Advanced Mathematical Methods for Chemistry

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Module – 07
Lecture – 05
Recap of Module 7, Practice Problems

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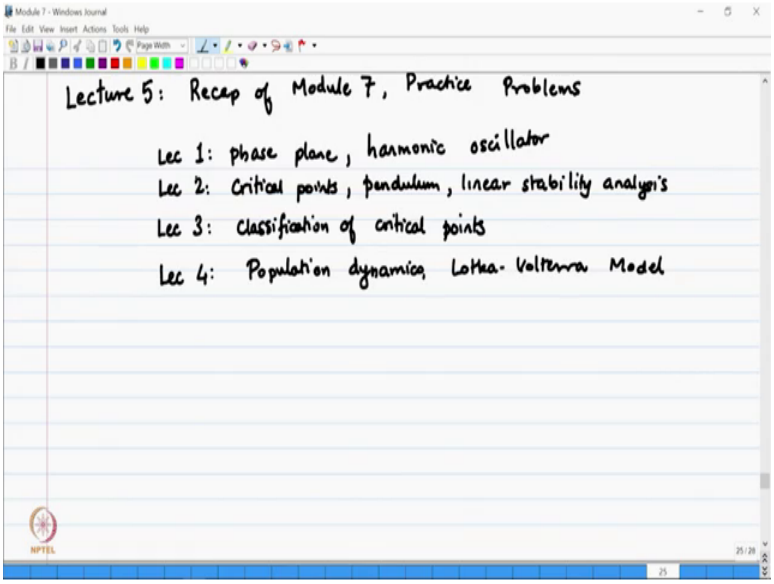

So in this module, in the first lecture; we learnt about the phase plane and the harmonic oscillator. We saw the description of the phase plane and how it can give a portrait of the of the harmonic oscillator problem. Then in the second lecture, we saw the critical point, we saw the meaning of critical points, we saw we looked at the problem of the pendulum and did linear stability analysis to get a phase portrait of the pendulum. In lecture 3, we saw the classification of critical points using the linearize system. In lecture 4, we saw population dynamics where we where we analyze the Lotka Volterra model.

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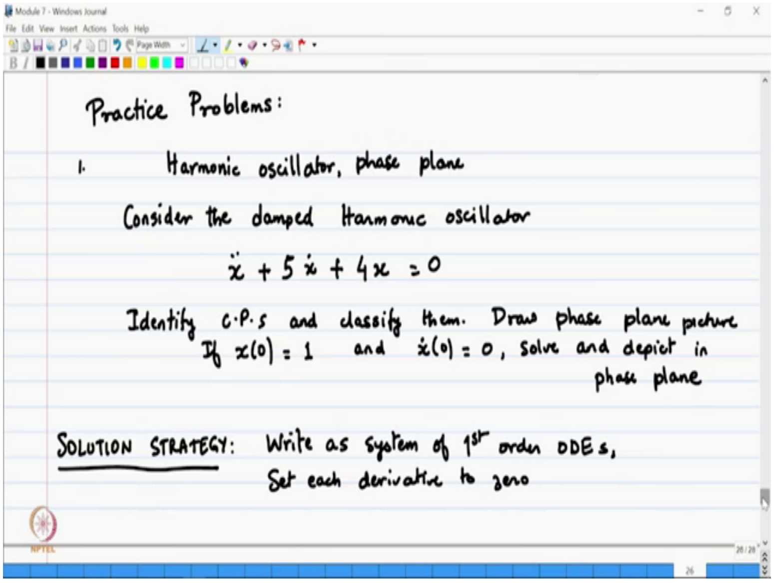

So, let us do a few practice problems. The first problem that I want to do is involves a harmonic oscillator and I have asked you to draw the phase plane of this harmonic oscillator. So, consider a damped harmonic oscillator given by this equation; x double dot plus 5 x dot plus 4 x equal to 0. Identify the critical points and classify them. Draw the phase plane picture, if x 0 equal to 1 and x dot of 0 equal to 0, solve and depict in phase plane. So, at t equal to 0 if you had this and this equal to 0 solve and depict in the phase plane.

So, the strategy to solve this is to write this as a system of first order ODEs set each derivatives to 0 and you solve that for the critical points Eigen values and so on. So, let us look at the solution.

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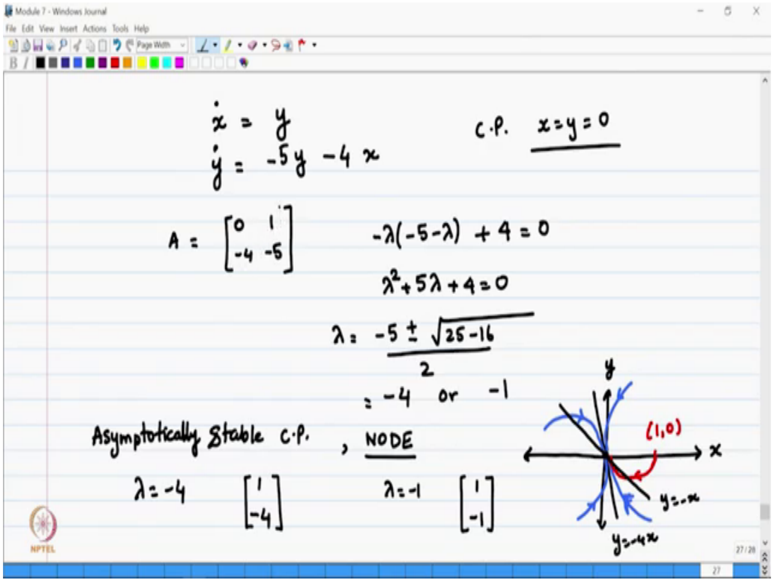

So, first we will write it as a system x dot equal to y and y dot equal to minus 5 y minus 4 x. So, clearly the critical point is x equal to y equal to 0 because if you set x dot equal to 0 you will get y equal to 0 and if you put y equal to 0 in this and you set y dot equal to 0 then x has to be 0. So, x equal to y equal to 0 is the only critical point of the system, since it is a linear system, this can only be the critical point. So, this is not a non-linear system this is a linear system.

So, we can go ahead, we can write the Eigen; we can write the matrix 0 1 minus 4 minus 5 we solve for the Eigen values of this matrix and you get the Eigen values by this simple quadratic equation. You will get Eigen values of minus 4 or minus 1. Now both the Eigen values are real and both are negative and they are not equal to each other. So, both are real, both are negative or are not equal to each other. So, that is an asymptotically stable critical point and in fact, it is a node and so if you take lambda equal to minus 4 then your Eigen vector is 1 minus 4 lambda equal to minus 1, your Eigen vector is 1 minus 1. So, basically if you look at the solutions; this is the more slowly; this is a smaller Eigen value and that is going to dominate the behavior at long times should do should do this again. So, the long time behave. So, let us just go ahead and draw the phase space picture.

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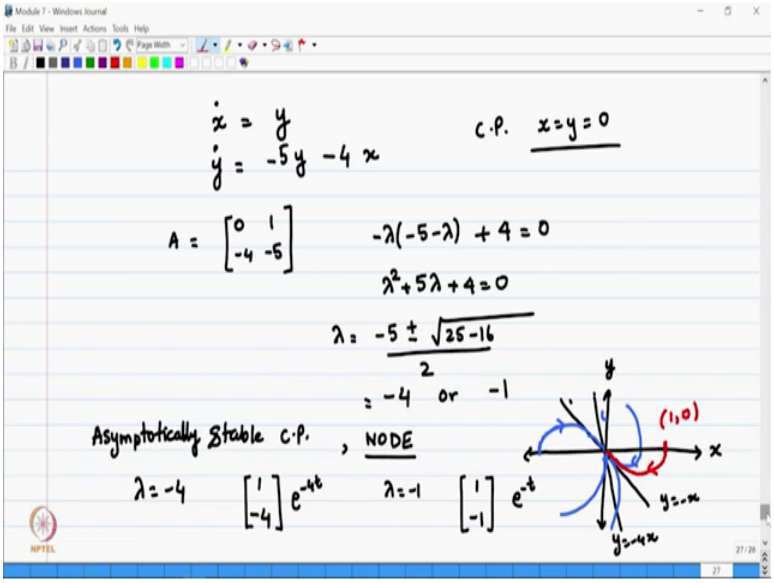

So, you have lambda equal to y equal to minus x and y equal to minus 4 x and what we said is that is that; this will have a term that looks like e to the minus t. This will have a term that looks like e to the minus 4 t. So, clearly this; do this again; 4 x and y equal to minus x. So, clearly it is the y equal to minus x that is going to dominate the behavior at long times. So, what the solutions will look like. So, suppose you start from somewhere then eventually you will go to 0 along this; asymptotically you will go along y equal to minus x.

So, asymptotically you will go; you will approach along y equal to minus x and you would; so, your solutions would look something like this. If you are in this part where x is greater than 0; so, if x is greater than 0 then you will be approaching along something like this if y is greater than 0. So, if y is greater than 0 then x dot is positive. So, if you are at this region, you will get a graph that that shows x dot increasing and then it asymptotically go to x dot equal to 0. So, this is what it will look like if you are somewhere here then what will happen is that you will go major series this point. So, so if you are somewhere in this in this region; suppose you start with x and y both greater than 0. Now x dot equal to y. So, y is greater than 0. So, y will decrease and x will increase till it becomes parallel to this line and then and then it will turn and go asymptotically towards this.

So, that is what your trajectories will look like when they cross the y; when they cross the x axis they will always be perpendicular because at this point y equal to 0. So, the rate of change of x is 0. So, it will cross in this manner and similarly you can extend for the other values also. So, in this case, if y is negative then your points will essentially go in this manner and approach the origin and so on.

So, this is what your points look like. Now suppose I start with a point at x equal to 1, y equal to 0. So, what will be the behavior of this point? So, since x is greater than 0 x since y is equal to 0 x dot and you started at this at this point. So, x dot is going to be 0, so, it is going to be straight and if you see y dot is negative. So, y has to decrease. So, y will go down and it will follow this and it will eventually come towards this point. So, this is what the picture of this of this oscillator is of this damned harmonic oscillator is.

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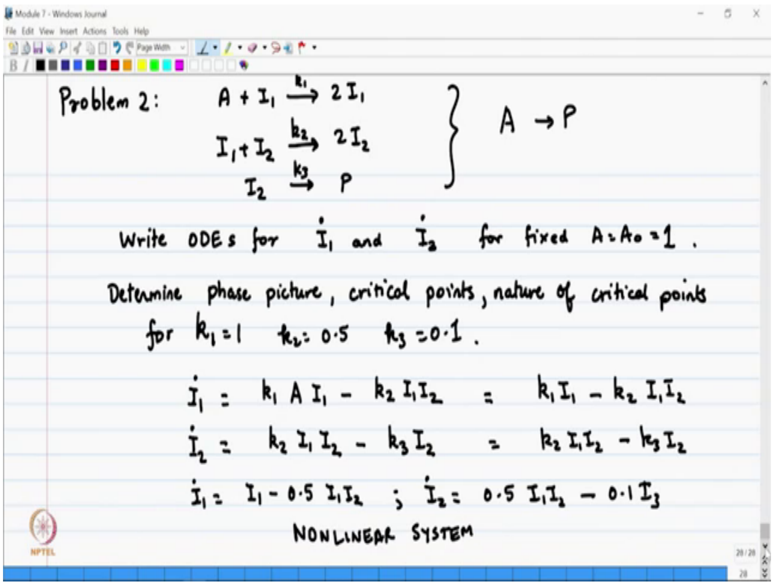

Now, the next problem is a chemical reaction. So, in this chemical reaction, I am writing the overall scheme. So, the overall reaction is overall reaction is A going to P. Some reactant going to a product and there are various steps in this reaction. So, the first step is A reacting with; I call it I 1 to give 2 I 1. So, I 1 might just be an excited state of A or you know it might just be some modified form of A. Then you have I 1 plus I 2 I 1 and I 2 are 2 intermediates that gives 2; I 2 and then I 2 going to P and these are the rate constants. So, I have asked you to write the ODEs for I 1 dot and I 2 dot for fixed A equal to A 0 equal to 1 and then you determine the phase picture critical point since nature of critical points for this problem.

So, this is fairly straight forwards. So, if I write I 1 dot using your typical kinetics. So, I 1 here, so I 1 dot; you can write it as k 1 times A is a concentration of A times I 1 and you have minus k 2 times I 1 I 2. And similarly I 2 dot is equal to k 2 I 1 I 2 minus k 3 I 2 and if A is equal to A 0 equal to 1, then this looks like k 1 I 1 minus k 2 I 1 I 2 and this looks like k 2 I 1 I 2 minus k 3 I 2.

So, this is the first thing that you have to write to the ODEs for I 1 dot and I 2 dot at fixed A equal to A 0 equal to 1. Then you have to determine the phase picture critical points and nature of critical points for k 1 equal to 1 k 2 equal to 0.5 and k 3 equal to 0.1. So, let us write the equation. So, if I can write the equations as I 1 dot is equal to k 1 that is I 1 minus 0.5 I 1 I 2 and I can write I 2 dot is equal to minus 0.5 I 1 I 2 minus 0.1 I 3.

So, what are the critical points of this equation? So, this is a non-linear equation; non-linear system. So, let us determine the critical points. So, so what are the critical points?

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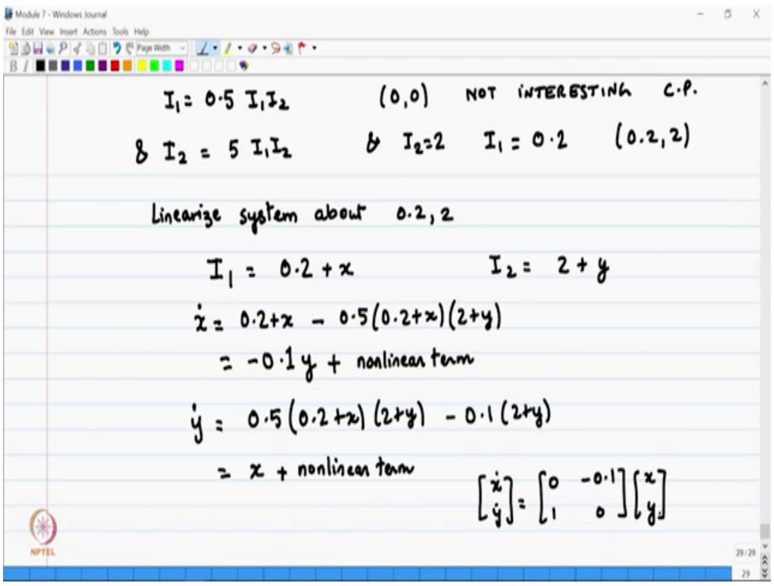

So, I 1 is equal to 0.5 I 1 I 2. So, and I 2; it should be I 2 and I 2 is equal to 5 times I 1 I 2. So, the critical points are 0, 0 which is uninteresting one and; what is the other critical point not interesting critical point; the other critical point is suppose. So, so you get I 2 equal to 2 and I 1 equal to I 1 equal to 0.2.

So, this critical point is 0.2 comma 2. So, now, now let us linearize about. So, suppose you linearize system about this point; what will happen? So, what you will get is I 1. So, you say I 1 equal to 0.2 plus x, I 2 is equal to 2 plus y, then I can write this equation as I 1 dot it will be x dot is equal to I 1 that is 0.2 plus x minus 0.5, 0.2 plus x into I 2 is 2 plus y and what you will get is you have the 0.2 will cancel because of the first term. So, and the x; so, you have 0.5 into x into 2. So, again that will cancel the x.

So, you will just have a term that involves y. So, you will have minus 0.5 y plus the x y term; plus the x y term which is non-linear plus non-linear term and y dot is equal to you. So, if you write for y dot what you will get is oh sorry not 0.5 y for 0.5 into 0.2 into y. So, that is 0.1 y and if you look at y dot y dot will have. So, y dot is 0 0.5 times 0.2 plus x 2 plus y minus 0.1 into 2 plus y and in this case again you will you will find that the factor of 0.5 to 0.2 is 0.1; 0.1 is A, 2 is 0.2. So, that will cancel the 0.2 and then you have 0.5 into 0.2 into y that is 0.1 y which will cancel that. So, what you will be left with is 0.5 into x into 2 that is x. So, just 0.5 into a point into x into 2 that is x and A plus non-linear term.

So, our linearize system looks like this; looks as x dot y dot is equal to 0 minus 0.1, 1, 0. So, this is what are linearize system looks like.

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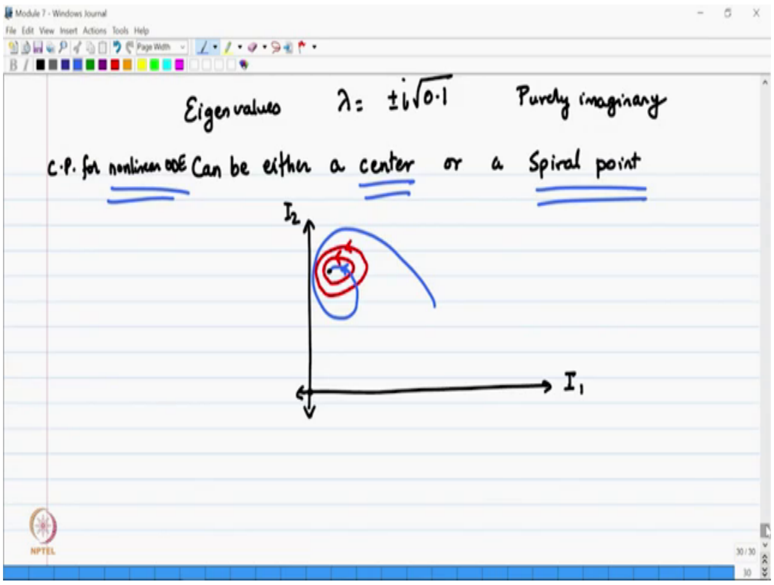

Now, Eigen values clearly the Eigen values are purely imaginary lambda is equal to plus minus square root of 0.1 I. So, purely imaginary and if it is purely imaginary, we know that it can be either a center or a spiral point. So, this point is either a center or a spiral point and that whether it is a center or a spiral point. This is for the non-linear equation. So, C.P for non-linear ODE, this can be either a center or a spiral point it is very important that this is for the non-linear ODE; for the linear ODE clearly; this will be a center, but for non-linear ode it can be it can also be a spiral point.

So, this is the; so what does a phase picture look like. So, let us just try to draw some characteristics of the phase plane. So, I 1 I 2 the 0 0 is a not. So, interesting point, but the other point is given by I 1 that is 0.2 and 2. So, 0.2 and 2, so, if it is a stable point then the trajectories will look like; if it is a the trajectories will look like this around this or if it is a I mean or if it is an unstable point; if it as a spiral point then your trajectories will go spiraling towards this. So, you can we will just we will just show what happens if it looks like a center. So, if it looks like a center; then we go back to our non-linear equations. So, so what we had was yeah. So, these are our non-linear system of equations.

So, I 1 dot is I 1 minus 0.5 I 1 I 2 and if you go around the critical point. So, if you look at the linear system then you have x dot equal to minus 0.1 y. So, if in this case y is greater than 0. So, the rate of change of x is negative around this point. So, so if x is; so, you have for y in this region. So, you have you have trajectories like this; you could also have it could also be a spiral. So, for some other values of the non-linear equation it is slightly more difficult to analyze, but you could also have a you could also have a spiral point which where the trajectories go spiraling towards this point could also have something like this it really it really you have to do a bit more analysis of this of this non-linear equation in order to get this.

So, I will conclude this module for now. So, this is the end of module seven and in this I have tried to show you certain ways to analyze non-linear differential equation. These are purely qualitative ways that give you some sort of picture of the non-linear differential equation and these are very interesting techniques and often you can get very good idea about non-linear equations by analyzing the critical points.

Thank you.