Oscillatory Systems: Approach from Nonlinear Dynamics

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ABSTRACT

The aim of this chapter is to present a brief outline of the background theories essential for understanding numerous non-equilibrium phenomena, such as chemical and biological oscillations, spirals and so on. Oscillations are one of the most common phenomena in chemical and biological systems. Oscillations of chemical origin have been present since life originated. Every living system contains thousands of chemical and biological oscillators. The systematic study of oscillating chemical reactions and subsequently the broader field of Nonlinear Dynamics is of considerably fundamental domain of research in recent decades. The chapter starts with a brief outline of some background history of chemical oscillations followed by the basic thermodynamic explanations and stability analysis. A short glimpse of Phase plane analysis and Limit cycles are given. One dimensional stability analysis is followed by two dimensional one. Relaxation oscillation is explained both theoretically and graphically.

Keywords: Steady State; Equilibrium; Phase Plane; Non-Equilibrium Process; Oscillatory Systems

Introduction

Dynamics is an interesting topic which explains how a physical variable of interest progresses with time. Harmonic oscillator is an example of linear motion which is well known from Newtonian Mechanics. In this motion the frequency of the oscillator is not dependent onamplitude. Whenever the system is not linear its motion changes the behavior. It is not so simple because of the dependency of its frequency over its amplitude. The result is the motion may vary from purely rhythmic to chaotic region. Nonlinear dynamics has its origin in Physics to Newtonian mechanics developed earlier in mid-1600s, it is now treated as an interdisciplinary subject today (Epstein 1998, Strogatz 1995, Murray 1993, Gillespie 1977, Goldbeter 2006) which has its application in almost all branches of Physics, Chemistry and Biology (Grossman 1990, Hillborn 1994, Jalan 2005, Julvez 2015). Although it developed early but the subject could not found its applicability because the classical three-body system was not under the ability of the Newtonian method. The Poincare developed a new geometric technique in studying such systems (Strogatz). From this a new area of Nonlinear Dynamics has been developed which has enlarged application in different area of science specially in chemistry and biology.

In order to go into the depth of aforementioned people have to get idea about the differences between temporal and spatio temporal oscillations. Oscillations are of two types. One is temporal that means it oscillates in time (Sen *et al.,* 2008, Sen *et al.,* 2009, Dhatt, Sen &

Chaudhury 2020, Murray 1993, Scot 1994) and the other is spatio temporal that means it can oscillate both in space and time. Temporal oscillation implies it is homogeneous in space (Bray 1921) where as the spatio-temporal oscillation has its coupling of the space part with the temporal part with diffusion (Epstein 1998, Ghosh et al., 2009, Sen et al., 2010). A chemical or biological oscillation is a periodic far-from-equilibrium phenomena which is part of non equilibrium thermodynamics. After looking back at the history of the subject it shows that long time has been taken to establish the fact that the oscillatory phenomena has no contradiction with the classical second law of thermodynamics. Belousov (1893-1970) submitted the manuscript of continuous conversion of yellow Ce⁺⁴ to colorless Ce⁺³ in 1951 but it was rejected. The editor outwardly stated that his work was simply impossible. The paper could be published on submission of some additional evidence which can contain some snapshots of different phases of oscillation. Tragic fact s that after laboring for six more years the work was again rejected, At 1961 Zhabottinsky a graduate student of Biophysics began looking at the same system. He replaced citric acid with malonic acid and obtained a better formulation. Zhabotinsky wrote his manuscript and sent to Belousov for his comments. More than ten papers on Belousov Zhabotinsky reaction had been published since 1951 moreover the the manuscript that Belousov originally wrote in 1951 was posthumously published in 1985 (Belousov 1951). So the above elaborative study described how difficult it was for the science community at that time to accept the oscillatory phenomena.

The classical theoretical model was first proposed by Alfred Lotka (1925) (Lotka, 1920). The model is used to explain predator prey system and the basic pillar to elaborate oscillation in chemistry and biology. It has three irreversible steps. X is the population of rabbits. It can reproduce auto catalytically, G is the grass. Since it is present in large it is assumed to be constant. Y represents the lynxes and D the dead lynxes.

$$G+X\rightarrow 2X$$

 $X+Y\rightarrow 2Y$
 $Y\rightarrow D$

The above kinetic elementary steps are not reversible: X will not convert into G, nor D convert into live ones. The behavior of the predator and prey species has been described in ecology. The following is the set of differential equations

$$\frac{dx}{dt} = k_x ax - k_y xy$$
$$\frac{dy}{dt} = k_y xy - k_d y$$

Here k_x is the rate constant of how fast rabbits reproduce; similarly k_y is the rate constant which indicates how fast lynxes reproduce and k_d is the mortality rate of lynxes. The predators and preys will oscillate in time for a particular set of parameters i.e. rate constants (Figure 1).

Population



Figure 1: Oscillations of Predators and Prey with time in Lotka Volterra model (Epstein, 1998)

While recalling the violation of second law of thermodynamics in chemical oscillations it is obvious that only oscillate are the intermediates. Reactants and products become steady after some time. There is vast differences between this chemical oscillator and physical one. Physical oscillator as it is known from simple pendulum always pass through equilibrium. Chemical oscillation is not an equilibrium phenomena rather it is away from equilibrium. During the oscillation of intermediates of chemical oscillation the free energy gradually decreases. Conversion of reactants having higher free energy to products having lower free energy leads to the oscillation of the intermediates. To maintain continuous oscillation supply of substrate concentrations must be thoroughly kept. That means the system must be open (Figure 2). Further chemical and thermodynamical study of BZ reaction made significant improvement in the domain of chemical oscillation (AM, 1964).



Figure 2: Explaining two different types of Oscillations. (a) Physical Oscillations where it Oscillates around Equilibrium, Inconsistent with Thermodynamics (b)Oscillations far from Equilibrium, Consistent with Thermodynamics. (Epstein, 1998)

Discussion

Linear Stability Analysis

For a system the equilibrium state is unique in nature but the steady states of a nonlinear system may not unique. The steady state of a dynamical system is also known as fixed point.(Epstein 1998, Strogatz 1995).Although at the fixed point the dynamics seizes but near the vicinity of the steady state the trajectories direction changes. Emphasis has been given on the dynamics around the fixed point or the domain of the steady state region. Generally the system is not exactly solvable. Approximation techniques has been taken or linearize the system truncating the nonlinearities. An one-dimensional dynamical system can be represented as,

$$\dot{x} = f(x)$$

Here f(x) can be a nonlinear function of x. The function f may not be explicitly time dependent. Then the system is autonomous or time independent and if it depends on time then it is nonautonomous or time dependent in nature. At the fixed point f(x) = 0

Let at a fixed point $x_s=0$. So $\frac{d}{dt} (\delta x) = 0$ for the above system. It has been disturbed the above system about $x_s as x_s = (x + \delta x) \cdot \delta x$ is the very small amount of perturbation. Thus it has been obtained

$$f(x + \delta x) = f(x_s) + f'(x_s)\delta x + O(\delta x^2)$$

where $O(\delta x^2)$ is the higherorder Taylor series expansion term and will generally negligible when $f'(x_s)$ is nonzero. Since $f(x_s)$ is zero at the steady state the following linear equation will arrive as $\frac{d}{dt}(\delta x) = f'(x_s)\delta x$

This linear equation easily tells that the extent of stability of the fixed point. That means If $f'(x_s)$ is positive then the fixed point is unstable; the system will go away from it whereas if it is negative then the fixed point is stable means the system will converge in it. Actually, for a one dimensional system the magnitude of $f'(x_s)$ gives a measure of stability and $1/f'(x_s)$ is a characteristic time scale which determines howsignificantly the solutions will grow or decay in the neighborhood of the fixed point x_s . A very important point about the one-dimensional flows is that the flow happens monotonically towards and away from the fixed point and existence of oscillatory solutions are thus forbidden.

Two Dimensional System

Two-dimensional systems are analyzed for the stability of fixed points, in almost the same manner as done in one dimensional ones, by linearizing them near those fixed points. Suppose a two-dimensional system of the form

$$\dot{x} = f(x, y)$$
$$\dot{y} = g(x, y)$$

and let $(x_{0,}y_{0})$ be the only fixed point of the system such that $f(x_{0},y_{0}) = 0 = g(x_{0},y_{0})$. Now to analyze the stability of the fixed point let people perturb the system around the fixed point by setting $x = x_{0}+\delta x$ and $y = y_{0}+\delta y$. After linearizing the system around the fixed point it has been obtained the dynamical equations for

$$\begin{pmatrix} \dot{\delta x} \\ \dot{\delta y} \end{pmatrix} = \begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix}$$

the perturbations δx and δy as

as where the matrix containing the terms f_x , f_y , g_x and g_y (indicating the values of partial derivatives with respect to *x* and *y* of the functions f(x,y) and g(x,y) at the fixed point) is known as stability matrix (*M*). It is assumed the solutions of δx and δy of the form $\delta x = Ae^{\lambda t}$ and $\delta y = Be^{\lambda t}$ then the eigenvalues are given by

$$\lambda = \frac{(TrM) \pm SQRT(TrM^2 - 4\Delta)}{2}$$

Where $TrM = f_x + g_y$ and $\Delta = f_x g_y - g_x f_y$. Now different possibilities of the solutions may arise for different values of TrM and Δ . Now different possibilities of the solutions may arise for different values of TrM and Δ .

(A) If $(TrM)^2 > 4 \Delta$, then there is always two real valued λ -s where dependingupon the signs of the corresponding eigenvalues three different kinds of stability of the fixed points are possible.

(i) If (*TrM*) >0 and Δ >0 both eigenvalues are positive leading to an unstable node (ii) If (*TrM*) <0 and Δ >0 both eigenvalues are negative leading to a stable node (iii) For (*TrM*) >0 and Δ <0 or (*TrM*) <0 and Δ <0 or (*TrM*) = 0 and Δ <0, one eigenvalue is positive and the other one is negative leading to saddle node.



Figure 4: Stabilities of the Fixed Point when $(TrM)^2 > 4 \Delta$ (Strogatz 1995)

(B) If $(TrM)^2 < 4 \Delta$, then the eigenvalues are always imaginary and appear as complex conjugate pair. Here also stability of the fixed point can be of different types.

(i) If (TrM) > 0 the both the imaginary eigenvalues have positive real part leading to a stable spiral

(ii) If (*TrM*) <0 the both the imaginary eigenvalues have negative real part leading to a stable spiral

(iii) If (TrM) = 0 and $\Delta > 0$, then this situation leads to a center.



Figure 5: Stabilities of the Fixed Point When $(TrM)^2 < 4\Delta$ (*Strogatz 1995*) Phase Plane Analysis; Limit Cycle: Excitable Systems and Relaxation Oscillations

Limit cycles are isolated closed trajectories in phase space i.e. limit cycle is the only closed trajectory in the neighborhood. This attractor can be stable or unstable depending upon the fact that all the neighboring trajectories can either get attracted to go or away from it (Figure 3).



Stable limit cycle

Unstable limit cycle

Half-stable limit cycle



Let people consider the equations of model be

$$\frac{du}{dt} = \frac{1}{\epsilon} f(u, v)$$
$$\frac{du}{dt} = g(u, v)$$

Here *f* and *g* are functions of the dynamical variables *u* and *v*. ϵ is a small number introduced as a scaling factor to maintain different time scales of dynamics. *u* reaches fast to a steady state, while *v* changes much more slowly. The term nullcline is defined as the curves on which the rate of changes of each of the dynamical variables are zero. From the intersections of the two nullclines one can obtain steady states. If the steady state falls on any one of the left or right branch then it is stable because all dynamical trajectories in its surroundings point in directing toward the intersection of the two nullclines. These types of systems are known as the excitable systems. On small perturbations of an excitable system it quickly returns to the steady state. As shown in Figure 6, upon applying small perturbation to the steady state the system jumps back to u nullcline because of the faster change of *u* due to $\frac{1}{\epsilon}$ term. Thus the steady state is concluded to be stable.



Figure 6: Phase Plane Analysis of Small Perturbation in the Steady States of Excitable Two Variable Model (Epstein 1998)

Now investigate what happens when large perturbation is applied to the steady state. Upon application of large perturbation the system reaches to the point A which is positive for f(u,v). Thus the perturbation continues to grow, pushing the system toward the right branch of the f = 0 nullcline. The concentration of v changes slowly compared to u. When the system reaches the f=0 nullcline at B, it starts to go up the nullcline as v increases (g(u;v) > 0), until it reached to the maximum at C, then it comes rapidly to the left-side branch of u-nullcline. The system then slides along this nullcline again back to the fixed point (Figure 7).



Figure 7: Phase Plane Analysis of Large Perturbation in the Steady States of Excitable Two Variable System (Epstein 1998)

If the intersection of the nullclines lies on the middle branch, the trajectories point awayfrom the steady state making it unstable. Since u changes very rapidly the analysis has tostart from the point A in Figure 6. The system will move slowly along the nullcline as v decreases from A to B. Upon reaching B, u will rapidly increase as the system jumps to the other branch of the f = 0 nullcline (C). This branch is in the positive region of g(u;v), so the system will move along the u-nullcline toward D as v slowly increases. Upon reaching D as v slowly increases, the system again 'falls off' this branch of the u nullcline and makes a rapid transition to E. It then proceeds back toward A, and the cycle repeats. Periodic temporal oscillations are obtained (Figure 8). These types of oscillations are called relaxation oscillations.



Figure 8: Phase Plane Diagram of Relaxation Oscillations (Epstein 1998)

A note has been taken on the extent of usefulness of the results of linear stability analysis. So long as a fixed point is a node or saddle or a spiral it is stable enough and the nonlinear terms left do not generally affect its stability. But when the fixed point is a center or degenerate nodes or star or non-isolated fixed point its stability is very much dependent on the nonlinear terms left. They should be taken care of to see what happens near such a fixed point.

Conclusion

So far it has been discussed the stability analysis of fixed point upon perturbed by small and large perturbations. Different types of dynamical behaviours are obtained. Oscillations are amongst them. The importance of oscillatory dynamics is noteworthy in the physical world and its origin is also supposed to be easily understood. A short glimpse has been given. Study of Nonlinear dynamics of oscillatory systems can reveal various phenomena. More insights will help to understand deeply the oscillatory phenomena and it will be done the same in upcoming issues.

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