Advanced Mathematical Methods for Chemistry

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Module - 07
Lecture - 01

Nonlinear Differential Equations, Phase Plane, Harmonic oscillator

So, now we will start module 7 and in this module I will take you through an extremely interesting topic and it is probably something that you have not seen before this is a qualitative methods for non-linear differential equations, I will tell you about the phase plane I will tell you about critical points and stability analysis. Now this topic is it is actually extremely powerful and many a time it is not a part of a standard textbooks, but still we will see that even the problems that you are familiar with way if you analyze using these methods you can get lot of useful information.

So, let us start this module. So, in the first lecture today I will be talking about I will be talking in general about what a non-linear differential equation is, and I will introduce to you the concept of the phase plane. And we will we will take the example of the harmonic oscillator, which is the actually not a non-linear differential equation to introduce the phase plane.

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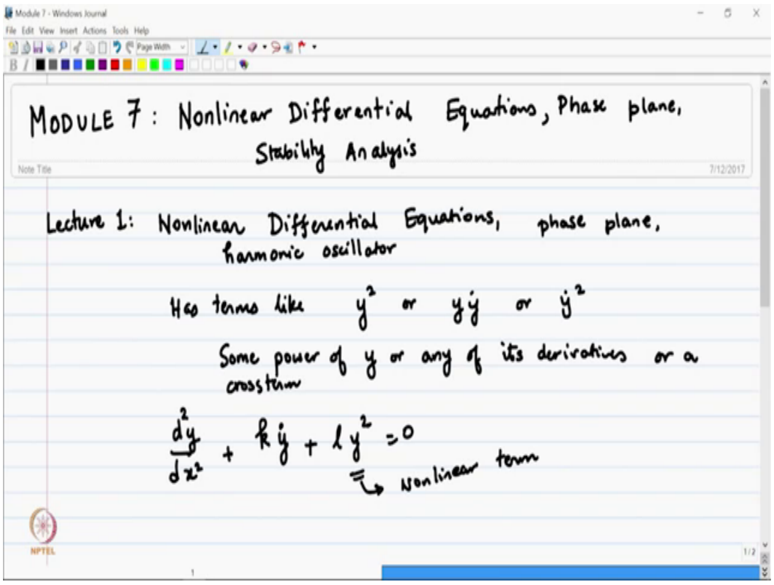

So, what is a non-linear differential equation a non-linear differential equation we if you if you remember what we said is that it has terms like a y square or yy dot or y dot square you know that is some power of y or any of its derivatives or a cross term.

So, for example, if you have d square y by d dx square, plus if you have if you have k y dot plus l y square equal to 0. So, this is a non-linear term. You need not have y square you can have y cube, you can have yy dot you can have y dot square, you can have all kinds of things, but anything that that is not linear any term is. So, it has a term that is not linear. Now what is the problem with this? So, linear differential equations there are standard ways to solve it.

So, linear differential equations have standard ways to solve it, non-linear equations are there are no standard tools to solve non-linear differential equations, no standard methods solution.

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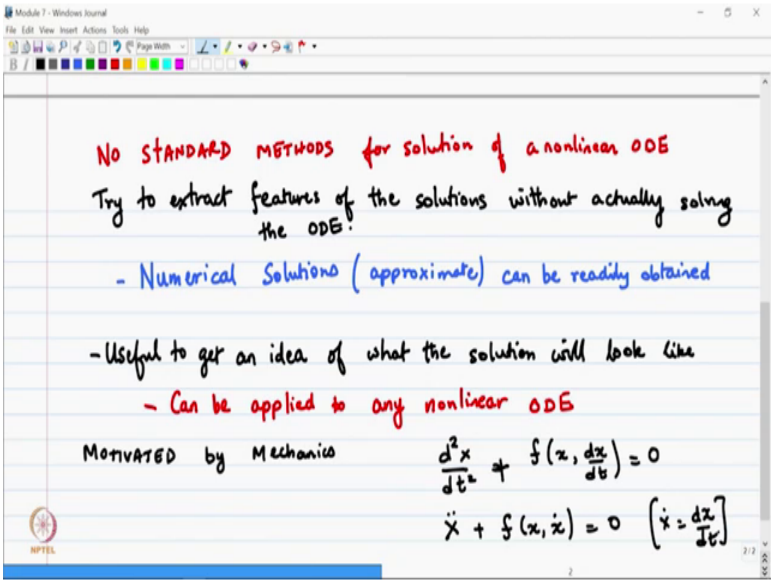

See if you have a linear of a non-linear ode; if you have a linear ode then if nothing you can use the power series method, but such things cannot be done for non-linear odes. So, now, what we are going to do is we are going to use, you are going to try to extract features of solution that is what are the properties of the solutions, without actually solving the equations.

So, this is what we are going to do. It should be emphasized that that you know we can relatively easy to find numerical solutions. Numericals are usually approximate, but they can be made fairly accurate. So, when you solve it numerically you get numbers as the answer as opposed to getting functions. So, numerical solutions can be readily obtained. So, using standard computer programs, you can get numerical solutions to non-linear odes.

So, this is not what we are doing. What we are doing is we are not going to look at numerical solutions; we are just going to try to develop certain methods where you can get extract features of the solution without actually solving the ode. This is very useful for example, so, useful to get an idea of what the solution will look like, and what we will see is that you know without explicitly solving, we will try to get a very good sense of what the solution will look like.

Now, this is a general method which can be applied to any non-linear. So, this is can be applied to any non-linear ode. So, the techniques that we will be discussing today they can be applied to any non-linear ode; however, we restrict for you know in most practical applications are based on mechanics. So, we will restrict are. So, motivated by mechanics and by mechanics I mean classical mechanics quantum mechanics wave equations etcetera. So, we will look at primarily we will look at equations that have this form.

So, I will write d square x by d t square is equal to f or write plus f of x dx by dt equal to 0 or the notation. So, this is a second derivative of some coordinate plus some function of the coordinate and the first derivative is equal to 0. You can also write this in a slightly different form. So, we will write it in a short notation which is which will be extremely useful, x double dot plus f of x, x dot equal to 0; where x dot equal to dx by dt x double dot will be the second derivative.

So, will primarily be looking at equations of this form and we will be seeing what the solutions look like.

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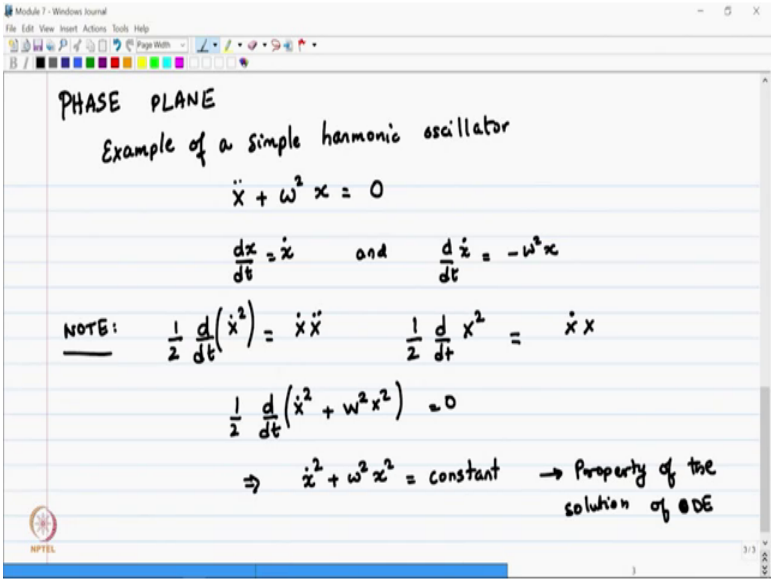

So, in order to introduce these solutions the first important concept is that of a phase plane. So, and to introduce this we take example of a simple harmonic oscillator. So, the fill a phase plane is a general idea, but just to introduce it I will use the example of a simple harmonic oscillator. Now remember phase plane is much more general than just for simple harmonic oscillators.

So, let us take the example of a simple harmonic oscillator, where we know the solutions and this will help us to introduce these methods. So, what is a simple harmonic oscillator I can write as x double dot plus omega square, this is an omega not a w, omega square x equal to 0. So, this is my simple harmonic oscillator, now I will write this as a dx by dt equal to x dot, and d by dt of x dot is equal to minus omega square x and what we will do is we will notice that if you look at d by dt. So, notice note. So, if you look at d by dt of x dot square. So, this is equal to 2 or let me put a half here. So, if I put a half here then that will cancel the 2. So, half d by dt of x dot square d by dt of this whole thing. So, that will be x dot into x double dot.

And we also notice that half d by dt of. So, half d by dt of x square it is equal to x x dot or rather let me write it the other way, let me write it as x dot times x . So, you notice that the only difference here you had x dot times x double dot here you have x dot times x, but you know that x double dot and x are related through this differential equation. So, what you can see immediately is that half d by dt of x dot square plus omega square x square equal to 0.

So, by using the property of this differential equation, we can write an expression like this and what this tells you is that this implies that x dot square plus omega square x square equal to constant. This is a property of the solution; this is not the solution of the differential equation. Remember this is not the solution of the differential equation, but you note that the solution will satisfy this property. So, now, what does this imply what does it imply?

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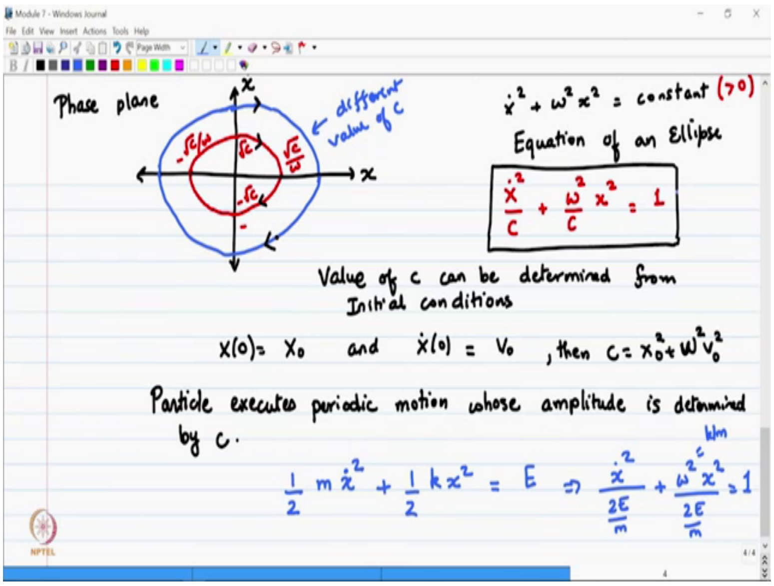

So, in order to see this we introduce; we look at the phase plane, what is the phase plane it is a plane showing x and x dot.

Now, remember our equation is x dot square plus omega square x square equal to constant. Now in this plane in this xx dot plane, this is an equation of an ellipse. So, what does the ellipse looks like? I will just draw this ellipse, you can find out all the where it intersects and so on it is not very hard. So, we know. So, suppose you say x dot square by its a C is a constant, plus omega square by C x square. I should emphasize that constant is strictly greater than 0 because this is all sum of squares everything is positive term here. So, equal to 1.

So, this is our equation for the ellipse, so, when x equal to 0, x dot square equal to C. So, when x equal to 0, so, this is equal to root C, this is equal to minus root C, when x dot equal to 0. So, the these are not the points that are plus 2 when x equal to 0 that is right here then this is equal to root C and minus root C when x dot equal to 0 that is along the x axis then x equal to square root of C by omega C by omega, this will be minus square root of C by omega.

So, for any value of x, x dot has to has to be has to satisfy this. Now if you change the value of C. So, C tells you the size of this ellipse. So, if you take different C, if you take some other constant then you will have a different ellipse is minus root C here, I will just write the root C in the inside here. So, if I change the value of C then I will get a different ellipse. So, this is a different value of C, now how do you determine the value of C. So, value of C, C can be determined from initial conditions. In other words if you take a X at 0 equal to X 0, and X dot X 0 equal to let me call it V 0 then C is equal to X 0 square plus omega square v square. So, that is what v 0 square.

And based on this you can determine there is something else you can get from here. Suppose you use our differential equation we know that dx by dt is x dot; that means, suppose you are. So, your trajectory will always have to be on one of these ellipses. So, suppose you start here each point has to be along this ellipse. So, what we said is dx by dt is x dot. So, let us say you are at a point here, now x dot is negative at in this point x dot is negative. So, dx by dt will be less than 0. So, the point will try to move in this direction as time goes you will move in this direction.

So, what happens is that your particle will have certain value of x and x dot and it will it always has to be on this ellipse, but as the particle moves it will move along this ellipse in this direction. So, there is a direction to the motion that is given in this plane. So, what will happen? As a particle moves based on this initial way based on the value of C, it will just go around this ellipse in this way, and you can show that it just executes this motion. And what is the property of this motion? Clearly this motion is periodic because after some time it comes back to where it started. So, after sometime it will come back to where it started.

So, it will go like this go along this circle and then come back to where it started; particle executes periodic motion whose amplitude is like if you take this inner circle the red a red ellipse, that has a much smaller amplitude whereas, the blue ellipse has a larger amplitude; amplitude is determined by C. So, this phase plane gives you a picture of what the solution is. Now you know the exact solution of the ellipse, you know the exact solution of the harmonic oscillator.

For example you take the if you take that classic harmonic oscillator what this represents is the same as half m x dot square plus half k x square equal to e, this is a kinetic energy and the potential energy and all I did was I just wrote this in this slightly different forms. So, I can write this as if I take the E in the denominator. So, I can write this as x dot square divided by 2 E by m plus now I will write this as omega square, x square where omega is nothing, but k by m divided by 2 E by m equal to 1 and now and now you can see that it is exactly in this form.

So, omega square is nothing, but k by m omega square equal to k by m. So, what this equation represents is the conservation of energy. This x this says that along any one motion the energy is conserved. So, this is again well known this is a well known property of the harmonic oscillator, but what we have seen through this is that you know we did not actually solve the differential equation, but we got lot of ideas. We got we got the fact that the solution is periodic and actually we can also calculate the amplitude, we can calculate the period of this oscillation, a lot of things we can get without actually solving the differential equation.

So, this is a general idea that I want to emphasize and this will be seen repeatedly throughout this topic.

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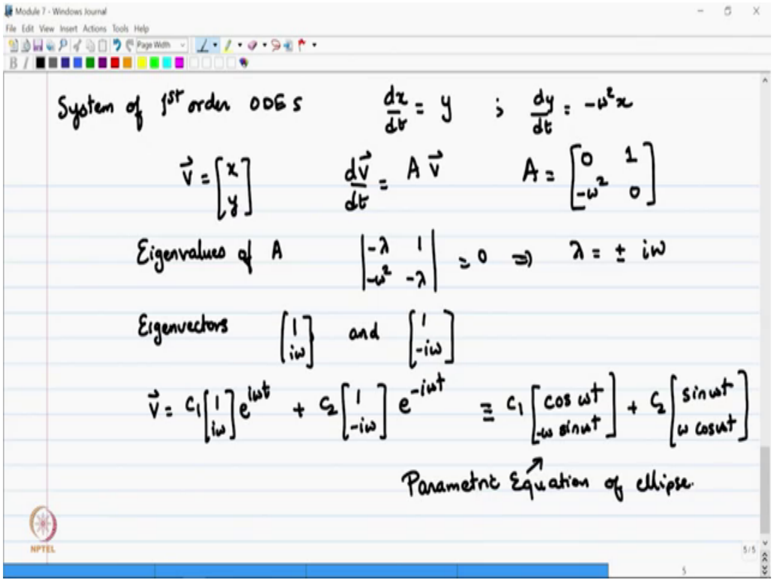

Now next let us look at a slightly more complicated. So, let us look at this in the using a system of differential equations, first order odes. So, you say y. So, you say dx by dt equal to y, and dy by dt equal to minus omega square x. So, we use our usual matrix method. So, you would recall V is equal to xy and what you will say is dV by dt is equal to A v where A is a matrix that whose first term is 0 1 minus omega square 0.

So, we have a linear system and if you have a linear system then we can calculate the Eigen values of A, what are the Eigen values of A? So, the Eigen values of A is you can do this. So, what you will get is if you want to calculate the Eigen values of A, you will write determinant of minus lambda minus lambda 1 minus omega square equal to 0, implies lambda equal to plus or minus i omega. So, lambda square is minus omega square. So, lambda equal to plus minus i omega, and the corresponding Eigen vectors in this case you can easily see that the Eigen vector should have this property. So, it will be 1, i omega and one minus i omega.

So, if the first constant is arbitrarily chosen as 1, you will get the second one as i omega and minus i omega based on the value of lambda. So, I can write the solution V is equal to C 1, 1 i omega e to the i omega t plus C 2 1 minus i omega e to the minus i omega t or alternatively equivalently I can write this in terms of sins and cosines. So, I can write this as C 1 and what I can do is I can write it as because if I do not want to write in terms of imaginary functions.

So, e to the i omega t I can write as a some of cosine and sine. So, I can do a few manipulations and I can write it in terms of constants, these are not exactly the same as this. So, I can write it as cos omega t omega sin omega t, let me put A minus sign here plus C 2 sin omega t, and omega cos omega t. So, these are the 2 I can absorb all these and write this in this form. What is important is that this; what we see here is a parametric equation of an ellipse. So, this is a parametric equation of an ellipse of ellipse this is exact and this will give you exactly this picture that we had earlier.

Now, we will not say anything more about the harmonic oscillator; now let us go to the damped harmonic oscillator. Before I mentioned that let me when you write this equation in this form you immediately realize that there is a.

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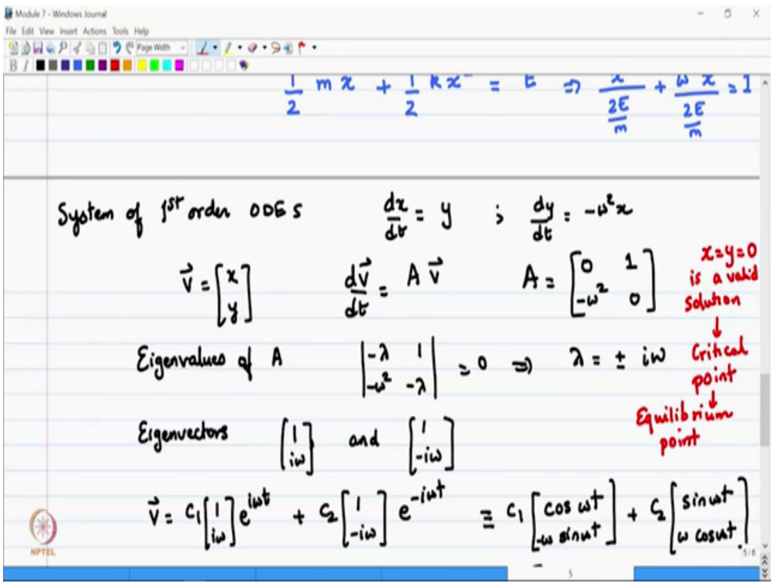

So, x equal to y equal to 0 is a solution is a valid solution and this is a, this is called a Critical point.

So, x equal to y equal to 0 is a critical point because once x equal to y equal to 0 then it cannot change. So, it is a valid solution for some values of C. So, depending on what you are depending on what this constant is if this constant is 0 then x equal to y equal to 0 is a valid solution that is called a critical point this is called an equilibrium because once it is called an equilibrium point because once x equal to y equal to 0 then there is no change in the solution.

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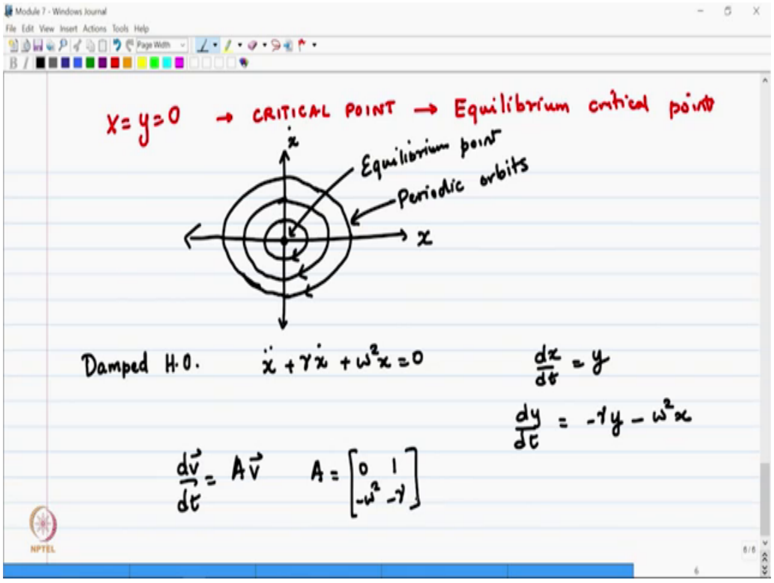

This is an important idea that that x equal to y equal to 0, this is a critical point.

So, any point with x equal to y equal to 0 if for a non for such a system of equations is called a critical point and in this case, it is called an equilibrium critical point. So, now, let us just look at the phase space picture. So, the phase portrait; so, looks like something like this. So, you have x y I am writing y instead of x dot. If I want to I can write x dot also you have this equilibrium critical point and then you have a family of ellipses based on based on what your value of that constant is.

So, this is what the solution to the simple harmonic oscillator looks like in the phase plane, a family of concentric ellipses and in all cases the motion is this way. So, this is a equilibrium point and these are all periodic orbits; periodic solutions are called as periodic orbits, for obvious reasons I called as a periodic orbits. So, this is the property. So, if you just by analyzing this differential equation we will get that x equal to y 0, y equal to 0 is your critical point which is an equilibrium point and there are periodic orbits to this solution.

So, a lot of information just by looking at the differential equation now let us take the case for the damped harmonic oscillator. So, in this case you have x double dot plus gamma x dot plus omega square x equal to 0. So, gamma is a damping constant and now if you do exactly by this method what you will get is dx by dt equal to y and dy by dt is equal to minus gamma times y, minus omega square times x. So, I can write my dv by dt is equal to Av, where A is equal to 0 1 minus omega square minus gamma.

So, the only difference from the previous solution was that for z you have a minus gamma here. So, if you want to calculate the Eigen values of this equation.

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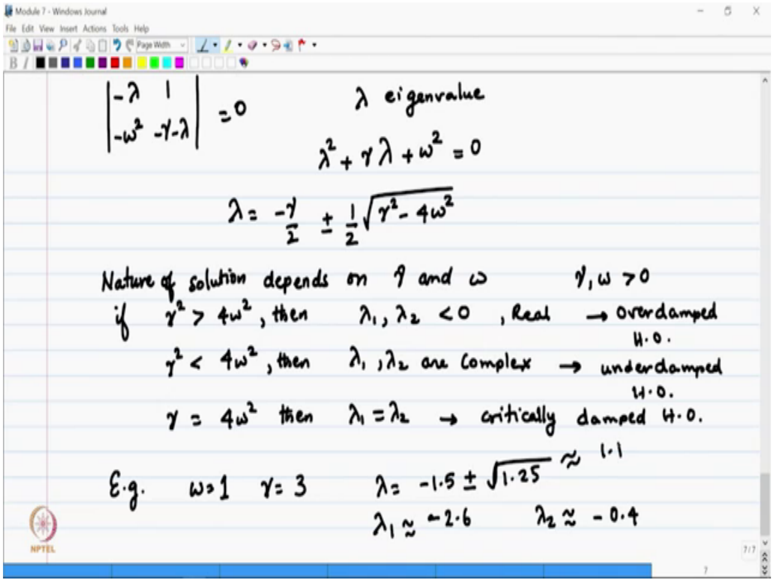

So, what you will write is determinant of minus gamma 1 minus omega square, minus gamma minus lambda equal to 0. So, where lambda is Eigen value; what do you get? you will get lambda square plus gamma times lambda plus omega square equal to 0 or you will get lambda is equal to minus gamma by 2 plus minus half square root of gamma square minus 4 omega square.

These are the Eigen values, now in this case your solution depends on the ray on the relative values of gamma and omega, so, nature of solution on gamma and omega. So, we have gamma omega, both are greater than 0 and we saw that if gamma square is greater than 4 omega square, then both solutions are then the lambda 1 and lambda 2 less than 0 real. So, this is over damped oscillator.

So, now this is the over damped oscillator and then if you have gamma square is less than 4 omega square, then lambda 1 lambda 2 are imaginary are complex and this is the under damped harmonic oscillator and finally, if gamma equal to 4 omega square then lambda 1 equal to lambda 2 this is critically damped. Now we can ask a question; what is the nature of the solution. So, what is the nature of the behavior and obviously, we have to choose certain values of a gamma and omega.

So, let us just take an example. So, I want to take the first case where gamma square is greater than 4 omega square. So, let me take let me take omega equal to 1 and gamma equal to 3. So, example omega equal to 1 gamma equal to 3 then lambda is equal to minus 1.5 plus minus square root of root 5 by 2. So, this is 9 minus 4 that is 5. So, root 5 by 2. So, this is what you have and if I want I can take the 2 inside, and I can write square root of 1.25. So, I will write it in this form and if you write square root of 1.25 will be approximately about 1.1. So, I can say lambda 1 approximately equal to minus 2.6, lambda 2 approximately equal to minus 0.4.

So, if I have plus 1.1. So, this is approximately equal to 1.1. So, then you have these 2 Eigen values.

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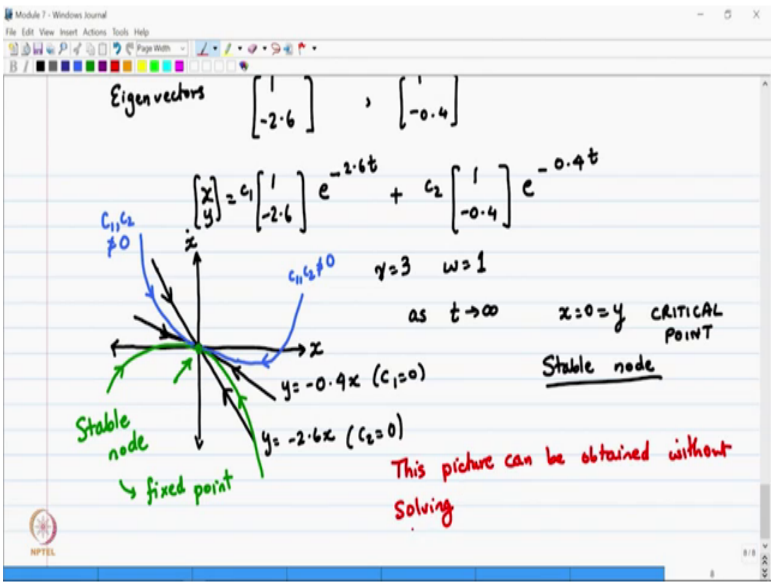

So, the solution now what about the Eigen vectors? In this case you have to work out the Eigen vectors and you can you can show quite easily that these let us work out the Eigen vectors. The Eigen vectors are given by 1 minus 2.6 and 1 minus 0.4. So, in this case your solution has the form x equal to 1 minus 2.6, C 1 e to the minus 2.6 t plus C 2 1 minus 0.4 e to the minus 0.4 t.

So, that is what your solution looks like now we can just look at the phase portrait of this, we obviously, the solution depends on the values of C 1 and C 2 which are governed by the initial conditions. Now if we just look at the phase portrait yeah. So, what you will say is you will come back to this picture; you will come back to this expression for the harmonic oscillator for the damped harmonic oscillator. So, you have dx by dt equal to x. So, you have this term dy by dt is given by this expression.

So, suppose you make a plot on the x x dot plane, x x dot plane this is for the value that we took gamma equal to 3 omega equal to 1. So, now, as I said the solution depends on C 1 and C 2. So, as t tends to infinity, we can clearly see that this should be xy. We can clearly see that that x equal to 0 equal to y. So, this is the critical point you can see that it is a see; it is called a stable node because once you reach that point then it does not you know there is no more evolution of the equation, for whatever value of C 1 and C 2 you take it will always end at that.

Now, you can ask the question how does it approach this stable node, how does the solutions go to this do they go this way, do they go this way, do they go this way, how do they go. Now in order to do this, we have to look at the relative values of x and y; obviously, let us consider one case where you only have C 1 where C 2 is 0. So, if C 2 is 0 what you can see is that y the x dot y which is x dot is just some multiple of x, it is just minus 2.6 times x. This is nothing, but a straight line of slope minus 2.6. So, it will look like this times x.

Now, what is happening is that y will always satisfy this for all t, and this is if C 2 equal to 0. So, if C 2 equal to 0 then you go in this way. So, based on the value of C 1 you either go this way towards this point or you go this way towards this point. X equal to 0 y equal to 0. So, if your initial condition initial condition is what tells you what the value of C 1 is, such that y is greater than 0 then you will go to 0 in this way. So, the ratio of y to x is given by this minus 2.6. So, this is one case when C 1 equal to 0.

What happens when C 2 equal to 0? Then you have another graph which is which looks like E to the minus 0.4 x. So, that will be a slightly smaller slope. So, it will look like this. So, this is y equal to minus 0.4 x; if both C 1 and C 2 are non-zero. So, if C 1 and C 2 are both non-zero. So, this is a case where C 1 equal to 0, this is the case where C 2 equal to 0. If both C 1 and C 2 are not equal to 0 now what will happen is that as you increase t this will go to 0 much faster, this will this will go to 0 much slower.

So, exponential of a larger negative number will be smaller than exponential of a smaller negative number. So, eventually what will happen is that your solution will tend to follow this. For very large times it will go, it will go towards this it will look like this. At very large times and it will be some linear combination and it will look something like this. So, this is what your trajectory will look like, if you start from the other side then it will look like this, this is C 1 C 2 both not equal to 0. So, we will have some trajectory like this. So, this will be for that value.

Now, if you started from the other side, then you have to approach this and you have to approach it from top. So, it will actually come like this, it will approach this graph in this way. So, this is what the solution will look like for some value of C 1 C 2 not equal to 0, you could also have solutions where based on the value of C 1 C 2 you could have also you could also have something like this.

So, whatever it is you end up at this, this is called a stable node it is a critical point or it is sometimes called a fixed point. So, x equal to y equal to 0 so that is a critical point and this is your stable node. So, the damped harmonic oscillator has this kind of solution. I should emphasize one thing that you know you know we got this by actually looking at the solutions, but you can get this picture just by looking at the equation and fin phase plane.

So, if you just look at the equation in this form. So, this picture can be obtained without solve solving. And that is what I am going to show you in the last part of this lecture. So, this point is a stable node or a fixed point, let us look at another case where gamma square is less than 4 omega square. So, what does it look like for gamma square less than 4 omega square. So, if gamma square is less than 4 omega square, then I mean you can take a you can take certain values of gamma and omega.

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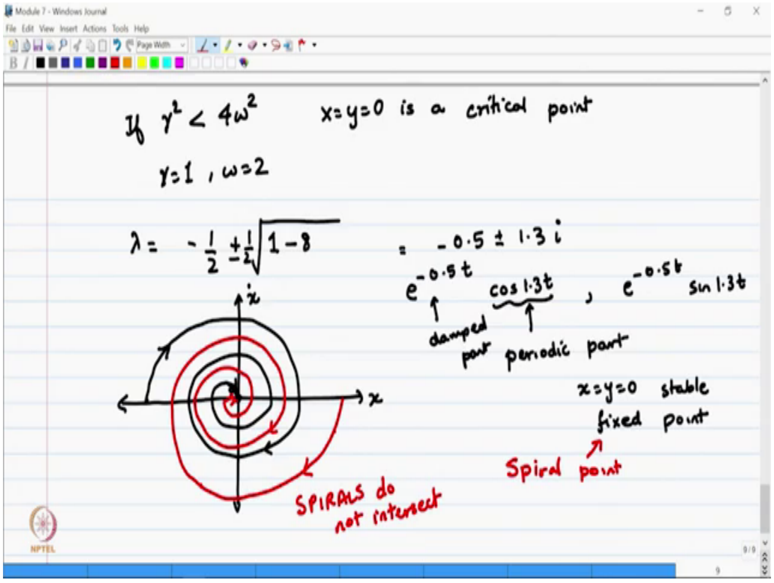

But I will just show what the solution will look like in this case. So, again x equal to y equal to 0 is a critical point. So, gamma square is less than 4 omega square, the let me let me just take value of gamma equal to 1 omega equal to 2. So, then the solution looks like. So, we have our Eigen values looks like minus gamma by 2. So, it is minus half plus minus square root of. So, lambda equal to minus half plus minus square root of 1 minus 8 by 2, is equal to minus 0.5 and you have square root of 7. Square root of seven is approximately about you can say about 2.6.

So, you have plus minus 1.3 times I that is what it looks like. These are the Eigen values what you see is that the solution looks like e to the minus 0.5 t into basically something like cos omega t or e to the minus 0.5 t into sin omega t. So, these are what your solutions will look like. So, these are the independent solutions and we can go ahead and write the expressions, I will not bother with that, but what I want to show is what the phase plane will look like in this case.

So, in this case, so, this is a 1.3 t; in this case what we you know before we draw the phase plane may mention that this is the periodic part and this is the damped part. As you can see as t goes to infinity this will go to 0 this will go to 0 x equal to is a stable fixed point.

Now, what is the nature of the solutions? So, if this at very small t this is approximately equal to 1. So, if t equal to 0 then you have the simple harmonic oscillator, gamma equal to 0 you have a simple harmonic oscillator and that you saw was the periodic was the was those ellipses. Now in this case you have an ellipse, but it is damped. So, the amplitude of the ellipse is decreasing. So, what you have is something that goes like this and eventually it ends at this point. So, your solutions will look something like this.

So, it look like your periodic solutions, but they will end up at this point. You can look at several other solutions so, for example, if you can take another solution that you may start here then it will go like this. What is important is that these are 2 trajectories; that means, that means if you start here you will go like this all the way till you end up here. So, this point is called a spiral point because each trajectory will spiral. So, based on where you start off with you will end up with one of these spirals, spiral points and notice that spirals do not intersect no trajectories can cross because you know the solution is unique. So, you will always go in this way.

So, you will always go in a particular way. So, you can never have these 2 curves crossing each other, because the motion is perfectly determined. So, once you have specified whether you start here or here you will end up at this, you will end up following these trajectories. So, wherever you start along this curve, you will end up following this trajectory and finally, ending up at this at this spiral point.

What I try to show you here is how true is I described the phase plane picture, I used a harmonic oscillator we used a simple harmonic oscillator and a damped harmonic oscillator. Now these are linear equations, but what I want to say is that the phase picture that we described here will be used to analyze non-linear differential equations. I will discuss that in the next lecture.

Thank you.