the first order differential equation, if you have a differential equation in this form, then we have seen that the condition that this differential equation is an exact differential is that dou M by dou y equal to dou N by dou x. And if this condition is satisfied then what you have here is an exact differential and it can be solved very easily and we have seen how to solve it.

Now, the question is suppose you have a differential equation that is not exact, suppose this is not satisfied. So, if this is true then d u equal to M d x plus N d y, you can write in that form, I have omitted the dependence on x and y. So, it will be it is understood that M is a function of x and y N as N, then d u is an exact differential and the solution can be written as n d u equal to 0 or u equal to constant. And we saw in the last class how you can solve for u.

Now, what happens suppose this is not an exact differential, so N of x y d y is not exact, that is dou M by dou y is not equal to dou N by dou x. So, if you have this situation then there exist it is possible to show that there exist a variety of integrating factors alpha which is, in general a function of x y. So, there exist a large number of integration factors or there exists one or more integration factors such that alpha M d x plus alpha N d y is exact, so I am just multiplying this, this original differential equation by alpha.

So, I have the same differential equation, but then the you have dou by dou y of alpha M is equal to dou by dou x of alpha N, where is a function of x and y, so alpha is a function of x and y. So, there exist these integration factors such that this is exact now, the question is how if this exists how would you go about to finding the alpha. So, in general it is not easy to find alpha because alpha will satisfy a differential equation.

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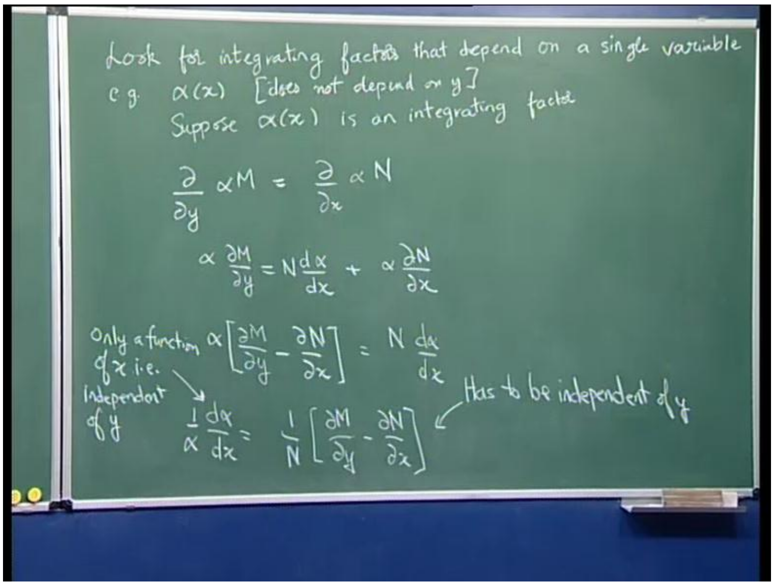

We assume or rather we look for integration factors that depend on a single variable. For example, alpha of x, so we specifically look for such integrating factors not all and you may or may not find it. But suppose alpha x is an integrating factor. Suppose alpha x this is independent of y, so suppose alpha x is an integrating factor. Then dou by dou y of alpha M is equal to dou by dou x of alpha N. Now, alpha depends only on x, so this can be written as alpha dou M by dou y is equal to and in this case you will have both terms, so in this case since we are differentiating with respect to y alpha is independent of y it comes outside the differential.

So, I have alpha times dou M by dou y and now in this case partial derivative with respect to x of alpha N will have two terms. First one will involve derivative with respective x of alpha and the second one will involve derivative with respect to x of N.

So, the first term will be d alpha by d x into N plus alpha dou N by dou x. Notice this is a ordinary differential because alpha depends only on x whereas, this is a partial derivative because n depends on both x and y.

And now I can rearrange this equation to write it as alpha dou M and by dou y minus dou N by dou x. So, I bring this M this side is equal to N d alpha by d x and this implies alpha d alpha by alpha is equal to 1 over N dou x into d x that you write it slightly differently I will write it as 1 over alpha d alpha by d x is equal to this. Now, the left hand side depends only on x, so the left hand side is only a function of x independent of y i e independent of y.

So, since alpha is only a function of x d alpha by d x will only be a function of x and 1 over alpha d alpha by d x will only be a function of x. So, the condition for alpha to be an integration factor is that the right hand side should also be independent of y. So, the right hand side has to be independent of y and so the condition for that to exist an integration factor alpha which depends only on x is that 1 over N dou M by dou y minus dou N by dou x has to be independent of y.

So, if this condition has satisfied if this is only a function of x then you can calculate the integration factor by integrating out. So, the condition for there to exist an integration factor alpha which is only a function of x is that one over alpha d alpha by d x or has to equal this right hand side. Or in other words 1 over N d M by d y minus d N by d x has to be a function only of x.

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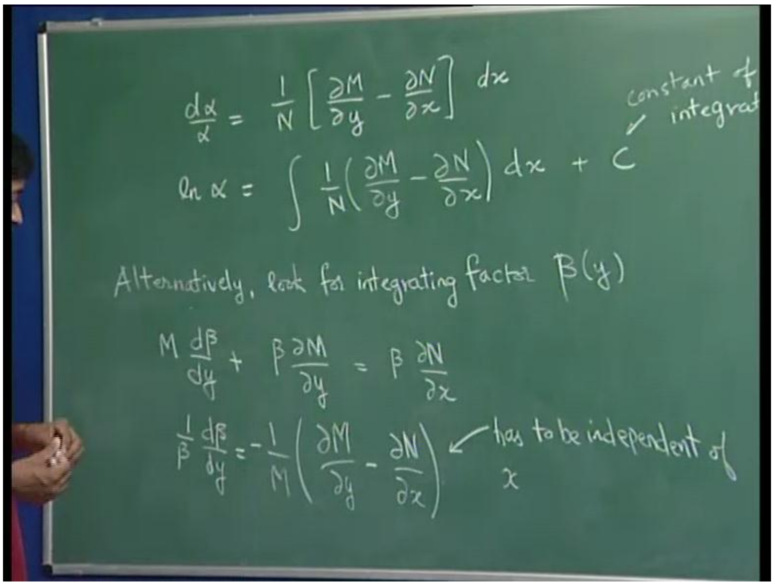

Now, if this is a function of x then we can integrate it out, so you can say d alpha by alpha is equal to dou y x d x and you can you can integrate this out. So, you will say natural log of alpha is equal to integral plus a constant. So, you just integrate both sides and you have a constant of integration. So, the strategy is you calculate this quantity and you see if it is a function of x, if it is a function x then you are done you have your integration factor.

Now, another way to do this instead of looking for an integration factor that depends only on x we, will look for an integration factor. So, alternatively look for integrated factor beta, which is only a function of y, it is independent of x. And you can go through the same arguments so you say that the instead of alpha you will have beta and you have the same condition but, beta depends only on y. So, in this case it will come outside the integral.

And you can show that your condition will look liked y into M plus dou M by dou y is equal to beta dou N by dou x. And if you rearrange this you will get something like 1 over beta d beta by d y is equal to minus 1 over M dou M dou y minus dou N by dou x and now the left hand side depends only on y. So, the condition is that the right hand side should depend only on y, so this has to be independent of x. So, if this is independent of x if this right hand side is independent of x then you can find this integration factor beta of y and you can calculate beta in the same way by integrating out.

So, what we notice is that in both these conditions you have the same expression dou M by dou y minus dou N by dou x. In one case you divided by N and you should get a function that is independent of y, in the other case you divided by M to get a function that is independent of x. So, the usual strategy when we solve these differential equations is to first calculate this quantity see, if you divided by M or N do you get the appropriate function that is independent of one variable.

And if you get that and then you know that an integration factor exists. So, let us look at an example of applying this integration factor. So, let us take a specific example of a problem and see how we can calculate the integration factor.

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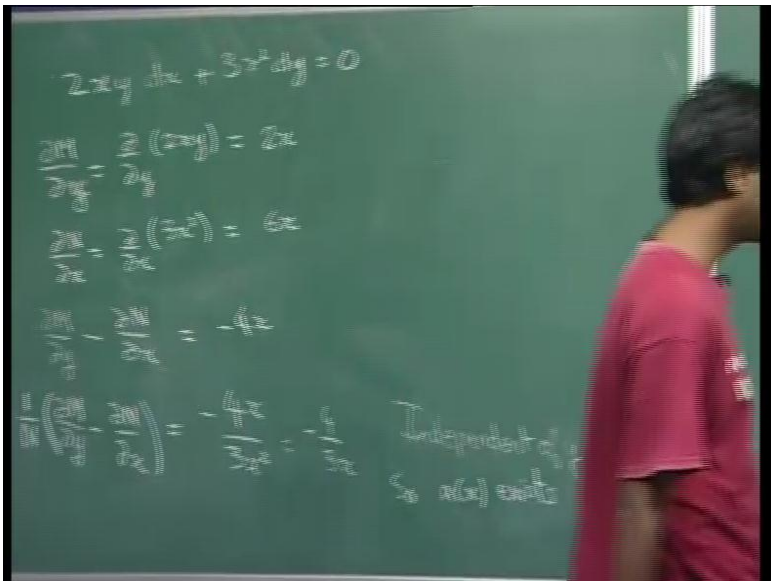

So, the problem is plus x square d y equal to 0 now the first thing you will say is that this can be solved by separation of variables. But let us go ahead and try to use the integration factor so what we will do is dou M by dou y is d by d y of this is equal to 2 x. So, you say that 4 x now if I divide this by so if I now look at 1 over N is equal to minus 4 x by 3 x square is equal to minus 4 by 3 x and it is independent of y. So, 1 over 1 dou M by dou y minus dou N by dou x is independent of y. So, alpha x exists so we have an integration factor that depends only on and you can calculate this integration factor.

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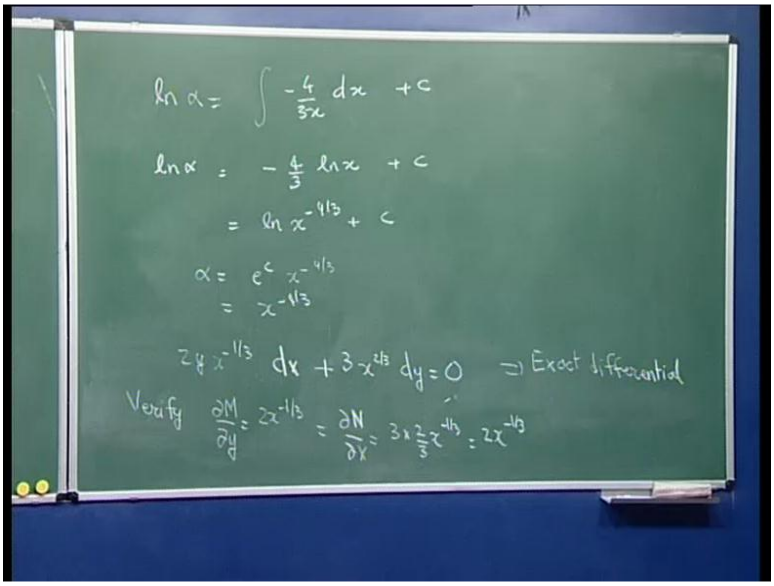

So, you say that l n alpha is equal to integral minus 4 by 3 x d x plus constant is equal to plus constant. And if you work this out you will get l n of x to the power minus 4 by 3 plus constant, and you can write alpha is equal to e raise to c 4 by 3. And this is just another constant e raise to c is just another constant so alpha is equal to x to the power minus 4 by 3. So, the constant of integration we do not need to worry about this. So, we just choose this as your integrating factor.

Now, if I choose this as an integration factor then your differential equation becomes 2 y, now if you multiply this by x to the minus 4 by 3. So, will get x to the minus 1 by 3 d x plus 3 now you have x to the 2 by 3 d y equal to 0. So, I just multiplied this differential equation by x to the minus 4 by 3 and when you do this then you can calculate you can verify that 1 by 3 is equal to dou N by dou x, so you have 3 into 2 by 3. So, that is 3 into 2 by 3 x to minus 1 by 3 equal to 2 x to minus 1 by 3.

So, clearly 2 x to the minus 1 by 3 is equal to dou M by dou y and it is equal to dou N by dou x. So, this is an exact differential, and once you know that this an exact differential you can find your u by the methods that we discussed earlier.

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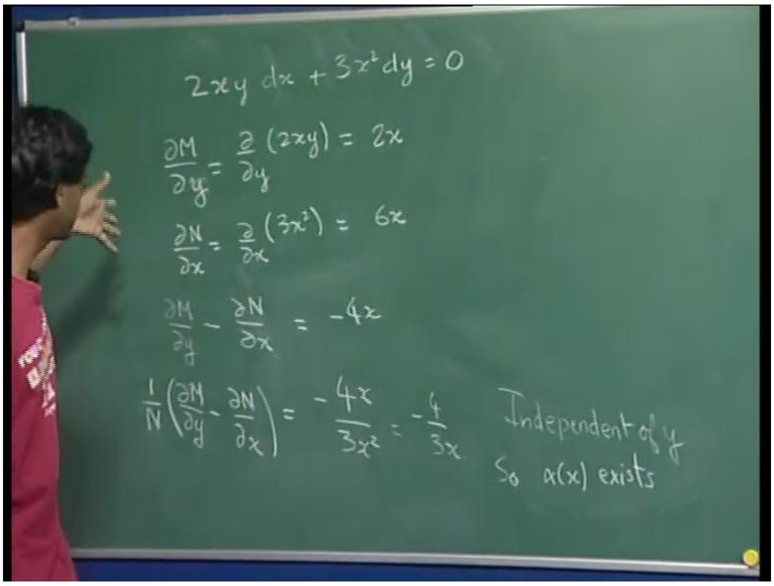

So, this is a procedure for finding the integration factor first you calculate dou M by dou y minus dou N by dou x. Then you look at your M and N and you see whether dividing by N you get a function only of x or dividing by M you get a function only of y. In this case actually we could have also found that integration factor that depends only on y because; if you divide this by M then you will get a function only of y. So, you can do it either way and you should get the same answer.

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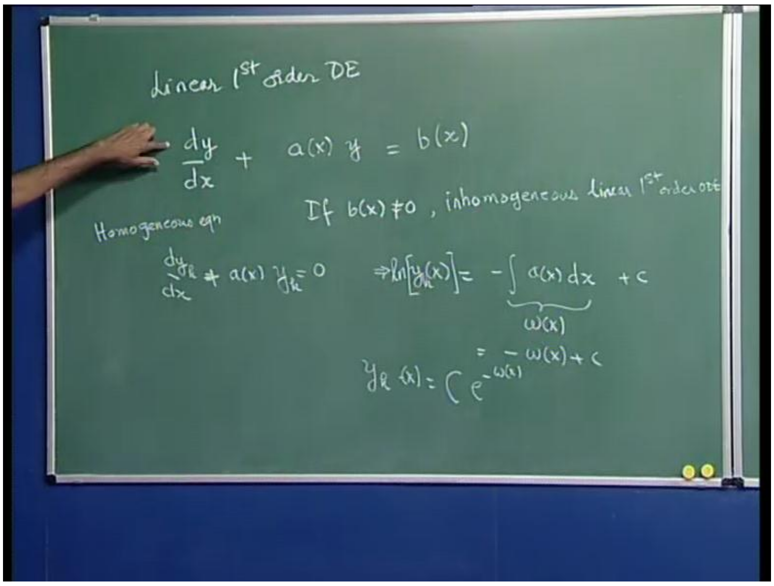

Now, we can look at a general linear first order differential equation. And this is of the form d y by d x plus a of x into y equal to b of x. So, it is linear because each term contains either y or it is derivative up to first power, and this is inhomogeneous. So, this is if b of x is not equal to 0 then it is inhomogeneous linear 1, now the question is how will we solve this. So, in order to solve this we can use the methods of method of integration factors and we can and you can go through the details and work out the solutions.

In all in order to write the solution we will first look at the homogeneous equation. So, the homogeneous equation d y by d x plus a of x y equal to 0. So, this homogeneous equation can be solved by separation of variables you take so if I take this on the right that bring the y below. So, this is just integral minus a of x d x plus constant. So, this is the solution of the homogenous equation and I will call this y h.

So, the solution of the homogeneous equation is given by this oh sorry it should be e to the minus. So, l n of y is equal to this. Now, let me call this quantity w of x then this is minus plus some constant, in other words the homogeneous equation has a solution. So, e to the minus w of x times e to the c and on that e to the C I will just write it as a constant capital C. So, this is the solution of the homogeneous differential equation so the homogeneous equation means you put b of x equal to 0. Now, the inhomogeneous equation the solution of this differential equation is related to the solution of this homogeneous equation in this form.

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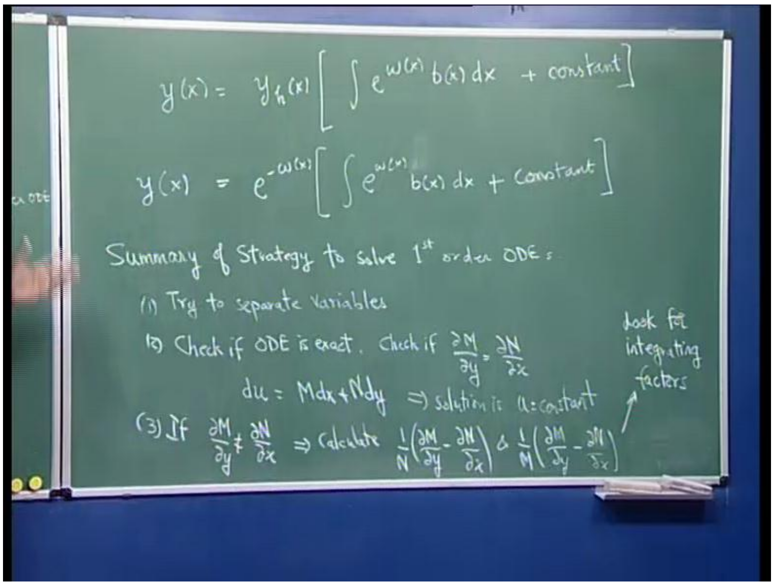

Now, the in homogeneous equation the solution of this differential equation is related to the solution of this homogeneous equation in this form is equal to h of x times integral d x plus constant. So, you can show by the method of integration factors. You look for an integration factor that depends only on x and you can show that the integration factor will give you this final solution. And so finally, you will get e to the minus w x plus.

So, this is the general solution of an inhomogeneous linear first order differential equation. And I leave it as an exercise you to verify that this is indeed the solution and as I said you can do this by method of integration factors. So, that concludes the part of involving first order differential equations, I will just summarize the strategy, so order O D E s. So, the summary the strategy to solve first order differential equations is first thing is to try to separate variables.

If you are able to separate variables then you will separate it and you solve the differential equation. If you are not able to separate then the next strategy is to check if O D E is exact. So, you check if your ordinary differential equation is an exact differential in other words check if dou N by dou x. So, if this is satisfied then you can find the solution as u is equal to d u equal to M d x plus N d y, so we can write d u equal to M d x plus N d y and solution is u equal to constant.

So, once you know that your ordinary differential is exact then you can solve this. And the third strategy if it is not exact, if by dou y not equal to dou x. Then the strategy is calculate 1 over N and so you calculate both these terms 1 over M to 1 over N times dou M by dou y minus dou N by dou x and 1 over M times dou M by dou y minus dou N by dou x. Then you check if this is only a function of x or you check if this will be a function of y, if this is only a function of x then you can find the integration factors.

If this is only a function of y you can find the integration factors. And then look for integrating factors. So, this is the general strategy for solving first order differential equations, and in case this is not independent of y and this is not independent of x. Then there exists no integration factors and you can not solve the differential equation using these procedures.

So, now we will start discussing second order differential equations and how you solve second order differential equations. So, it turns out that second order differential equations are the most commonly encountered type of differential equations in most applications. Some common ones that you have seen are the Schrodinger equation, and the diffusion equation and so on.

But, in general second order differential equations are some of the most commonly encountered differential equations. So, now what are the techniques that we use to solve second order differential equations, and for now we will restrict ourselves to ordinary second order differential equations, so ordinary D E.

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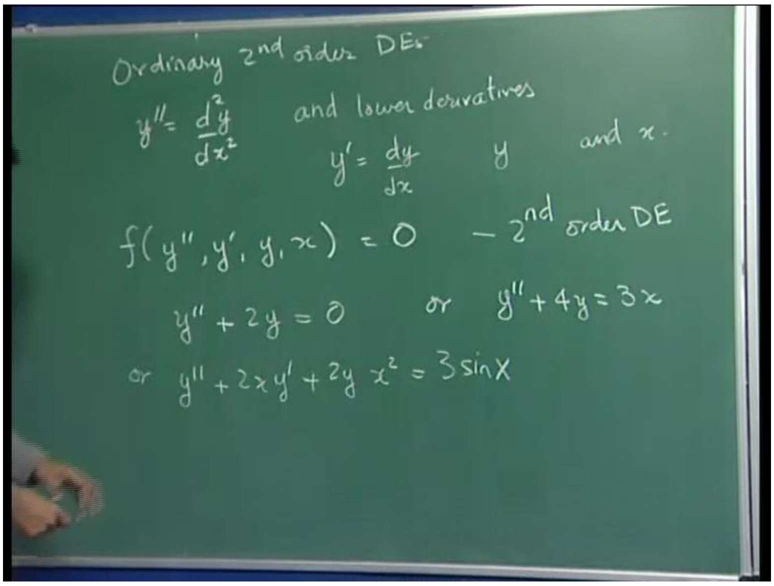

Now, second order differential equation is something that contains y double prime. So, second derivative of y square it contains y double prime, and it contains lower derivatives. So, the lower derivatives will be y prime and x.

So, it is an equation containing y double prime, y prime, y and x. So, you can write it as some function of y prime y x equal to 0. So, this is our second order differential equations. For example, you can have y double prime plus 2 y equal to 0, it is an example of a differential equation. So, it contains this particular equation contains only y double prime and y, but in general it can contain all those. So, or we can have 3 x or you can have, so this contains y double prime, y prime, y and x. So, it can contain some or all of these and that is what forms a second order differential equation.

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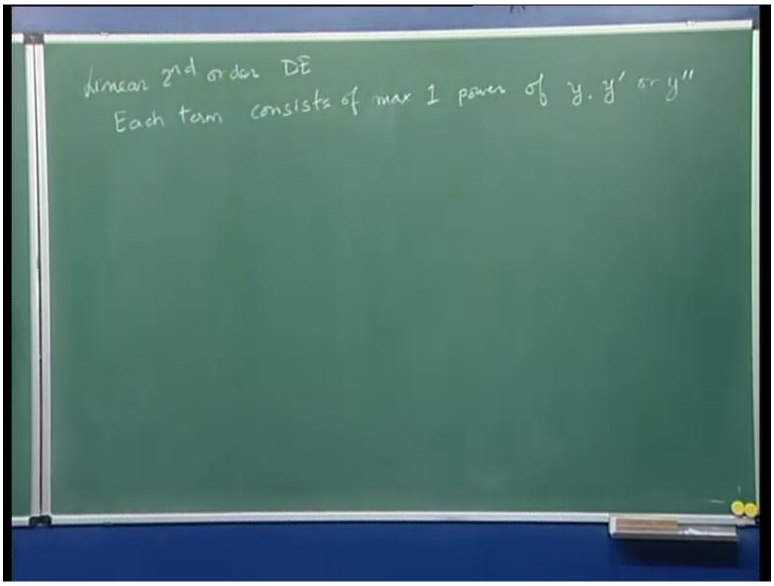

Now, let us look at some types of second order differential equation a linear order differential equation. So, a linear second order differential equation is one in which each term consists of only 1 power of y prime or y double prime or I should not say only 1. So, at most 1, so right way to say this of maximum 1 power of y prime or y double prime.

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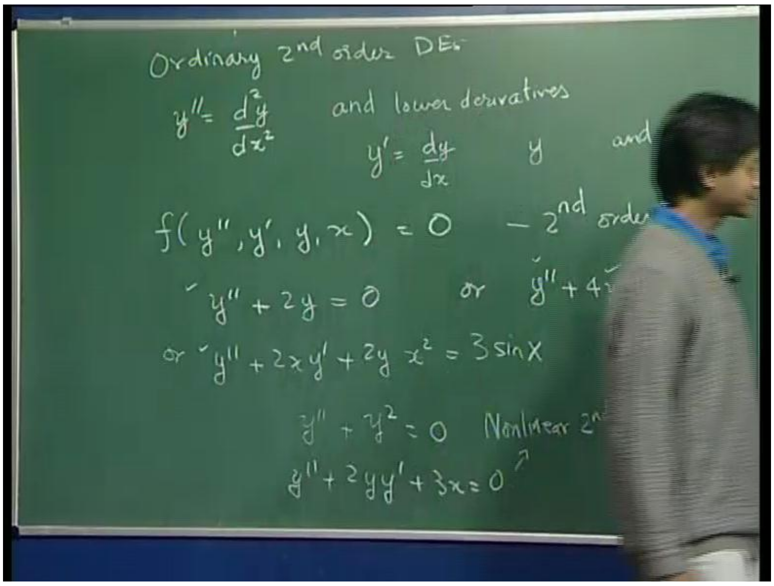

So, for example, if you look at these equations if you notice if you look at this equation the first term contains y double prime second term contains y. So, this is a linear second order differential equation. Similarly, you look at this contains y double prime this contains only 1 y prime this contains y, this is also a linear second order differential equation. So, these are all linear similarly, this also contains each term contains only 1 power of y.

So, an example of on the other hand if you had something like y double prime plus y square equal to 0. Now, this contains y to the second power. So, this is a non-linear O D E similarly, you could have a non-linear second order O D E of the form. So, this term contains 1 power of y prime and 1 power of y, so effectively it contains two powers of y or it is derivatives. So, this is another non-linear, so you can have linear or non-linear second order differential equation.

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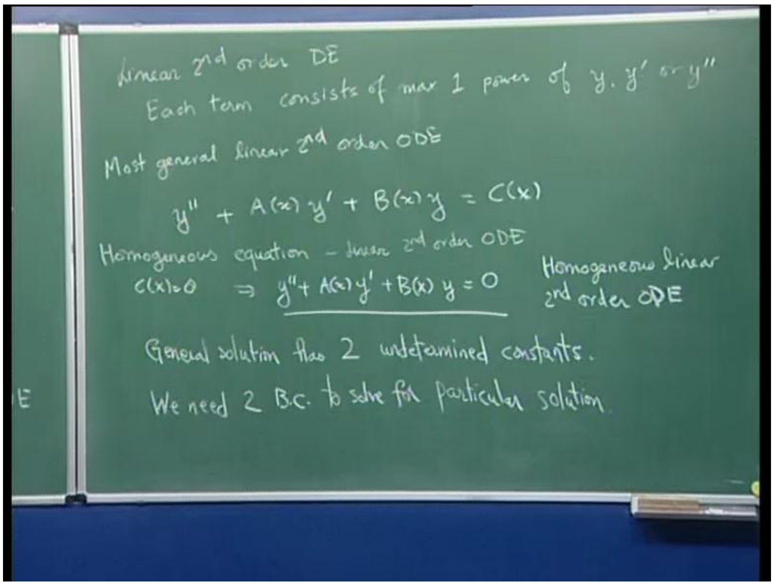

So, the most general linear second order O D E. Now, what is the most general form of this linear second order differential equation that is you can write it as y double prime plus a of x y prime plus b of x y equal to c of x. So, this contains second derivative of y, this contains first derivative of y and some function of x, this contains y and some function of x and this contains a constant. So, this is the most general linear second order ordinary differential equation.

Now, we have already learn what are a homogeneous equation is one in which each term contains y to the same power of y or it is derivatives. So, homogeneous equation linear second order O D E. So, a homogeneous linear second order differential equation that is a special class of these where, c of x equal to 0. So, that implies this is homogeneous linear O D E. So, this is one class of linear second order differential equations is the homogenous one.

Now, there is something very interesting that happens with these homogeneous equations and that is what we will explore in the rest of today’s class what I want to mention right the beginning is that if you have a second order differential equation, then the general solution it has 2 undetermined constants. So, in the general solution of a second order differential equations has two undetermined constants.

And so we need 2 boundary conditions in order to solve for the particular solution. So, this is a this is a brief summary of second order differential equations and what we will do now is to look at various cases, we will look at methods to solve them, we will look at how a general solution can be constructed and so on. So, that will be the topic of the rest of this class, and the next few lectures. So, now let us look at the homogeneous equations.

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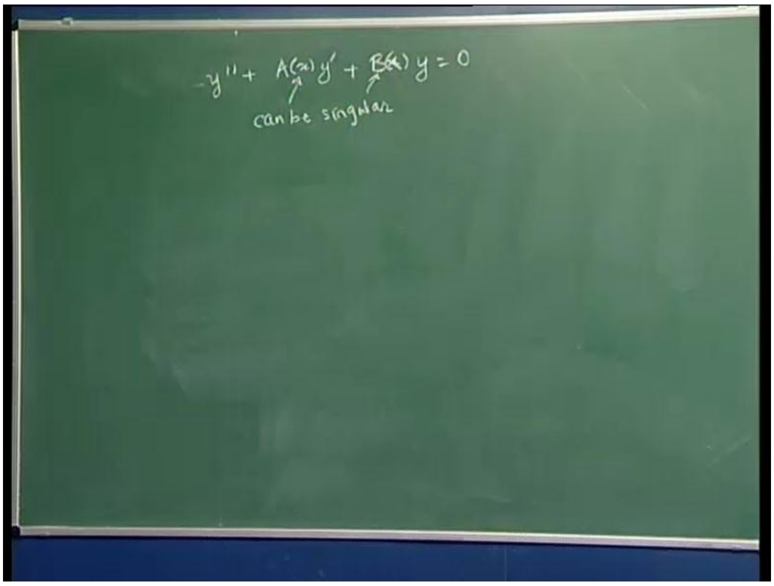

So, of the form y double prime plus A x y prime plus B of x y equal to 0. Now, some of you might wonder why I did not put a some function of x here. And the answer is that you can take that function of x and you can include it in the A x.

So, suppose I had c of x here, then I just divide the whole equation by c of x and I take the factor of c of x into the A of x. So, in a sense A of x can be singular, so it can go to infinity at some points and so on. Now, the question is A of x and B of x both of them can be divergent at some point. So, there might be certain values of x for which these functions go to infinity. So, now let us go to certain properties of the solutions now the property of the solutions that we are most interested in is the following.

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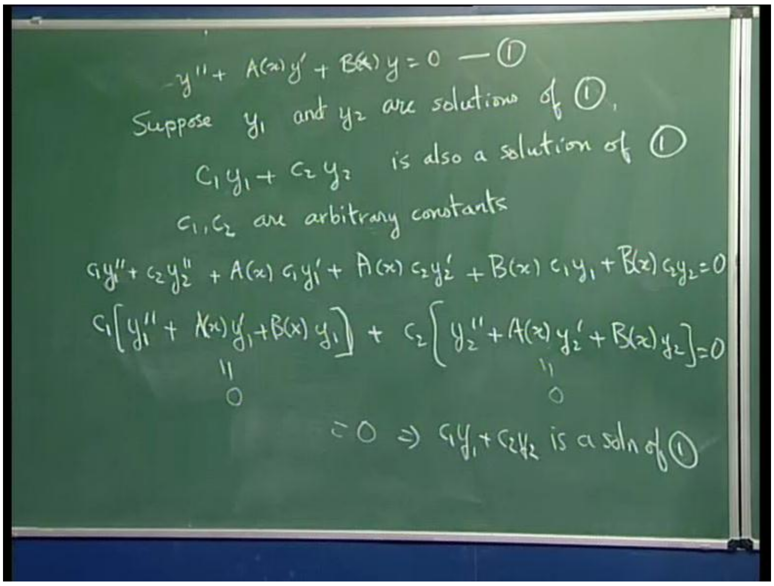

Suppose y 1 and y 2 are solutions of I will call this equation 1 of 1. So, suppose y 1 and y 2 are solutions of 1, then c 1 y 1 plus c 2 y 2 is also a solution of 1. So, where c 1 c 2 are arbitrary constants, so suppose y 1 and y 2 are solutions of this equation and clearly a any linear combination of these two will also be a solution of this equation. It is very easy to prove you can just substitute in this equation, what I will get is c 1 y 1 double prime plus c 2 y 2 double prime plus A of x c 1 y 1 prime plus A of x c 2 y 2 prime plus B of x c 1 y 1 plus B of x c 2 y 2 equal to 0.

And what you can see immediately is that you take the c 1 terms we will get c 1 y 1 double prime plus A of x y 1 y 1 prime plus c 2 y 2 double prime plus A of x y 2 prime equal to 0. So, what I did is I substituted in this equation and when I substitute this when I take the terms containing C 1, so I have first term is C 1 y 1 double prime then I have a C 1 y 1 prime a of x. So, y 1 prime A of x C 1 and I will get C1 B of x y 1, so B of x y 1 and similarly, with C 2.

Now, this is equal to 0 because y 1 is a solution of this differential equation, and. So, this whole thing is equal to 0. And that implies C 1 y 1 plus C 2 y 2 is the solution of one. So, this is the a very important property that says, that if you have two solutions of the differential equation any linear combination of them is also a solution to this second order homogeneous differential equation.

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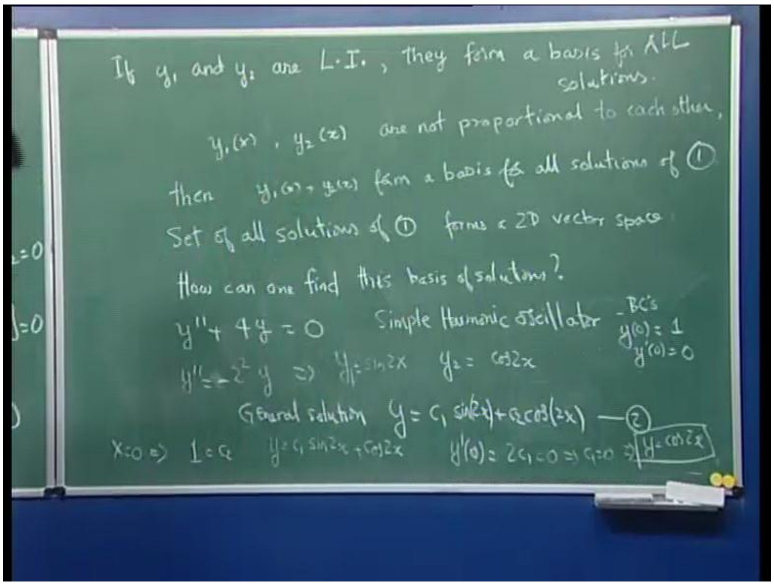

Now, the next question is or the next comment is that is in if y 1 and y 2 are linearly independent they form a basis for all solutions and I should say this with a little bit of caution, because there might be some solutions that might not be expressible in this form. So, the statement is that if y 1 and y 2 are linearly independent. So, y 1 is a function of x, y 2 is a function of x. So, if these two are linearly independent and when I say that they are linearly independent; that means, they are not proportional to each other.

Then y 1 of x, y 2 of x form a basis for all solutions, so if they are not proportional to each other they form a basis for all solutions of 1. So, the point is you have this differential equation. So, if you know two linearly independent solutions then any solution can be expressed as a linear combination of these solutions, so that is the idea. So, in a sense if you have a vector space you say that any vector can be written as a linear combination of the basis vectors.

So, same way if you have the set of solutions any solution can be expressed as a linear combination of these two solutions. Now, incidentally you also notice that 0 y equal to 0 is a trivial solution of this equation. So, y equal to 0 satisfies this equation in a very trivial way. So, actually you can show that the set of solutions forms a vector space, this satisfies the axioms of a vector space. So, you can set of all solutions of 1 forms a 2 D vector space.

So, it forms a 2 D vector space because if y 1 and y 2 are solutions then any linear combination of them is also a solution. So, this is a very useful property, so the question. So, the biggest question is how do we find the basis. So, how one find this basis of solutions so just to reiterate what we want to do is to find two linearly independent solutions. Two solutions to this differential equation which are not proportional to each other, so now, the question is how do you find this basis and that is the challenge of these second order differential equations.

And we will look at various strategies for finding this solution of these differential equations. So, let us take a very simple example and we will and see how this works we will take an example where they are familiar with the solutions. And then later on we will go to more complicated cases, so let us take the example y double prime plus 4 y is equal to 0. And you will immediately tell me that this equation is of the form of a simple harmonic oscillator.

So, this is a simple harmonic oscillator and the solution is of the form. So, this is y double prime plus 2 square y or y double prime equal to minus 2 square y implies y equal to y 1 equal to sin x sin 2 x y 2 equal to cos x. So, y 1 is sin 2 x y 2 is cos 2 x and these 2 are these 2 are linearly independent and so they form a basis. So, the general solution y equal to C 1 sin 2 x plus C 2 cos 2 x.

So, the general solution to this differential equation can be written in this form and depending on the boundary conditions you can put the boundary conditions and you can solve for C 1 and C 2. So, suppose I give the boundary conditions, so suppose I say boundary conditions y of 0 equal to 1 y prime of 0 equal to 0. So, these are my 2 boundaries suppose I had these two as my boundary conditions then what you will do is y of 0 is if I substitute if I put x equal to 0 in this.

So, I will call this 2 so put x equal to 0 in 2. So, x equal to 0 implies the sin 2 x term will go away we will have cos 2 x is 1 cos 2 into 0 that is 1. So, you will have C 2 equal to 1. So, 1 equal to c 2, so you have determined c 2 and if you do that then you have y equal to C 1 sin 2 x plus cos 2 x. So, then you take the derivative, so y prime is equal to or y prime at 0 is equal to. So, if I take the derivative here I will get 2 C 1 cos 2 x and if I put x equal to 0 cos 2 x is cos 0 which is 1. So, I have 2 c 1 in this case derivative is 2 sin 2 x.

When x equal to 0 that derivative goes to 0. So, 2 C 1 equal to 0 implies C 1 equal to 0, so we have determines. So, the C 2 is 1 C 1 is 0. So, the particular solution y is equal to cos 2 x implies y equal to cos 2 x. So, this is the particular solution with no undetermined constants. So, what we had is we had a differential equation y double prime plus 4 y equal to 0 and the solution was written as y is equal to C 1 sin 2 x plus C 2 cos 2 x.

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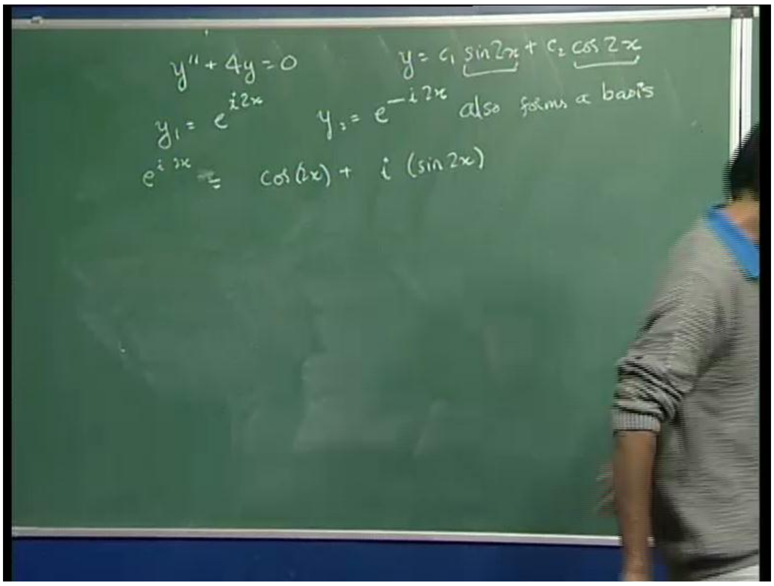

That was a general solution and we said that the basis vectors are sin 2 x and cos 2 x form a basis. Now, the next thing is let us try to do it in a slightly different way now, instead of saying sin 2 x and cos 2 x suppose I could have said y 1 is equal to e to the i 2 x and y 2 is equal to 2 x. So, what all I said this is also a solution to this differential equation. And I could have used this as a solution, so this also forms a basis and you can see that. So, that implies that our original basis is not a unique basis they can be other basis also.

And that should be fairly obvious because you can write e to the i into 2 x is equal to cos 2 x plus i sin 2 x, and so we wrote y 1 as a linear combination of these 2 basis. So, this implies that you can go from one basis to the other and so if cos 2 x and sin 2 x are a basis also e to the 2 i x and e to the minus 2 i x also form a basis. So, you should not be surprised if you get very different looking forms of basis, because indeed the basis are not unique.