Nonlinear Oscillation and Control in the BZ Chemical Reaction

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Nonlinear Oscillation and Control
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DEDICATION

To my parents, my wife and my son.

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SUMMARY

In this thesis, we investigate the oscillatory Belousov-Zhabotinsky (BZ) reaction determined by a reversible Lotka-Volterra model in a closed isothermal chemical system. The reaction consists in two zones, oscillation zone and transition zone. By applying geometric singular perturbation method, we prove the existence of the central axis $W^o_{\sigma,\varepsilon}$ in the oscillation zone, and a strongly stable two-dimensional invariant manifold $M^t_{\sigma,\varepsilon}$ in the transition zone. And $M^t_{\sigma,\varepsilon}$ contains a one-dimensional stable invariant manifold $W^t_{\sigma,\varepsilon}$ which is the part of the central axis in the transition zone. We also find that the time spending in the oscillation zone is in the algebraic order in σ. And in the vicinity of the equilibrium, there is no oscillation as indicated by Onsager's reciprocal symmetry relation. Furthermore, the damped oscillation is studied in terms of the action-action-angle variables. In the end, we apply the model reference control technique to control the oscillation amplitude in the BZ reaction.

CHAPTER I

INTRODUCTION

Chemical and biochemical oscillations are one of the most important aspects of nonlinear dynamics of living cellular systems [23, 49, 53]. The study of oscillating chemical reaction has a long history. The first discovery of the oscillation in a chemical system dates back to 1828 when G.T. Fechner published a report, in [17], about the oscillating current in an electrochemical cell. Throughout the nineteenth century, the related work on oscillating reaction was done by F. Schönbein in 1836, J.P. Joule in 1844 and W. Ostwald in 1898, etc, see [56]. However, because the system they studied were heterogeneous, it was believed that no homogeneous oscillation exists.

The theoretical discussion of the oscillating reaction was first formulated by Alfred Lotka in 1910. It mainly appeared in his series of work in the period between 1910 and 1920. But cited from [45], he also remarked that "*no reaction is known which follows the above law*". This may be one of the reasons why no further analysis on the oscillating reaction continued along Lotka's idea during that period. However, just as Lotka remarked in [45] that "*as a matter of the fact the case here considered was suggested by the consideration of the matters lying outside the field of physical chemistry*", his ideas leads to a successful development in the ecological problem with periodic behavior. Inspired by Lotka's idea, Vito Volterra, an Italy mathematician and physicist, studied the mutual interaction of two species and found the periodic fluctuation, see [70].

Nevertheless the oscillating chemical reaction was not recognized widely in the chemistry community. One reason is the wrong impression that all the solutions of chemical reagents must approach the equilibrium state in the monotonic way, because of the laws thermodynamics. The other is the relatively low level development of the theoretical tools

for analyzing the mechanism behind complex reaction [22].

In 1951, Boris Belousov, a Russian chemist, discovered the temporal oscillation in a liquid phase reaction consisting of bromate, citric acid and ceric ions Ce^{4+} and started the modern study of oscillating reaction. But his manuscript about this discovery was rejected for some journal publication because of the resistance to oscillating reaction, and finally was published in an unrefereed abstract in a conference on radiobiology in 1957.

In 1961, Anatol Zhabotinsky redid the experiment by Belousov's recipe and confirmed Belousov's discovery. In the following years, at least ten papers about the BZ reaction were published. Especially after Zhabotinsky presented some of his work at a conference in Prague in 1968 where Western and Soviet scientists were allowed to meet, the study on BZ reaction was immediately widely spread. And because of the great contribution to the oscillating reaction, Belousov and Zhabotinsky were awarded Lenin Prize in 1980, the highest medal in Soviet Union. Unfortunately, Belousov had passed away ten years eariler.

A short survey on this history can be found in [16, 22, 77].

In reality, there are two types of reactions where the oscillation can be observed. The first type is *open* system, where the exchange of matter and energy with surroundings is allowed [16]. Open systems have a wide range of dynamical behavior. Most of currently existing models exhibiting oscillating reaction dynamics are of this type. For example [35] studied composite double oscillation, [65] the chaos, [67, 72, 48] for period-doubling bifurcation and so on. The advantage of this type of mathematical models is that the system's long-time behavior can be defined in rigorous mathematical terms[52, 36]. One of the leading group in this field, especially thermodynamics [51, 54], is the Brussels school of which Prigogine is a member.

The second type is *closed* system. According to the second law of thermodynamics, closed system eventually tend to the equilibrium state. And from the law of mass action kinetics [62], there exists a free energy function which plays the role of a Lyapunov function. But to study the chemical oscillation in a closed reaction system, one has to deal with

the quasi-stationary phenomenon, which is usually more difficult to be rigorously defined in mathematics. And such a system usually involves in multi-scale dynamics and becomes a singular perturbation problem.

Actually studying the singularly perturbed systems, such as models of physical phenomena with multiple different scales in time and space, is an important branch of applied mathematics. Phenomena with different scales are widely observed in many areas of science and engineering such as population dynamics, neurobiology, ecology, and so on. For example, the singular perturbation method is employed to study a predator-prey model of three dimensions with two different time scales in [44], and the traveling wave solution in a tissue interaction model with three different time scales in [1].

Compared with the regular perturbation, in singular perturbation, one always has to deal with the non-uniform limiting behavior. Therefore singular perturbation technique offers a lot for understanding the physical phenomena with multi-scale behavior.

When studying singularly perturbed problem, one often encounters a problem about the persistence of invariant manifold under the perturbation. It was proved in [47] that an invariant manifold is persistent under any smooth perturbation if and only if it is normally hyperbolic. Roughly speaking, an invariant manifold is normally hyperbolic if the growth the rate of the linearized flow about the invariant manifold dominates in the normal direction.

A straightforward way is to first locate the invariant manifold for the unperturbed system; second, linearize the unperturbed system around the invariant manifold; and then study the stability which allows one to determine the persistence of the invariant manifold under perturbation. The first two steps are relatively easy to do, but the last one is not trivial at all because the coefficient matrix of the linearized system will depend heavily on t.

Mainly there are two approaches for checking normal hyperbolicity in the last step, and essentially they are equivalent. One is to calculate so-called Lyapunov type numbers γ_L and σ_L. This is the key of the Fenichel's geometric singular perturbation theory [21], which is

the consequence of his previous work on the invariant manifold theorem in [18, 19, 20]. Fenichel proved that if $\gamma_L < 1$ and $\sigma_L < 1$, then the invariant manifold is persistent under perturbation. The second one is to study the exponential dichotomy, see [60, 9]. If the coefficient matrix of the linearized system has uniform exponential dichotomy, then the invariant manifold is persistent.

The application of singular perturbation technique to chemical reaction was introduced by Roussel and Fraser in [57]. Mathematically it involves mainly in the invariant manifold theorem and system reduction.

In this thesis, we will mainly consider the Belousov-Zhabotinsky(BZ) reaction given by a reversible Lotka-Volterra(LV) model

$$A + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X, \qquad X + Y \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2Y, \qquad Y \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} B.$$
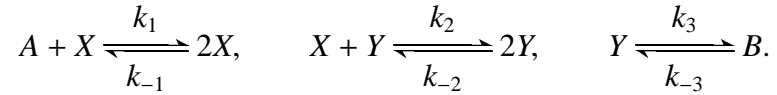
where k_{-1}, k_{-2}, k_{-3} are reverse reaction rates and k_1, k_2, k_3 are forward reaction rates. Note that if all the reverse reaction rates are equal to zero, then we will have the standard LV system of irreversible reaction considered in [45]. By an appropriate rescaling and the assumption that the reverse reaction is much slower than the forward reaction, then we will have a three-dimensional LV system with two small parameters of different order. It results in a singularly perturbed system.

$$\begin{cases} \dfrac{du}{d\tau} & = \ u(w - v) - \varepsilon(\sigma u^2 - v^2) \\ \dfrac{dv}{d\tau} & = \ v(u - 1) - \varepsilon v^2 + \varepsilon\left(\xi - u - v - \frac{w}{\sigma}\right) \\ \dfrac{dw}{d\tau} & = \ -\sigma(wu - \varepsilon\sigma u^2), \end{cases}$$

Note that the unperturbed system, where $\sigma = \varepsilon = 0$, is a standard Lotka-Volterra system and admits a first integral. Thus it is a conserved system.

It is important to notice that σ introduce a singular perturbation, and the partially perturbed system, where $\varepsilon = 0, \sigma > 0$, connects the periodic orbits in different levels of unperturbed system in certain way. In addition, it has an invariant manifold W_σ which serves as the oscillation axis. However W_σ is not normally hyperbolic by the computation

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of Lyapunov type number $\sigma_L \geq 2$, thus it is not ensured that W_σ can persist under any smooth perturbation.

Furthermore, the reaction zone of the perturbed system, where $\varepsilon > 0$, consists of two zones, oscillation zone and transition zone. In the oscillation zone, ε produces a regular perturbation. Because $\sigma_L \geq 2$ for W_σ, the existence of the invariant manifold $W_{\sigma,\varepsilon}^o$ cannot be obtained directly from the persistence of W_σ by Fenichel's theorem. Nevertheless, the existence of $W_{\sigma,\varepsilon}^o$ under the specific perturbation we study is true and it can be proven, instead, by means of exponential dichotomy, which is an important technique to study the invariant manifold in a singularly perturbed system [61] and integral manifold and its stability [79, 80], etc.. While in the transition zone, ε produces a singular perturbation. By Fenichel's geometric singular perturbation theory, we prove that there exists a two-dimensional strongly stable manifold $M_{\sigma,\varepsilon}^t$ in there. And there is also a one-dimensional stable manifold $W_{\sigma,\varepsilon}^t$ on $M_{\sigma,\varepsilon}^t$. All the solutions away from $W_{\sigma,\varepsilon}^t$ will eventually approach $W_{\sigma,\varepsilon}^t$ in the monotonic way.

Due to the regular perturbation of ε in the oscillation zone, we can approximate the oscillation time by studying the partially perturbed system, and show that the total time spending in the oscillation zone is in the algebraic order of σ, which means the oscillation will last in a long but finite time. And in the transition zone, the time spending on the transition from the oscillation axis to the vicinity of the equilibrium is in the algebraic order of ε.

By computing the eigenvalues of the linearized system around the unique interior equilibrium point, we can show that all the eigenvalues are negative and real, thus this equilibrium point is stable but there can be no trace of oscillation near the equilibrium, as dictated by Onsager's reciprocal relations. Moreover, a Lyapunov function, the total free energy of the reaction system, can be constructed to show that the equilibrium point is a global attractor in the reaction zone. This is exactly what the second law of thermodynamics [24] states, that is, the free energy of a closed isothermal system decreases until it reaches its

minimum which corresponds to the equilibrium state of the system.

To study the damped oscillation, we study the action variable, the area of the enclosed region swept by a complete unperturbed oscillation, and prove that it is monotonically decreasing in time. Thus the reaction shows the damped oscillation around and shrinking to the oscillation axis. But considered in the framework of Hamiltonian system, the action variable is not monotone but oscillatory instead from the numerical simulation.

The reversible LV model in the open system yields a two-dimensional system with two parameters w and β. It is proved that the oscillation around equilibrium exists in a wide range of w, but does not when $w < \delta = \sigma\varepsilon$. Thus the open system exhibits the similar dynamical behavior to the closed system as w varying monotonically. Mathematically, the open reaction system is a two-dimensional approximation to the three-dimensional closed reaction system by treating slowly changing quantities as constant.

According to all the theoretical analysis and numerical simulation, the important observation of this reversible LV system is summarized and can be found in [43], where a mechanical analog to this chemical system is also provided by a mechanical system with time-dependent increasing damping. The analytical results matches the lab observation of BZ reaction. The reaction starts with the nonlinear oscillation of varying frequencies. After a long time, the oscillation disappears. And the reaction eventually approaches the equilibrium state.

At the end, we study the control of the BZ reaction. Chemical system is a complex system because the reaction mechanism is not well understood [73]. Model reference control has advantage of controlling unknown system(plant). It is composed of two processes, system identification and controller generation. Once the real plant is identified, the controller will be trained to drive the plant's output to follow the reference signal. So far model reference control(MRC) already has a wide application in engineering such as controlling robot's arm [26, 41], flight vehicles [37, 38, 39, 40, 68], mechanical oscillators [32], etc. Some applications of MRC to biological system like susceptible-infectious-recovered(SIR)

epidemic disease models are given in [6]. Here we apply MRC to the BZ reaction and successfully control the oscillation amplitude and eliminate the oscillation to have a monotonic reaction. This provides another example of application of MRC to a biological system.

The rest of this thesis will be arranged in the following way. First, we will introduce the BZ chemical reaction, its history, lab experiment and mathematical modeling in Chapter 2. Then we study the open reaction in Chapter 3. Chapter 4 accommodates a large paragraph of the analysis about closed reaction, which is carried out step by step from unperturbed system, partially perturbed system to the perturbed system. And the damped oscillation is considered in terms of action-action-angle variables to complete this chapter. Chapter 5 is about the model reference control of the BZ closed reaction with numerical simulation provided.

CHAPTER II

BELOUSOV-ZHABOTINSKY CHEMICAL REACTION

2.1   History of BZ Reaction

The oscillating chemical reaction was first discovered by Fechner in 1828 and some related work followed throughout the nineteenth century. However, because of the lack of mathematical tools for analysis on such systems, and the wrong understanding during that time that chemical oscillation is not allowed due to the second law of thermodynamics, oscillating reaction was not recognized in the science community.

The modern study on the chemical oscillation was started by Russian chemist Boris Belousov. Belousov finished his chemical education in Zurich. After the World War I began, he returned to Russia and served in a military laboratory. Little is known about how he started the research and discovered the chemical reaction in the lab. In 1951, when he already retired from the army, he wrote a paper about the temporal oscillation he discovered. But his paper was rejected for publication in some journals, and even with a comment that his "supposedly discovered discovery was impossible", see page 161 in [78]. Years later, his paper finally was published in a conference on radiobiology 1958. His original manuscript in English translation can be found in the Appendix in [22].

In the middle of 1950's, a young biochemist, S.E. Shnoll, who was interested in periodic behavior in biochemistry, learned about Belousov's work. He got Belousov's original recipe of oscillating reaction and suggested a graduate student, A.M. Zhabotinsky, in Moscow State University to look into this reaction in 1961. Zhabotinsky repeated and confirmed Belousov's oscillating reaction. After an international meeting held in Prague in 1968, where Zhabotinsky presented some results on this interesting phenomenon, BZ reaction inspired the interest of chemical experimentalists and theoreticians. Since then, the

biological and biochemical oscillation becomes a widely studied subject and BZ reaction is regarded as a standard model of oscillating chemical reaction.

In 1980, ten years after Belousov passed away, Belousov and Zhabotinsky were awarded the Lenin Prize, the highest medal in the Soviet Union, for their pioneering work in the chemical oscillation. A detailed history about the BZ reaction can be found in [77].

2.2   Lab Experiment of BZ reaction

Belousov's original recipe of oscillating reaction is as follows

Citric acid,	2.00g,
$Ce(SO_4)_2$,	0.16g,
$KBrO_3$,	0.20g,
$H_2SO_4(1:3)$,	2.0ml,
H_2O,	to a total volume of 10.0ml.

When all the reagents above are well mixed at the room temperature, there will be several quick color change from yellow to colorless and back. As a matter of fact, Ce^{4+} shows yellow and Ce^{3+} colorless. Oxidized by bromate, Ce^{3+} is changed to Ce^{4+}, and then Ce^{4+} is reduced to Ce^{3+}. This oxidation-reduction process repeats and thus the solution color changes from yellow to colorless, back and forth.

2.3   Mathematical Modeling of BZ Reaction

The first theoretical study on oscillating chemical reaction is due to Alfred Lotka in his papers [45, 46]. Because at that time, no chemical reaction was known to follow Lotka's rule, his model was not widely recognized in the chemistry community. However, ecologist did benefit a lot from his idea. Motivated by Lotka's idea, Vito Volterra successfully studied a variety of ecological problems where the oscillation occurs. Because of the great contribution of Lotka and Volterra, the oscillating model of this type is cited as Lotka-Voltera

model, which is already the standard model widely studied by many scientists and mathematicians. Takaguchi even wrote a book [64] mainly to study the global dynamics of this model.

Besides Lotka-Volterra model, there are many other different models for BZ reaction, for example, Field-Körös-Noyes model. The detailed discussion about it can be found in [49]. In this thesis, we mainly consider the Lotka-Volterra model.

The standard Lotka-Volterra reaction system consists of four chemical species A, B, X and Y and three irreversible steps given by

$$A + X \xrightarrow{k_1} 2X$$
$$X + Y \xrightarrow{k_2} 2Y$$
$$Y \xrightarrow{k_3} B,$$
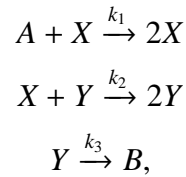
where k_i is the reaction rate in each step. Because each step is irreversible, a system of differential equations can be written as

$$\begin{cases} \dot{x} &= k_1 c_A x - k_2 xy \\ \dot{y} &= k_2 xy - k_3 y \end{cases} \tag{1}$$

where x, y, c_A and c_B denote the concentration of the corresponding species X, Y, A and B.

Note that if we consider a reaction in an open system, that is, the reaction system allows exchange of energy and/or matter with the environment, then by adding A to keep it constant, system (1) will have periodic oscillation for any given initial condition (x_0, y_0) with $x_0, y_0 > 0$. And the period of the oscillation varies and depends on the initial conditions. In contrast, if the reaction is in a closed system, then obviously c_A will be decreasing and satisfy equation

$$\dot{c}_A = -k_1 c_A x.$$

In section 4.3, we will see that the reaction in a closed system will oscillate when it is away from the equilibrium, and eventually approach the equilibrium in the monotonic way.

On the other hand, if we assume that all the reactions are reversible, with backward

reaction rates k_{-i}, then we will have

$$A + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X, \qquad X + Y \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2Y, \qquad Y \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} B. \tag{2}$$
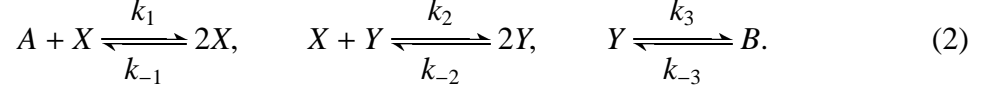
Similarly, the reversible Lotka-Volterra system in a closed system will be given by

$$\begin{cases} \dfrac{dx}{dt} &= k_1 c_A x - k_{-1} x^2 - k_2 xy + k_{-2} y^2, \\ \dfrac{dy}{dt} &= k_2 xy - k_{-2} y^2 - k_3 y + k_{-3} c_B, \\ \dfrac{dc_A}{dt} &= -k_1 c_A x + k_{-1} x^2, \\ \dfrac{dc_B}{dt} &= k_3 y - k_{-3} c_B. \end{cases} \tag{3}$$

For the sake of simplicity, under the following transformation,

$$u = \tfrac{k_2}{k_3} x, \qquad v = \tfrac{k_2}{k_3} y, \qquad w = \tfrac{k_1}{k_3} c_A, \qquad z = \tfrac{k_2}{k_3} c_B,$$

$$\tau = k_3 t, \qquad \varepsilon = \tfrac{k_{-1}}{k_1} = \tfrac{k_{-2}}{k_2} = \tfrac{k_{-3}}{k_3}, \qquad \sigma = \tfrac{k_1}{k_2}, \qquad \delta = \varepsilon \sigma \tag{4}$$

we will have an equivalent system in the dimensionless form

$$\begin{cases} \dfrac{du}{d\tau} &= u(w - v) - \varepsilon(\sigma u^2 - v^2) \\ \dfrac{dv}{d\tau} &= v(u - 1) - \varepsilon v^2 + \varepsilon z \\ \dfrac{dw}{d\tau} &= -\sigma(wu - \varepsilon \sigma u^2), \\ \dfrac{dz}{d\tau} &= v - \varepsilon z. \end{cases} \tag{5}$$

In addition, if we assume that the first forward reaction is much slower than the second one, and all the reverse reactions are even much slower than the corresponding forward reactions, then we have $0 < \varepsilon \ll \sigma \ll 1$. By the law of mass action, $u + v + \frac{w}{\sigma} + z$ is conservative. Let $\xi = u + v + \frac{w}{\sigma} + z$, then system (5) is reduced into a 3D system

$$\begin{cases} \dfrac{du}{d\tau} &= u(w - v) - \varepsilon(\sigma u^2 - v^2) \\ \dfrac{dv}{d\tau} &= v(u - 1) - \varepsilon v^2 + \varepsilon \left(\xi - u - v - \tfrac{w}{\sigma}\right) \\ \dfrac{dw}{d\tau} &= -\sigma(wu - \varepsilon \sigma u^2). \end{cases}$$

In the case of open system in which A and B can be kept constant by the experimenter by providing chemical energy, the reaction is given by

$$\begin{cases} \dfrac{dx}{dt} &= k_1 c_A x - k_{-1} x^2 - k_2 xy + k_{-2} y^2, \\ \dfrac{dy}{dt} &= k_2 xy - k_{-2} y^2 - k_3 y + k_{-3} c_B, \end{cases} \tag{6}$$

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and its dimensionless form is

$$
\begin{cases}
\dfrac{du}{d\tau} &= u(w - v) - \varepsilon(\sigma u^2 - v^2) \\
\dfrac{dv}{d\tau} &= v(u - 1) - \varepsilon v^2 + \beta
\end{cases}.
$$

where w and $\beta = \varepsilon z$ are treated as parameters.

In the following chapters, we will first study the 2D reversible Lotka-Volterra reaction in an open system, and then analyze in details the 3D reversible LV reaction in a closed system.

CHAPTER III

REVERSIBLE LV REACTIONS IN AN OPEN SYSTEM

In this section, we will consider the reversible BZ reaction (2) in an open chemical system, that is, a system that can exchange matter and/or energy with its surroundings, see [16]. Suppose that species A and B in system (2) are being controlled by an experimenter at constant level of c_A and c_B, by providing chemical energy, then only the concentrations of species X and Y are dynamic, and satisfy equation (6)

$$\begin{cases} \dfrac{dx}{dt} &= k_1 c_A x - k_{-1} x^2 - k_2 xy + k_{-2} y^2, \\ \dfrac{dy}{dt} &= k_2 xy - k_{-2} y^2 - k_3 y + k_{-3} c_B. \end{cases}$$

Such a reaction is called *driven*. The amount of energy for every A molecule becoming B molecule is the difference between μ_A and μ_B:

$$\Delta \mu_{AB} = \mu_A - \mu_B = \ln \left(\frac{k_1 k_2 k_3 c_A}{k_{-1} k_{-2} k_{-3} c_B} \right) \tag{7}$$

and the driving force for the chemical reaction system is given by

$$\gamma = e^{\Delta \mu_{AB}} = \frac{k_1 k_2 k_3 c_A}{k_{-1} k_{-2} k_{-3} c_B} = \frac{w}{\varepsilon \delta \beta} \tag{8}$$

in the representation of dimensionless form. Under the rescaling in (4) with $\beta = \varepsilon(\xi - u - v - \frac{w}{\sigma})$, we will have the following dimensionless system of driven reversible reaction

$$\begin{cases} \dot{u} &= u(w - v) - \delta u^2 + \varepsilon v^2 \\ \dot{v} &= v(u - 1) - \varepsilon v^2 + \beta. \end{cases} \tag{9}$$

Mathematically, system (9) can also be regarded as a two-dimensional approximation of 3D closed system to some extent. Note that this is not the usual approximation by letting small parameter $\sigma = 0$, but by treating β and w as constant, instead. This makes sense

because both w and β are slow variables. It is obvious for w, and also for β by setting $\beta = \varepsilon z$ and resulting in $\dot{\beta} = \varepsilon(v - \beta)$ in (5). According to the analysis in the following sections, we can see that both open system and closed system exhibit the similar dynamical transition from oscillation to non-oscillation as w is varying.

From the following argument, we see that reversible driven LV system (9) behaves significantly different from the traditional LV system.

Theorem 3.0.1. *For any $w, \beta > 0$, system (9) has a unique positive equilibrium $(\bar{u}, \bar{v})$, and it is asymptotically stable.*

<u>Proof:</u> Note that the positive equilibrium point, $(\bar{u}, \bar{v})$, satisfies

$$v = f(u) = \frac{(u-1) + \sqrt{(u-1)^2 + 4\beta\varepsilon}}{2\varepsilon}, \qquad v = g(u) = -\delta u^2 + wu + \beta.$$

Because $f(u)$ is increasing in u, $-g$ is convex with $\lim\limits_{u \to \infty} -g(u) = \infty$ and

$$f(0) = \frac{-1 + \sqrt{1 + 4\beta\varepsilon}}{2\varepsilon} = \frac{2\beta}{1 + \sqrt{1 + 4\beta\varepsilon}} < \beta = g(0),$$

we know that the two curves determined by $v = f(u)$ and $v = g(u)$ intersect at only one point for $u \geq 0$, that is, $(\bar{u}, \bar{v})$ is unique.

The Jacobi matrix of system (9) is

$$J = \begin{bmatrix} w - \bar{v} - 2\delta\bar{u} & 2\varepsilon\bar{v} - \bar{u} \\ \bar{v} & \bar{u} - 1 - 2\varepsilon\bar{v} \end{bmatrix} = \begin{bmatrix} -\delta\bar{u} - \dfrac{\varepsilon\bar{v}^2}{\bar{u}} & 2\varepsilon\bar{v} - \bar{u} \\ \bar{v} & -\varepsilon\bar{v} - \dfrac{\beta}{\bar{v}} \end{bmatrix}$$

and

$$\begin{aligned}
\mathrm{tr}(J) &= -\delta\bar{u} - \frac{\varepsilon\bar{v}^2}{\bar{u}} - \varepsilon\bar{v} - \frac{\beta}{\bar{v}}, \\
\det(J) &= \left(\delta\bar{u} + \frac{\varepsilon\bar{v}^2}{\bar{u}}\right)\left(\varepsilon\bar{v} + \frac{\beta}{\bar{v}}\right) - \bar{v}(2\varepsilon\bar{v} - \bar{u}), \\
\Delta = \mathrm{tr}^2 - 4\det &= [(w - \bar{v} - 2\delta\bar{u}) - (\bar{u} - 1 - 2\varepsilon\bar{v})]^2 + 4\bar{v}(2\varepsilon\bar{v} - \bar{u}) \\
&= \left[\left(\delta\bar{u} + \frac{\varepsilon\bar{v}^2}{\bar{u}}\right) - \left(\varepsilon\bar{v} + \frac{\beta}{\bar{v}}\right)\right]^2 + 4\bar{v}(2\varepsilon\bar{v} - \bar{u})
\end{aligned}$$

Obviously the trace $\mathrm{tr}(J) < 0$. And since

$$\det(J) = \left(\delta\bar{u} + \frac{\varepsilon\bar{v}^2}{\bar{u}}\right)\frac{\beta}{\bar{v}} + \varepsilon\delta\bar{u}\bar{v} + \frac{\varepsilon^2\bar{v}^3}{\bar{u}} - \bar{v}(2\varepsilon\bar{v} - \bar{u})$$

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and

$$\frac{\varepsilon^2 \bar{v}^3}{\bar{u}} - \bar{v}(2\varepsilon\bar{v} - \bar{u}) = \frac{\bar{v}}{\bar{u}}\left(\varepsilon^2 \bar{v}^2 + \bar{u}^2 - 2\varepsilon\bar{u}\bar{v}\right) = \frac{\bar{v}}{\bar{u}}(\varepsilon\bar{v} - \bar{u})^2 \geq 0,$$

we can see that the determinant $\det(J) > 0$. Therefore the equilibrium $(\bar{u}, \bar{v})$ must be asymptotically stable, and it is a stable node if the discriminant $\Delta > 0$ and a stable spiral point if $\Delta < 0$. And $\Delta = 0$ provides the critical values for transition from a node to a spiral point.

Lemma 3.0.2. *The following statements are equivalent.*

$$\bar{v} = (<, >)\beta \iff \bar{u} = (>, <)\frac{w}{\delta} \iff \gamma = \frac{w}{\varepsilon\delta\beta} = (<, >)1.$$

<u>Proof:</u> Note that $\gamma = \frac{w}{\varepsilon\delta\beta}$ in terms of new variables (β, w). If $\bar{v} = \beta$, then $\bar{u} = 0$ or $\bar{u} = \frac{w}{\delta}$. As $\bar{u} = 0, \beta = \bar{v} = f(\bar{u}) = f(0) < \beta$ is a contradiction. Thus $\bar{u} = \frac{w}{\delta}$, and then

$$\beta = f(\frac{w}{\delta}) = \frac{(\frac{w}{\delta} - 1) + \sqrt{(\frac{w}{\delta} - 1)^2 + 4\beta\varepsilon}}{2\varepsilon} \implies w = \varepsilon\delta\beta \implies \gamma = 1.$$

Similarly, if $\bar{v} = g(\bar{u}) < \beta$, then $\bar{u} > \frac{w}{\delta}$ and

$$\beta > \bar{v} = f(\bar{u}) > f(\frac{w}{\delta}) = \frac{(\frac{w}{\delta} - 1) + \sqrt{(\frac{w}{\delta} - 1)^2 + 4\beta\varepsilon}}{2\varepsilon} \implies w < \varepsilon\delta\beta.$$

This completes the proof because all the above derivations are revertible.

Lemma 3.0.3. *If $w \leq \varepsilon\delta\beta$, the $\Delta > 0$.*

<u>Proof:</u> Note that the discriminant

$$\Delta = [(w - \bar{v} - 2\delta\bar{u}) - (\bar{u} - 1 - 2\varepsilon\bar{v})]^2 + 4\bar{v}(2\varepsilon\bar{v} - \bar{u})$$

Since $w \leq \varepsilon\delta\beta$ is equivalent to $\bar{v} \leq \beta$, then

$$\bar{u} = \varepsilon\bar{v} - \frac{\beta}{\bar{v}} + 1 \leq \varepsilon\bar{v} < 2\varepsilon\bar{v},$$

which implies that $\Delta > 0$. $\qquad\qquad\square$

Theorem 3.0.4. *Let D be the domain where the discriminant is nonpositive, that is,*

$$D(\beta, w) = \{(\beta, w), \quad \beta, w \geq 0 \quad and \quad \Delta(\beta, w) \leq 0\}.$$

Then D is bounded and $\frac{\delta}{2} < \min_{D} w < \frac{\delta}{1 + \delta}$.

Proof: Set

$$v_* = \frac{2w}{1 + 4\varepsilon\delta}, \qquad u_* = 2\varepsilon v_*.$$

Claim that $v_* > (=, <)f(u_*)$ if and only if $\beta < (=, >)v_*(1 - \varepsilon v_*)$. Because f is monotone and its inverse $f^{-1}(v) = \varepsilon v - \frac{\beta}{v} + 1$, we have

$$v_* > f(u_*) \iff 2\varepsilon v_* = u_* < f^{-1}(v_*) = \varepsilon v_* - \frac{\beta}{v_*} + 1 \iff \beta < v_*(1 - \varepsilon v_*).$$

Similarly we can prove the rest of the claim. On the other hand, it follows from $u(w - v) - \delta u^2 + \varepsilon v^2 = 0$ that $\bar{u} \geq \frac{4\varepsilon w}{1+4\varepsilon\delta} = u_*$ because the existence of real roots infers that $u^2 - 4\varepsilon(wu - \delta u^2) \geq 0$, that is, u_* is the minimum of $\bar{u}$.

Note that the discriminant

$$\Delta = [(w - \bar{v} - 2\delta\bar{u}) - (\bar{u} - 1 - 2\varepsilon\bar{v})]^2 + 4\bar{v}(2\varepsilon\bar{v} - \bar{u})$$

and $\Delta \geq 0$ if $2\varepsilon\bar{v} - \bar{u} \geq 0$. As $\beta \geq v_*(1 - \varepsilon v_*)$,

$$\bar{v} = f(\bar{u}) \geq f(u_*) \geq v_* \geq \frac{1 + \sqrt{1 - 4\beta\varepsilon}}{2\varepsilon},$$

thus $\varepsilon\bar{v}^2 - \bar{v} + \beta \geq 0$, that is, $2\varepsilon\bar{v} - \bar{u} = \frac{1}{\bar{v}}(\varepsilon\bar{v}^2 - \bar{v} + \beta) \geq 0$ and consequently $\Delta \geq 0$. This shows that

$$D \subset U = \{(\beta, w), \quad 0 \leq \beta \leq v_*(1 - \varepsilon v_*)\} \subset [0, \frac{1}{4\varepsilon}] \times [0, \frac{1}{2\varepsilon} + 2\delta]$$

which is bounded.

In addition, if $\beta = 0$ and $w = \frac{\delta}{1+\delta}$, then $\bar{u} = \frac{w}{\delta}$ and $\bar{v} = 0$ and hence $\Delta = 0$. Moreover, if $(\beta, w) \in D$, then $\beta \leq v_*(1 - \varepsilon v_*)$. From Lemmas 3.0.2 and 3.0.3 it follows that if $(\beta, w) \in D$, then $w > \varepsilon\delta\beta$ or equivalently $\bar{u} \leq \frac{w}{\delta}$. When $w \leq \frac{\delta}{2}$, we know $\beta \leq \delta$. Hence

$$\bar{u} \leq \frac{1}{2}, \qquad \bar{v} \leq v_{\max} = g(\frac{w}{2\delta}) = \frac{w^2}{4\delta} + \beta \leq 2\delta$$

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and

$$\Delta = [(1 + w) - (1 + 2\delta)\bar{u} - (1 - 2\varepsilon)\bar{v}]^2 + 4\bar{v}(2\varepsilon\bar{v} - \bar{u}) > 0.$$

Thus it follows immediately that $\dfrac{\delta}{2} \leq \min_{D} w \leq \dfrac{\delta}{1 + \delta}$. $\qquad\qquad\square$

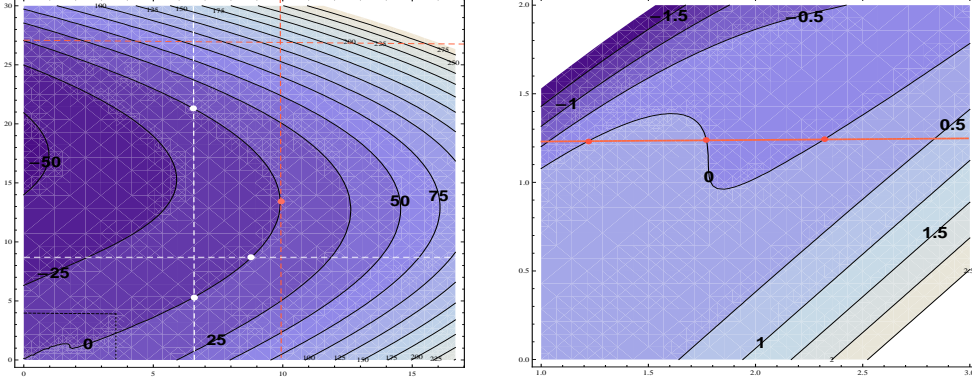The contour plot of the discriminant is given in Figure 1.

Figure 1: Contour Plots(and zoomed in) of the discriminant against (β, w).

Theorem 3.0.5. *Set*

$$\gamma_c = \min_{(\beta, w) \in D} \left\{ \frac{w}{\varepsilon\delta\beta} \right\}.$$

Then γ_c is well defined. Suppose the minimum is attained at $(\beta_c, w_c) \in D$, then (β_c, w_c) satisfies $\Delta(\beta_c, w_c) = 0$ and the following equation

$$\frac{w}{\beta} = -\frac{\Delta_\beta}{\Delta_w} = -\frac{\Delta_w^e \left[(1 + 4\varepsilon\delta)(\bar{v} - \bar{u}) - (1 - 2\varepsilon)w\right] + 2(4\varepsilon\bar{v} - \bar{u})(w - 2\delta\bar{u}) - 4\varepsilon\bar{v}^2}{\Delta_w^e \left[-\bar{u}^2 + \bar{u}(1 + \bar{v} - w) + w - \bar{v}(1 - 2\varepsilon w)\right] + 2\bar{v}(1 - 2\varepsilon\bar{v})}. \qquad (10)$$

where $\Delta_w^e = w - \bar{v} - 2\delta\bar{u} - \bar{u} + 1 + 2\varepsilon\bar{v}$. Furthermore, $\gamma_c \sim \frac{1}{2\varepsilon\delta}$.

<u>Proof:</u> From the fact that D is bounded and $\min_{D} w > 0$, we know that if $(\beta, w) \in D$, then $\frac{w}{\varepsilon\delta\beta} > 0$ and $\inf_{D} \dfrac{w}{\varepsilon\delta\beta}$ exists. And since D is closed, inf can be replaced by min and then

$$\gamma_c = \min_{(\beta, w) \in D} \left\{ \frac{w}{\varepsilon\delta\beta} \right\} > 0$$

is well defined. Note that

$$\min_{(\beta, w) \in U} \left\{ \frac{w}{\beta} \right\} \geq \min_{w \in [0, \frac{1}{2\varepsilon} + 2\delta]} \frac{w}{v_*(1 - \varepsilon v_*)} = \min_{w \in [0, \frac{1}{2\varepsilon} + 2\delta]} \frac{1 + 4\varepsilon\delta}{2(1 - \frac{2\varepsilon w}{1 + 4\varepsilon\delta})} = \frac{1}{2} + 2\varepsilon\delta,$$

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thus

$$\gamma_c = \min_{(\beta,w)\in D} \left\{ \frac{w}{\varepsilon\delta\beta} \right\} \geq \min_{(\beta,w)\in U} \left\{ \frac{w}{\varepsilon\delta\beta} \right\} \geq 2 + \frac{1}{2\varepsilon\delta}.$$

On the other hand, when $(\bar{u}, \bar{v}) = (u_*, v_*)$, $\beta = v_*(1 - \varepsilon v_*)$ and $\Delta = (w - 1)^2$. Therefore if $w = 1$ and $\beta = \frac{2(1-2\varepsilon+4\varepsilon\delta)}{(1+4\varepsilon\delta)^2}$, $\Delta = 0$, that is $(\frac{2(1-2\varepsilon+4\varepsilon\delta)}{(1+4\varepsilon\delta)^2}, 1) \in D$. Thus

$$\gamma_c \leq \frac{1}{\frac{2(1-2\varepsilon+4\varepsilon\delta)\varepsilon\delta}{(1+4\varepsilon\delta)^2}} = \frac{(1 + 4\varepsilon\delta)^2}{2\varepsilon\delta(1 - 2\varepsilon + 4\varepsilon\delta)} \leq 2 + \frac{2}{\delta} + \frac{1}{2\varepsilon\delta}.$$

And from geometric viewpoint, it is obvious that if γ_c is attained at $(\beta_c, w_c) \in D$, then (β_c, w_c) solves $\Delta = 0$ and satisfies

$$\frac{w}{\beta} = -\frac{\Delta_\beta}{\Delta_w},$$

which provides an exact expression for the switching point γ_c. $\quad\square$

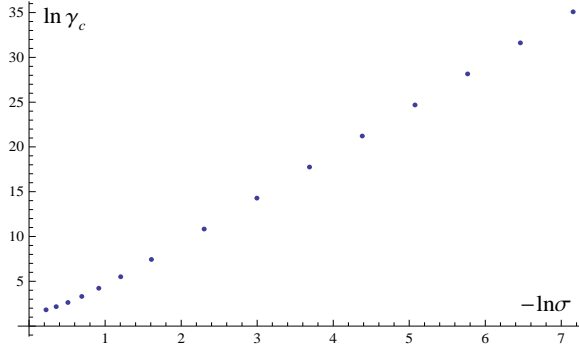The dependence of γ_c on σ is given in Figure 2.

Figure 2: Log-Log plot of the critical driving force against parameter σ.

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CHAPTER IV

REVERSIBLE LV REACTION IN A CLOSED SYSTEM

4.1 Overview of the 3D LV system

As shown in the introduction, the closed reaction system is given by a three dimensional Lotka-Volterra system

$$
\begin{cases}
\dfrac{du}{d\tau} &= u(w - v) - \varepsilon(\sigma u^2 - v^2) \\
\dfrac{dv}{d\tau} &= v(u - 1) - \varepsilon v^2 + \varepsilon\left(\frac{\xi}{\sigma} - u - v - \frac{w}{\sigma}\right) \\
\dfrac{dw}{d\tau} &= -\sigma(wu - \varepsilon\sigma u^2).
\end{cases}
\tag{11}
$$

In this section, we will first take an overview on this system for some general properties like invariance and global stability.

4.1.1 Positively Invariant Set.

To study the closed BZ chemical reaction, we propose a mathematical model in terms of the 3D reversible Lotka-Volterra system (11) where each state variable represents the concentration of corresponding chemical reactant. Before any further detailed analysis on this system, we must ensure that this system is properly chosen in the sense that each variable remains positive during the time evolution. In this section, we will find, in the first octant, an invariant set under the flow induced by system (11) and then we can see that all the variables remain positive if they start at a positive initial point.

Definition 4.1.1. *Consider a vector field $V(x)$ on $\mathbb{R}^n$. The set $\mathcal{I}$ is called flow-invariant for V if all the trajectories $x(t)$ of $\dot{x} = V(x)$ meeting $\mathcal{I}$ at t_0 will remain in $\mathcal{I}$ for $t > t_0$. That is, if $x(t_0) \in \mathcal{I}$, then $x(t) \in \mathcal{I}$ for $t > t_0$.*

There are several different versions about the invariant set theorem due to La'Salle [63], Bony [4], Brezis [5] and so on. La'Salle's invariant set theorem mainly deals with

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stability by constructing a Lyapunov function, but it is only about the local invariance. Bony and Brezis' theorems are more geometric and they are deeply connected, see [55] for the detailed discussion between these two theorems. Here we will use the one due to Bony.

Definition 4.1.2. *Let $x \in I$ and $B(x')$ be an open ball centered at x' such that $x \in \partial B(x')$ and $B(x') \cap I = \emptyset$. Then the vector $\vec{v}(x) = x' - x$ is called normal to I at x in the sense of Bony.*

Theorem 4.1.3. *[4]. Let $V(x)$ be a vector field in $\mathbb{R}^n$ and $I \subset \mathbb{R}^n$ such that*

   1. *For any $x, y \in I$, $|V(x) - V(y)| \le K|x - y|$, $K > 0$ is the Lipchitz constant;*

   2. *$\vec{v}(x) \cdot V(x) \le 0$ if $\vec{v}(x)$ is normal to I.*

Then I is flow-invariant for V.

Theorem 4.1.4. *For any fixed $\xi > 0$, let $\mathcal{T}$ be the tetrahedron defined by*

$$\mathcal{T} = \left\{ (u, v, w) \in \mathbb{R}^3, u, v, w > 0, \text{ and } u + v + \frac{w}{\sigma} \le \xi \right\}.$$

Then $\mathcal{T}$ is positively invariant under the flow induced by equation (11).

<u>Proof:</u> Let $\partial \mathcal{T}$ be the boundary surface of $\mathcal{T}$, then $\partial \mathcal{T} = S_1 \cup S_2 \cup S_3 \cup S_4$, where

$$S_1 = \{(u, v, w) \in \mathcal{T}, \ u = 0\}, \quad S_2 = \{(u, v, w) \in \mathcal{T}, \ v = 0\},$$
$$S_3 = \{(u, v, w) \in \mathcal{T}, \ w = 0\}, \quad S_4 = \left\{(u, v, w) \in \mathcal{T}, \ u + v + \frac{w}{\sigma} = \xi\right\}.$$

Denote by $V(X)$ the vector field on the right side of equation (11) with $X = (u, v, w)$, and by $\vec{n}$ the regular outer normal vector to $\partial \mathcal{T}$ (perpendicular to $\partial \mathcal{T}$). Then

$$
\begin{aligned}
V(X) \cdot \vec{n}_1 &= -\varepsilon v^2 \le 0, & \vec{n}_1 &= (-1, 0, 0)^T, & \text{on} \quad S_1, \\
V(X) \cdot \vec{n}_2 &= -\varepsilon(\xi - u - \tfrac{w}{\sigma}) \le 0, & \vec{n}_2 &= (0, -1, 0)^T, & \text{on} \quad S_2, \\
V(X) \cdot \vec{n}_3 &= -\varepsilon \sigma^2 u^2 \le 0, & \vec{n}_3 &= (0, 0, -1)^T, & \text{on} \quad S_3, \\
V(X) \cdot \vec{n}_4 &= -v \le 0, & \vec{n}_4 &= (1, 1, \tfrac{1}{\sigma})^T, & \text{on} \quad S_4.
\end{aligned}
$$

Note that $\vec{n}$ is also the normal vector to $\mathcal{T}$ in the sense of Bony because $\mathcal{T}$ is convex. Therefore it follows, from Bony's flow-invariant set theorem, that $\mathcal{T}$ is a positively invariant set under the flow induced by equation (11). □

We will call $\mathcal{T}$ the *reaction zone* in the closed system (11), over which all the analysis is carried on in the rest of the paper.

4.1.2   Dissipative Dynamics.

Because System (11) allows a positively invariant set $\mathcal{T}$ which is compact, there must exist at least one equilibrium point P in $\mathcal{T}$. And if P is asymptotically stable, the system may be dissipative. In this section, we will prove the dissipative dynamics by finding the unique interior equilibrium point and its global stability in $\mathcal{T}$.

First we will recall some useful results on the sufficient conditions for all the roots of a polynomial to be real and negative and the estimate of the eigenvalues.

Theorem 4.1.5. *[30, 33]. The real parts of all roots of the polynomial*

$$p(x) = x^3 + a_2 x^2 + a_1 x + a_0 = 0$$

are negative if and only if

$$a_2 > 0, \qquad a_2 a_1 - a_0 > 0, \qquad a_0(a_2 a_1 - a_0) > 0.$$

Theorem 4.1.6. *[42]. Let $p(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0$ be a polynomial of degree $n \geq 2$ with positive coefficients $a_i > 0$. If*

$$a_i^2 - 4a_{i-1}a_{i+1} > 0, \qquad i = 1, 2, \ldots, n-1,$$

then all the roots of the polynomial $p(x)$ are real and distinct. See [42].

Let $A = \left(a_{ij}\right)$ be a square complex matrix. Around every element a_{ii} on the diagonal of the matrix, we draw a circle with radius equal to the sum of the norms of the other elements on the same row, $r_i = \sum\limits_{j \neq i} |a_{ij}|$, or on the same column, $c_i = \sum\limits_{j \neq i} |a_{ji}|$. Such disks are called Gershgorin's disks.

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Theorem 4.1.7. *[31]. For any square matrix A, every eigenvalue of A must lie in one of Gershgorin's disks.*

Now we are ready to prove a main result.

Theorem 4.1.8. *System (11) has a unique interior equilibrium point*

$$P_3 = \left(\frac{\varepsilon^2 \xi}{r(\varepsilon)}, \frac{\varepsilon \xi}{r(\varepsilon)}, \frac{\sigma \varepsilon^3 \xi}{r(\varepsilon)} \right) \in \mathcal{T}, \qquad r(\varepsilon) = 1 + \varepsilon + \varepsilon^2 + \varepsilon^3.$$

And the Jacobian $J(P_3)$ at P_3 has three negative real eigenvalues satisfying

$$|\lambda_1 + (1 + \varepsilon)| \sim \varepsilon^2, \qquad |\lambda_2 + \varepsilon \xi| \sim \varepsilon^2, \qquad \left| \lambda_3 + \sigma \varepsilon^2 \xi \right| \sim \sigma^2 \varepsilon^3,$$

and hence P_3 is an asymptotically stable node,

Proof: It follows from the simple calculation that system (11) has three equilibrium points

$$P_1 = (0, 0, \sigma \xi), \qquad P_2 = (\frac{\xi}{1 + \varepsilon}, 0, \frac{\sigma \varepsilon \xi}{1 + \varepsilon}), \qquad P_3 = \frac{\varepsilon \xi}{r(\varepsilon)} \left(\varepsilon, 1, \sigma \varepsilon^2 \right).$$

Note that P_1 and P_2 are on the boundary $\partial \mathcal{T}$, and only P_3 is in the interior of $\mathcal{T}$. First we will consider the Jacobi matrix at P_3,

$$J(P_3) = \frac{1}{r(\varepsilon)} \begin{pmatrix} -\varepsilon(1 + \sigma \varepsilon^2)\xi & \varepsilon^2 \xi & \varepsilon^2 \xi \\ -\varepsilon r(\varepsilon) + \varepsilon \xi & -(1 + \varepsilon)r(\varepsilon) - \varepsilon^2 \xi & -\dfrac{\varepsilon r(\varepsilon)}{\sigma} \\ \sigma^2 \varepsilon^3 \xi & 0 & -\sigma \varepsilon^2 \xi \end{pmatrix}$$

whose characteristic polynomial is $P(\lambda) = \lambda^3 + a_2 \lambda^2 + a_1 \lambda + a_0$, where

$$a_2 = \frac{1}{r(\varepsilon)}(1 + \varepsilon)[r(\varepsilon) + \varepsilon(1 + \sigma \varepsilon)\xi] > 0, \qquad a_0 = \frac{1}{r(\varepsilon)}\sigma \varepsilon^3 \xi^2 > 0,$$

$$a_1 = \frac{1}{r(\varepsilon)}[r(\varepsilon) - 1 + \sigma \varepsilon(r(\varepsilon) - 1) + \sigma \varepsilon^3)]\xi + \frac{\sigma \varepsilon^2}{r^2(\varepsilon)}(r(\varepsilon) - 1)\xi^2 > 0.$$

Because, for $\varepsilon \ll \sigma$ sufficiently small, $a_2 \sim 1$, $a_1 \sim \varepsilon \xi$ and $a_0 \sim \sigma \varepsilon^3 \xi^2$, we have

$$a_2 > 0, \qquad a_2 a_1 - a_0 > 0, \qquad a_0(a_2 a_1 - a_0) > 0.$$

Thus it follows from Routh-Hurwitz Theorem 4.1.5 that all the eigenvalues of $J(P_3)$ have negative real parts. In addition, since $a_0, a_1, a_2 > 0$ and

$$a_2^2 - 4a_1 a_0 > 0, \qquad a_2 - 4a_1 > 0,$$

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Kurtz's Theorem [42] implies that all the eigenvalues $J(P_3)$ are real. And consequently P_3 is an asymptotically stable node.

On the other hand, note that the diagonal entries of $A = J(P_3)$ are

$$a_{11} = -\varepsilon(1 + \sigma\varepsilon^2)\xi, \qquad a_{22} = -(1 + \varepsilon)r(\varepsilon) + \varepsilon^2\xi, \qquad a_{33} = -\sigma\varepsilon^2\xi$$

and the radii for the three Gershgorin's disks with center at a_{11}, a_{22} and a_{33} are

$$r_1 = 2\varepsilon^2\xi, \qquad r_2 = \frac{\varepsilon}{\sigma}r(\varepsilon) + \varepsilon|\xi - r(\varepsilon)|, \qquad r_3 = \sigma^2\varepsilon^3\xi.$$

respectively, by row, and

$$c_1 = \varepsilon|\xi - r(\varepsilon)| + \sigma^2\varepsilon^3\xi, \qquad c_2 = \varepsilon^2\xi, \qquad c_3 = \sigma^2\varepsilon^3\xi + \frac{\varepsilon}{\sigma}r(\varepsilon).$$

respectively, by column. Since the following three Gershgorin's disks

$$D_i = \{z, |z - a_{ii}| \le \min\{r_i, c_i\}\}, \qquad i = 1, 2, 3$$

are not overlapping, by Theorem 4.1.7, there must be exactly one eigenvalue in one disk. Thus we have the following estimate

$$|\lambda_1 + (1 + \varepsilon)| \sim \varepsilon^2, \qquad |\lambda_2 + \varepsilon\xi| \sim \varepsilon^2, \qquad \left|\lambda_3 + \sigma\varepsilon^2\xi\right| \sim \sigma^2\varepsilon^3.$$

And the associated eigenvectors are approximately given by

$$\vec{v}_1 \sim \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \qquad \vec{v}_2 \sim \begin{bmatrix} 1 \\ (\xi - 1)\varepsilon \\ 0 \end{bmatrix}, \qquad \vec{v}_3 \sim \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

$\square$

Remark 4.1.9. *Theorem 4.1.8 indicates that when the reaction is close to the equilibrium state, the oscillatory behavior disappears. This is the usual phenomenon observed in most of the chemical experiments. Moreover, the three eigenvalues of $J(P_3)$ are all of different scales. By intuition, around P_3, the solution must be attracted to P_3 in the following way,*

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first along the direction of $\vec{v}_1$ (associated with the negatively largest eigenvalue λ_1), then of

$\vec{v}_2$ and finally of $\vec{v}_3$ (associated to the negatively smallest eigenvalue λ_3). This can be also

observed by asymptotic expansion around P_3 to have

$$\{(u, v, w), u = \varepsilon^2\xi, v = \varepsilon\xi, w = \sigma\varepsilon^3(\xi + Ce^{-\sigma\xi t})\},$$

as shown in Figure 3.
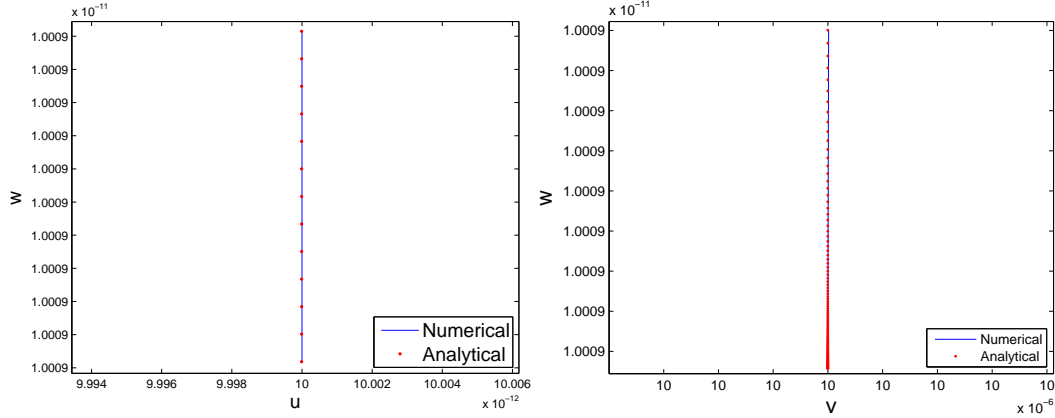
Figure 3: In the Vicinity of Equilibrium.

Furthermore, we will draw a stronger conclusion that P_3 is a global attractor in $\mathcal{T}$.

Set $z = \xi - u - v - \frac{w}{\sigma}$ and denote $\mathbb{R}^{4+} = \{(u, v, w, z) | u, v, w, z > 0\}$. Due to the invariance

of $\mathcal{T}$, we may consider the 4D version of system (11)

$$\dot{Y} = \tilde{V}(Y), \qquad Y \in \mathbb{R}^{4+},$$

where

$$Y = \begin{bmatrix} u \\ v \\ w \\ z \end{bmatrix}, \qquad \tilde{V}(Y) = \begin{bmatrix} wu - uv - \varepsilon(\sigma u^2 - v^2) \\ vu - v - \varepsilon\left(v^2 - z\right) \\ -\sigma(wu - \varepsilon\sigma u^2), \\ \mu v - \varepsilon z, \end{bmatrix},$$

Let $P_3 = (u^*, v^*, w^*)$ and $z^* = \xi - u^* - v^* - \frac{w^*}{\sigma}$. Define function

$$L(Y) = u \ln\left(\frac{u}{u^*}\right) + v \ln\left(\frac{v}{v^*}\right) + \frac{w}{\sigma} \ln\left(\frac{w}{w^*}\right) + z \ln\left(\frac{z}{z^*}\right).$$

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Lemma 4.1.10. *Under the side condition $Y \cdot \vec{n} = \xi$, where $\vec{n} = (1, 1, \frac{1}{\sigma}, 1)^T$, $L(Y) \geq 0$, and $L(Y) = 0$ if and only if $Y = Y^* = (u^*, v^*, w^*, z^*)$.*

<u>Proof:</u> Under the side condition $Y \cdot \vec{n} = \xi$ additionally, the Lagrange multiplier method reads

$$\nabla L(Y) = \lambda \vec{n},$$

or more explicitly

$$\ln\left(\frac{u}{u^*}\right) + 1 = \ln\left(\frac{v}{v^*}\right) + 1 = \ln\left(\frac{w}{w^*}\right) + 1 = \ln\left(\frac{z}{z^*}\right) + 1 = \lambda$$

which implies that

$$u = u^* e^{\lambda - 1}, \quad v = v^* e^{\lambda - 1}, \quad w = w^* e^{\sigma \lambda - 1}, \quad z = z^* e^{\lambda - 1}.$$

Thus we have $\lambda = 1$ and consequently

$$u = u^*, \quad v = v^*, \quad w = w^*, \quad z = z^*.$$

Note that $L(Y)$ is smooth in $\mathbb{R}^{4+}$, and its Hessian matrix $\nabla^2 L(Y) = diag\left\{\frac{1}{u}, \frac{1}{v}, \frac{1}{\sigma w}, \frac{1}{z}\right\}$ is positive definite, thus $L(Y)$ is convex on $\mathbb{R}^{4+}$ and it cannot attain the maximum in the interior. Therefore X^* must be the minimum and $L(Y) \geq L(Y^*) = 0$ for $Y \cdot \vec{n} = \xi$. $\qquad\square$

Lemma 4.1.11. *$L'(Y) \leq 0$ for all $Y \in \mathbb{R}^{4+}$ and under the constraint $Y \cdot \vec{n} = \xi$, $L'(Y) = 0$ if and only if $Y = Y^*$.*

<u>Proof:</u> It is easy to calculate that

$$
\begin{aligned}
L'(Y) &= \nabla L(Y) \cdot \dot{Y} = \nabla L(Y) \cdot \tilde{V}(Y) \\
&= \left[\ln\left(\frac{u}{u^*}\right) + 1\right]\left[u(w - v) - \varepsilon(\sigma u^2 - v^2)\right] + \left[\ln\left(\frac{v}{v^*}\right) + 1\right]\left[vu - \mu v - \varepsilon(v^2 - \mu z)\right] \\
&\quad + \frac{1}{\sigma}\left[\ln\left(\frac{w}{w^*}\right) + 1\right]\left[-\sigma(wu - \varepsilon\sigma u^2)\right] + \left[\ln\left(\frac{z}{z^*}\right) + 1\right]\left[\mu v - \varepsilon\mu z\right] \\
&= \ln\left(\frac{u}{u^*}\right)\left[u(w - v) - \varepsilon(\sigma u^2 - v^2)\right] + \ln\left(\frac{v}{v^*}\right)\left[vu - \mu v - \varepsilon(v^2 - \mu z)\right] \\
&\quad + \ln\left(\frac{w}{w^*}\right)(-wu + \varepsilon\sigma u^2) + \ln\left(\frac{z}{z^*}\right)(\mu v - \varepsilon\mu z) \\
&= (uw - \varepsilon\sigma u^2)\ln\left(\frac{uw^*}{wu^*}\right) + (uv - \varepsilon v^2)\ln\left(\frac{vu^*}{uv^*}\right) + (\mu v - \varepsilon\mu z)\ln\left(\frac{zv^*}{vz^*}\right) \\
&= uw\left(1 - \frac{\varepsilon\sigma u}{w}\right)\ln\left(\frac{\sigma\varepsilon u}{w}\right) + uv\left(1 - \frac{\varepsilon v}{u}\right)\ln\left(\frac{\varepsilon v}{u}\right) + \mu v\left(1 - \frac{\varepsilon z}{v}\right)\ln\left(\frac{\varepsilon z}{v}\right) \\
&= uwf\left(\frac{\varepsilon\sigma u}{w}\right) + uvf\left(\frac{\varepsilon v}{u}\right) + \mu vf\left(\frac{\varepsilon z}{v}\right),
\end{aligned}
$$

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where $f(x) = (1 - x) \ln x$. Because function $f(x) \leq 0$ for all $x > 0$ and $f(x) = 0$ if and only

if $x = 1$, it implies that $L'(Y) \leq 0$ for all $Y \in \mathbb{R}^{4+}$ and $L'(Y) = 0$ if and only if

$$f\left(\frac{\varepsilon \sigma u}{w}\right) = 0, \qquad f\left(\frac{\varepsilon v}{u}\right) = 0, \qquad f\left(\frac{\varepsilon z}{v}\right) = 0,$$

that is,

$$\frac{\varepsilon \sigma u}{w} = \frac{\varepsilon v}{u} = \frac{\varepsilon z}{v} = 1, \qquad \text{or} \qquad w = \sigma \varepsilon u, \quad u = \varepsilon v, \quad v = \varepsilon z.$$

Under the constraint $Y \cdot \vec{n} = \xi$, that is, $u + v + \frac{w}{\sigma} + z = \xi$, we have

$$u = u^*, \qquad v = v^*, \qquad w = w^*, \qquad z = z^*.$$

See Figure 4. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ □
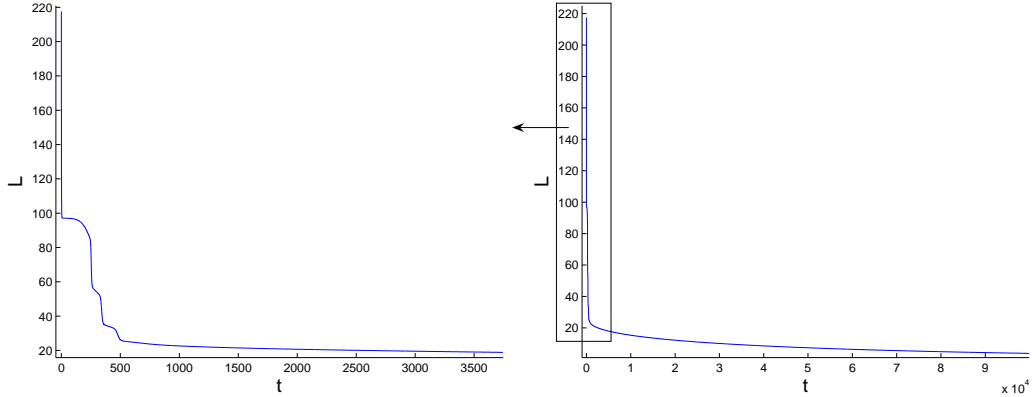
Figure 4: Lyapunov Function L.

Note that $\mathcal{T} = \mathbb{R}^{4+} \cap \{Y \cdot \vec{n} = \xi\}$, thus we have

Theorem 4.1.12. P_3 *is the global attractor of system (11) in* $\mathcal{T}$.

Indeed, L is a Lyapunov function, and physically it is exactly the free energy function. By the Second Law of Thermodynamics [24], the chemical reaction in the closed system must approach the equilibrium state eventually with the free energy decaying. Theorem 4.1.12 provides a mathematical statement for it. In addition, we also notice that system (11) is not a gradient system, this explains mathematically why the reaction does not proceed in the most rapidly decreasing direction, the negative of gradient, of the free energy. However, the physical interpretation behind is not well understood yet.

4.2   Unperturbed Lotka-Volterra System

In the previous section, we studied the long term behavior that, in the closed system, the reaction ends up at the equilibrium state in the monotonic way. But as a matter of fact, the oscillation lasts long before it vanishes. Experimentally, we may observe that the chemical solution changes color alternatively and the frequency may vary. To study this nonlinear oscillation, we have to concentrate on the region far away from the equilibrium. And since the unperturbed LV system with $\varepsilon = \sigma = 0$ exhibits oscillation, it is reasonable to think that the oscillatory behavior in chemical reaction is inherited directly from the oscillation in the unperturbed LV system

$$\begin{cases} \dot{u} &= u(w - v) \\ \dot{v} &= v(u - 1) \\ \dot{w} &= 0 \end{cases} \tag{12}$$

Since w remains constant in (12) and hence can be treated as a parameter, we will have a standard 2D LV system. And it admits a first integral

$$E = (u - 1 - \ln u) + \left[(v - w) + w \ln \left(\frac{w}{v} \right) \right] \qquad \forall w \geq 0.$$

For fixed $w > 0$ and $E > 0$, it produces a closed orbit. This simple system was already widely studied by many authors, especially on its period function T, such as the monotonicity of T with respect to energy E [71], critical point of T [7] and so on.

To study the oscillation time for the perturbed system (11), we need to know not only the dependence of T on E, but also the dependence on w, on which no work is done to my knowledge. In this section, we will study the dependence of period function T on parameter w. For completeness, the dependence of T on E is also included.

4.2.1   Period Function of planar Hamiltonian System.

In this section, we will temporarily replace E by h to denote the energy. And we will provide a representation of period function $T(h)$ and its derivative $T'(h)$ with respect to energy h. A similar form for the separable Hamiltonian was first given by Sabatini in

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[59] by the argument in terms of normalizer. And our proof is based on the elementary differential geometry.

Lemma 4.2.1. *Suppose that function $F(u, v) \geq 0$ is differentiable on an open set $O \subset R^2$ and $\nabla F(u, v) = 0$ only at $(u_0, v_0) \in O$. Let $h_0 > 0$ be such that the level curve*

$$\Gamma_h = \{(u, v) \in O, F(u, v) = h\}$$

is a Jordan closed curve for any $h \in (0, h_0)$. Then, for any continuous function $P(u, v)$,

$$\mathcal{A}(h) = \iint_{F(u,v) \leq h} P(u, v) du dv, \qquad \mathcal{L}(h) = \int_{\Gamma_h} P(u, v) ds,$$

are well-defined and differentiable for $h \in (0, h_0)$ if P is differentiable, and

$$\frac{d\mathcal{A}}{dh} = \oint_{\Gamma_h} \frac{P(u, v)}{|\nabla F|} ds, \qquad \frac{d\mathcal{L}}{dh} = \int_{\Gamma_h} \left[\frac{\kappa P}{|\nabla F|} + \frac{\nabla P \cdot \nabla F}{|\nabla F|^2} \right] ds,$$

where κ is the curvature of Γ_h.

<u>Proof:</u> Let $h \in (0, h_0)$ be fixed and $\varepsilon > 0$ sufficiently small such that $h + \varepsilon \in (0, h_0)$, then

$$\mathcal{A}(h + \varepsilon) - \mathcal{A}(h) = \iint_{h \leq F(u,v) \leq h+\varepsilon} P(u, v) du dv$$

For any $(u, v) \in \Gamma_h$, choose $(u+\delta_1, v+\delta_2) \in \Gamma_{h+\varepsilon}$ such that $\delta = (\delta_1, \delta_2)$ has the same direction as $\nabla F(u, v)$. Note that

$$F(u, v) = h, \qquad F(u + \delta_1, v + \delta_2) = h + \varepsilon,$$

it follows that

$$F(u + \delta_1, v + \delta_2) - F(u, v) = \varepsilon \Rightarrow \delta \cdot \nabla F + o(|\delta|) = \varepsilon,$$

that is,

$$|\delta||\nabla F| + o(|\delta|) = \varepsilon,$$

because δ and $\nabla F(u, v)$ have the same direction. Therefore, by inverse function theorem,

$$|\delta| = \frac{\varepsilon}{|\nabla F|} + o(\varepsilon).$$

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Furthermore, by the mean value theorem and by the uniform continuity of $P(u, v)$ on the δ-neighborhood $N_\delta(\Gamma_h)$ of Γ_h, we have

$$\mathcal{A}(h + \varepsilon) - \mathcal{A}(h) = \oint_{\Gamma_h} [P(u, v) + r(\varepsilon)]|\delta|ds = \oint_{\Gamma_h} [P(u, v) + r(\varepsilon)] \left[\frac{\varepsilon}{|\nabla F|} + o(\varepsilon) \right] ds,$$

where $r(\varepsilon) \to 0$ as $\varepsilon \to 0$. Hence it follows that

$$\frac{d\mathcal{A}}{dh} = \lim_{\varepsilon \to 0} \frac{\mathcal{A}(h + \varepsilon) - \mathcal{A}(h)}{\varepsilon} = \oint_{\Gamma_h} \frac{P(u, v)}{|\nabla F|} ds.$$

This completes the proof of the first part of the lemma.

For the second part, consider a pair of points $(u, v), (u', v') \in \Gamma_h$ sufficiently close to each other. Let ds be the length of the infinitesimal arc on Γ_h with two end points (u, v) and (u', v'), ds' the length of the according portion with end points $(u + \delta_1, v + \delta_2)$ and $(u' + \delta'_1, v' + \delta'_2)$ on $\Gamma_{h+\varepsilon}$, then

$$\frac{ds'}{ds} = \frac{R'}{R} + o(|\delta|) = \frac{R + |\delta|}{R} + o(|\delta|) = 1 + \kappa|\delta| + o(|\delta|)$$

where κ is the curvature of the curve Γ_h at point (u, v) and R is the radius of curvature. Thus

$$
\begin{aligned}
\mathcal{L}(h + \varepsilon) &= \int_{\Gamma_{h+\varepsilon}} P(u_1, v_1) ds' \\
&= \int_{\Gamma_h} P(u + \delta_1, v + \delta_2) \left[1 + \kappa|\delta| + o(|\delta|) \right] ds \\
&= \int_{\Gamma_h} [P(u, v) + \nabla P(u, v) \cdot \delta + o(|\delta|)][1 + \kappa|\delta| + o(|\delta|)] ds
\end{aligned}
$$

and then

$$
\begin{aligned}
\mathcal{L}(h + \varepsilon) - \mathcal{L}(h) &= \int_{\Gamma_h} [P(u, v) + \nabla P(u, v) \cdot \delta + o(|\delta|)][1 + \kappa|\delta| + o(|\delta|)] - P(u, v) ds \\
&= \int_{\Gamma_h} [P(u, v)\kappa|\delta| + \nabla P(u, v) \cdot \delta] ds + o(|\delta|).
\end{aligned}
$$

Recall that

$$\delta = |\delta| \frac{\nabla F}{|\nabla F|}, \qquad |\delta| = \frac{\varepsilon}{|\nabla F|} + o(\varepsilon),$$

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then we can obtain that

$$\frac{1}{\varepsilon}[\mathcal{L}(h+\varepsilon) - \mathcal{L}(h)]$$

$$= \frac{1}{\varepsilon}\int_{\Gamma_h}\left[P(u,v)\kappa|\delta| + \nabla P(u,v)\cdot\nabla F\frac{|\delta|}{|\nabla F|}\right]ds + o(\frac{|\delta|}{\varepsilon})$$

$$= \frac{1}{\varepsilon}\int_{\Gamma_h}\left(\kappa P + \nabla P\cdot\nabla F\frac{1}{|\nabla F|}\right)[\frac{\varepsilon}{|\nabla F|} + o(\varepsilon)]ds + o(1)$$

$$\to \int_{\Gamma_h}\left[\frac{\kappa P}{|\nabla F|} + \frac{\nabla P\cdot\nabla F}{|\nabla F|^2}\right]ds,$$

that is,

$$\frac{d\mathcal{L}}{dh} = \int_{\Gamma_h}\left[\frac{\kappa P}{|\nabla F|} + \frac{\nabla P\cdot\nabla F}{|\nabla F|^2}\right]ds.$$

$\square$

Lemma 4.2.2. *Consider a two-dimensional system*

$$\begin{cases} \dot{u} &= f(u,v) \\ \dot{v} &= g(u,v) \end{cases} \tag{13}$$

with analytic functions f and g on an open region $\Omega \subset R^2$. Then this system can be converted into a Hamiltonian system

$$\begin{cases} \dot{x} &= -H_y \\ \dot{y} &= H_x \end{cases} \tag{14}$$

under a transformation $x = x(u,v)$ and $y = y(u,v)$ if and only if this system admits a first integral $F(u,v)$.

Proof: Since the Hamiltonian is a conservative quantity, the necessary condition is trivial. Now let us assume that this systems has a first integral $F(u,v)$, then

$$\frac{dF}{dt} = \nabla F\cdot(\dot{u},\dot{v})^T = \nabla F\cdot(f,g)^T = 0 \Rightarrow F_u f + F_v g = 0.$$

Let

$$v(u,v) = \frac{F_u}{g} = -\frac{F_v}{f},$$

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which, obviously, is an integrating factor. Let $x = x(u, v)$ and $y = y(u, v)$ be a transform such that

$$\det(A) = v \qquad \text{with} \qquad A = \frac{\partial(x, y)}{\partial(u, v)} = \left(\begin{array}{cc} \dfrac{\partial x}{\partial u} & \dfrac{\partial x}{\partial v} \\ \dfrac{\partial y}{\partial u} & \dfrac{\partial y}{\partial v} \end{array} \right).$$

It is easy to check that under this transform, the original system becomes

$$\left. \begin{array}{l} \dot{x} = \dfrac{\partial x}{\partial u}\dot{u} + \dfrac{\partial x}{\partial v}\dot{v} \\ \dot{y} = \dfrac{\partial y}{\partial u}\dot{u} + \dfrac{\partial y}{\partial v}\dot{v} \end{array} \right\} \Rightarrow \left(\begin{array}{c} \dot{x} \\ \dot{y} \end{array} \right) = A \left(\begin{array}{c} \dot{u} \\ \dot{v} \end{array} \right) = A \left(\begin{array}{c} f \\ g \end{array} \right)$$

and $H(x, y) = F(u(x, y), v(x, y))$ is the corresponding first integral. And on the other hand, $H(x(u, v), y(u, v)) = F(u, v)$ implies that

$$\left. \begin{array}{l} -vf = F_v = H_x\dfrac{\partial x}{\partial v} + H_y\dfrac{\partial y}{\partial v} \\ vg = F_u = H_x\dfrac{\partial x}{\partial u} + H_y\dfrac{\partial y}{\partial u} \end{array} \right\}$$

$$\Rightarrow \left(\begin{array}{c} f \\ g \end{array} \right) = \frac{1}{v} \left(\begin{array}{cc} \dfrac{\partial y}{\partial v} & -\dfrac{\partial x}{\partial v} \\ -\dfrac{\partial y}{\partial u} & \dfrac{\partial x}{\partial u} \end{array} \right) \left(\begin{array}{c} -H_y \\ H_x \end{array} \right) \Rightarrow \left(\begin{array}{c} f \\ g \end{array} \right) = \frac{1}{v}A^*J\nabla H = A^{-1}J\nabla H$$

where A^* is the adjoint matrix of A and

$$J = \left(\begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right).$$

Therefore we can obtain the Hamiltonian system

$$\left(\begin{array}{c} \dot{x} \\ \dot{y} \end{array} \right) = J\nabla H = \left(\begin{array}{c} -H_y \\ H_x \end{array} \right).$$

Now it suffices to show the existence of such a transform. It is readily to see that

$$x = u, \qquad y = \int v(u, v)dv$$

satisfies

$$\frac{\partial(x, y)}{\partial(u, v)} = \left| \begin{array}{cc} 1 & 0 \\ \displaystyle\int \frac{\partial v}{\partial u}dv & v \end{array} \right| = v.$$

$\square$

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Remark. Note that the transform converting a two-dimensional system with first integral to a Hamiltonian system is not unique, for example, we can also choose

$$x = \int v(u, v)du, \qquad y = v$$

or

$$x = \int v(u, v)dv, \qquad y = -u$$

or

$$x = -v, \qquad y = \int v(u, v)du.$$

Lemma 4.2.3. *Suppose that system (13) admits a first integral $F(u, v)$ which satisfies the conditions in Lemma 4.2.1 and v is the integrating factor. Then, for any $h \in (0, h_0)$, its period function can be represented as*

$$T(h) = \mathcal{A}'(h), \qquad where \qquad \mathcal{A} = \iint_{F \leq h} |v|ds.$$

Proof: It is the immediate consequence of Lemma 4.2.1 that

$$\mathcal{A}'(h) = \oint_{\Gamma_h} \frac{|v|}{|\nabla F|}ds = \int_0^{T(h)} \frac{|v|\sqrt{f^2 + g^2}}{|\nabla F|}dt = \int_0^{T(h)} dt = T(h).$$

$\square$

Lemma 4.2.4. *Suppose that system (14) is the Hamiltonian form of system (13), both (13) and (14) admit period annulus and T_F and T_H are their period functions, respectively. Then $T_F(h) = T_H(h)$ for any $h \in (0, h_0)$.*

Proof: Consider the following two area integrals

$$A_F(h) = \iint_{F \leq h} |v|dudv = \iint_{H \leq h} |v||\det(A^{-1})|dxdy = \iint_{H \leq h} dxdy = A_H(h).$$

Immediately from Lemma 4.2.1, it follows that

$$T_F(h) = \mathcal{A}'_F(h) = \mathcal{A}'_H(h) = T_H(h).$$

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$\square$

Now we will consider a planar Hamiltonian system

$$\dot{X} = J\nabla H(X). \tag{15}$$

Theorem 4.2.5. *Suppose $F = H$ satisfies the conditions in Lemma 4.2.1, then the period function $T(h)$ of system (14) and its derivative have the following representation*

$$T(h) = \oint_{\Gamma_h} \frac{1}{|\nabla H|} ds, \qquad T'(h) = \oint_{\Gamma_h} \frac{(\nabla H)^T \left(J^T \mathcal{H} J - \mathcal{H} \right) \nabla H}{|\nabla H|^5} ds.$$

where $\mathcal{H}$ is the Hessian matrix of H.

Proof: For the Hamiltonian system the integrating factor is $\nu = 1$, then, by Lemma 4.2.3, we have

$$T(h) = \mathcal{A}'(h) = \oint_{H=h} \frac{1}{|\nabla H|} ds, \qquad \mathcal{A}(h) = \iint_{H \leq h} dxdy.$$

By letting $P = \frac{1}{|\nabla H|}$, Lemma 4.2.1 also implies

$$T'(h) = \oint_{\Gamma_h} \left[\frac{\kappa}{|\nabla H|^2} + \frac{\left(\nabla \frac{1}{|\nabla H|} \right) \cdot \nabla H}{|\nabla H|^2} \right] ds.$$

Note that the curvature of the level curve $H(x, y) = h$ is given by

$$\kappa = \frac{\dot{x}\ddot{y} - \ddot{x}\dot{y}}{(\dot{x}^2 + \dot{y}^2)^{\frac{3}{2}}}.$$

Let $\mathcal{H}$ be the Hessian matrix of H, note that

$$\ddot{x} = -\left(\frac{\partial^2 H}{\partial y \partial x} \dot{x} + \frac{\partial^2 H}{\partial y^2} \dot{y} \right), \qquad \ddot{y} = \frac{\partial^2 H}{\partial x^2} \dot{x} + \frac{\partial^2 H}{\partial x \partial y} \dot{y},$$

therefore

$$\dot{x}\ddot{y} - \dot{y}\ddot{x} = (\dot{x}, \dot{y}) \begin{pmatrix} \dfrac{\partial^2 H}{\partial x^2} & \dfrac{\partial^2 H}{\partial y \partial x} \\ \dfrac{\partial^2 H}{\partial x \partial y} & \dfrac{\partial^2 H}{\partial y^2} \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = (\nabla H)^T J^T \mathcal{H} J\nabla H$$

and hence

$$\kappa = \frac{(\nabla H)^T J^T \mathcal{H} J\nabla H}{|\nabla H|^3}.$$

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In addition,
$$\nabla\left(\frac{1}{|\nabla H|}\right) = -\frac{\mathscr{H}^T\nabla H}{|\nabla H|^3} = -\frac{\mathscr{H}\nabla H}{|\nabla H|^3},$$

then we have
$$\begin{aligned}
\frac{dT}{dh} &= \oint_{\Gamma_h}\left[\frac{(\nabla H)^T J^T \mathscr{H} J\nabla H}{|\nabla H|^3}\frac{1}{|\nabla H|^2} - \frac{(\nabla H)^T \mathscr{H}^T\nabla H}{|\nabla H|^3}\frac{1}{|\nabla H|^2}\right]ds \\
&= \oint_{\Gamma_h}\left[\frac{(\nabla H)^T J^T \mathscr{H} J\nabla H}{|\nabla H|^5} - \frac{(\nabla H)^T \mathscr{H}\nabla H}{|\nabla H|^5}\right]ds
\end{aligned}$$

Therefore
$$T'(h) = \oint_{\Gamma_h}\frac{(\nabla H)^T\left(J^T \mathscr{H} J - \mathscr{H}\right)\nabla H}{|\nabla H|^5}ds. \tag{16}$$

$\square$

Remark 4.2.6. *Note that*

$$\Phi(x, y) = (\nabla H)^T\left(J^T \mathscr{H} J - \mathscr{H}\right)\nabla H = (H_y^2 - H_x^2)(H_{xx} - H_{yy}) - 4H_{xy}H_x H_y,$$

which first appears in [59] where the author applied the normalizer to study the period function, but it seems to only provide a sufficient condition for the monotonicity of period function. By contrast, the equivalent representation of $T'(h)$ given in (16) provides a necessary and sufficient condition. And from this representation, we can see the derivative of the period function depends only on the geometric property of the graph of the Hamiltonian H. By Lemma 4.2.2, any planar system with a first integral has Hamiltonian structure. And Lemma 4.2.4 implies that, to find period function of a planar system with first integral, it is enough to calculate the period function for the period function of the associated Hamiltonian system.

Corollary 4.2.7. *Suppose that $f \in C^2(\mathbb{R}^+)$ is convex and $f'(0) = 0$. Then the period function T_{H_f} of the Hamiltonian system with Hamiltonian $H_f(x, y) = f(|x|) + f(|y|)$ is monotonically decreasing when f'' is increasing in $\mathbb{R}^+$ and T_{H_f} increasing when f'' is decreasing.*

Proof: Let $g(x) = f(|x|)$, then

$$g'(x) = f'(|x|)\frac{x}{|x|}, \qquad g''(x) = f''(|x|).$$

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Note that H is separable, that is, $H_{xy} = 0$, thus

$$\Phi(x, y) = (H_y^2 - H_x^2)(H_{xx} - H_{yy}) = \left[(f'(|y|))^2 - (f'(|x|))^2\right](f''(|x|) - f''(|y|)).$$

Because f is convex, that is, f' increasing, we know that $f' \geq 0$ in $\mathbb{R}^+$. Then $\Phi \leq 0$ and hence $T'(h) < 0$ as f'' increasing in $\mathbb{R}^+$, and similarly $T'(h) > 0$ as f'' decreasing. $\quad\square$

Example 4.2.8. *For any $\alpha > 2$, define $H_\alpha(x, y) = |x|^\alpha + |y|^\alpha$, then the corresponding period function is decreasing because $f(x) = x^\alpha$ is convex, $f(0) = 0$ and f'' increasing in $\mathbb{R}^+$. And the period function for $H(x, y) = |x| + e^{-|x|} + |y| + e^{-|y|}$ is increasing because $f(x) = x + e^{-x}$ is convex, $f'(0) = 0$ and f'' decreasing.*

4.2.2   Dependence of T on E.

For the standard Lotka-Volterra system, the period function is studied by many authors in many different ways. Here we only list the result in the following theorem.

Theorem 4.2.9. *For any $w > 0$, the period function of system*

$$\dot{u} = u(w - v), \qquad \dot{v} = v(u - 1) \tag{17}$$

is monotonically increasing in energy E.

See [71] for details of the proof.

In this section, we will go further to take a closer look at the period function to see how T depends on E. For this purpose, we will use an alternative representation of the period function. Note that the 2D Lotka-Volterra system in (17) has a first integral

$$F(u, v) = (u - 1 - \ln u) + \left[(v - w) + w\ln\left(\frac{w}{v}\right)\right] = E = constant.$$

Because F is a separable function, we introduce the following transformation

$$u - 1 - \ln u = E\cos^2\theta, \qquad (v - w) + w\ln\left(\frac{w}{v}\right) = E\sin^2\theta, \tag{18}$$

see [71] for the general discussion of the transformation for separable first integral. Under this transformation, we will have an equivalent system

$$\dot{E} = 0, \qquad \dot{\theta} = \frac{(v(\theta, w) - w)(u(\theta) - 1)}{2E\sin\theta\cos\theta}. \tag{19}$$

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Thus the period function can be written as

$$T(E, w) = \int_0^T dt = \int_0^{2\pi} \frac{dt}{d\theta} d\theta = \int_0^{2\pi} \frac{2E \sin\theta \cos\theta}{(v-w)(u-1)} d\theta. \tag{20}$$

Lemma 4.2.10. *Suppose that* $f(y) = y - 1 - \ln y$. *Then, for any* $x \in \mathbb{R}$, $f(y) = x^2$ *has a series solution* $y = \sum_{k=0}^{\infty} a_k x^k$ *where* $a_0 = 1$, $a_1 = \pm\sqrt{2}$, $a_2 = \frac{2}{3}$ *and*

$$a_{k+1} = \frac{1}{(k+2)a_1}\left(2a_k - \sum_{i=1}^{k-1}(i+1)a_{i+1}a_{k-i+1}\right), \qquad k \geq 2.$$

<u>Proof:</u> Consider equation $f(y) = x^2$. Then, by implicit differentiation, we have

$$\left(1 - \frac{1}{y}\right)y'(x) = 2x \Rightarrow (y-1)y' = 2xy. \tag{21}$$

Suppose that (21) has series solution $y = \sum_{k=0}^{\infty} a_k x^k$, then

$$\left(\sum_{k=0}^{\infty} a_k x^k - 1\right)\left(\sum_{k=0}^{\infty} k a_k x^{k-1}\right) = 2x \sum_{k=0}^{\infty} a_k x^k$$

which implies that $a_0 = 1$. And then we have

$$\left(\sum_{k=1}^{\infty} a_k x^k\right)\left(\sum_{k=0}^{\infty} k a_k x^{k-1}\right) = 2x \sum_{k=0}^{\infty} a_k x^k$$

$$\Rightarrow \left(\sum_{k=0}^{\infty} a_{k+1} x^{k+1}\right)\left(\sum_{k=1}^{\infty} k a_k x^{k-1}\right) = 2x \sum_{k=0}^{\infty} a_k x^k$$

$$\Rightarrow \left(\sum_{k=0}^{\infty} a_{k+1} x^k\right)\left(\sum_{k=0}^{\infty} (k+1) a_{k+1} x^k\right) = 2 \sum_{k=0}^{\infty} a_k x^k$$

$$\Rightarrow \sum_{k=0}^{\infty} \left(\sum_{i=0}^{k} (i+1) a_{i+1} a_{k-i+1}\right) x^k = 2 \sum_{k=0}^{\infty} a_k x^k$$

therefore we find the recurrent relation

$$a_1 = \pm\sqrt{2}, \qquad a_2 = \frac{2}{3}, \qquad \sum_{i=0}^{k}(i+1)a_{i+1}a_{k-i+1} = 2a_k, \qquad k = 2, 3, \ldots.$$

and

$$a_{k+1} = \frac{1}{(k+2)a_1}\left[2a_k - \sum_{i=1}^{k-1}(i+1)a_{i+1}a_{k-i+1}\right], \qquad k \geq 2,$$

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that is,

$$k = 2, \quad a_1 a_3 + 2a_2^2 + 3a_3 a_1 = 2a_2 \Rightarrow a_3 = \frac{a_2(1-a_2)}{2a_1} = \pm\frac{1}{9\sqrt{2}},$$

$$k = 3, \quad a_4 = \frac{1}{5a_1}(2a_3 - 5a_2 a_3) = \frac{a_3}{5a_1}(2 - 5a_2) = -\frac{2}{135},$$

$$k = 4, \quad a_5 = \frac{1}{6a_1}\left(2a_4 - 6a_2 a_4 - 3a_3^2\right) = \frac{1}{540a_1} = \pm\frac{1}{540\sqrt{2}}$$

$$\vdots$$

$\square$

Lemma 4.2.11. *For fixed $w > 0$, the period function $T(E, w)$ satisfies the following in-equality*

$$ET'_E \le T \Rightarrow T(E, w) \begin{cases} \le T(1, w)E, & as \quad E \ge 1 \\ \\ \ge T(1, w)E, & as \quad E \le 1 \end{cases}.$$

Proof: From the transformation in (18), it follows that

$$u_E = \frac{u \cos^2 \theta}{u - 1}, \qquad v_E = \frac{v \sin^2 \theta}{v - w}.$$

Hence

$$
\begin{aligned}
T'_E &= \int_0^{2\pi} \left(\frac{2 \sin\theta \cos\theta}{(v-w)(u-1)} - \frac{2E \sin\theta \cos\theta}{(u-1)^2(v-w)} \frac{u \cos^2\theta}{u-1} - \frac{2E \sin\theta \cos\theta}{(u-1)(v-w)^2} \frac{v \sin^2\theta}{v-w} \right) d\theta \\
&= \int_0^{2\pi} \frac{2 \sin\theta \cos\theta}{(v-w)(u-1)} \left(1 - \frac{uE \cos^2\theta}{(u-1)^2} - \frac{vE \sin^2\theta}{(v-w)^2} \right) d\theta \\
&= \int_0^{2\pi} \frac{2 \sin\theta \cos\theta}{(v-w)(u-1)} \left(1 - \frac{u(u-1-\ln u)}{(u-1)^2} - \frac{v\left(v-w+w\ln\frac{w}{v}\right)}{(v-w)^2} \right) d\theta
\end{aligned}
$$

Define

$$g(x) = \frac{x(x - 1 - \ln x)}{(x - 1)^2},$$

then $g(x)$ is an increasing function and $0 \le g(x) \le 1$ for $x \ge 0$, and

$$T'_E = \int_0^{2\pi} \frac{2 \sin\theta \cos\theta}{(v-w)(u-1)} \left[1 - g(u) - g\left(\frac{v}{w}\right) \right] d\theta.$$

Since T is increasing in E and $\frac{2 \sin\theta \cos\theta}{(v-w)(u-1)} > 0$ for $\theta \in [0, 2\pi]$, we have

$$ET'_E \le T \Rightarrow \begin{cases} T(1, w) \le T(E, w) \le T(1, w)E, & as \quad E \ge 1 \\ \\ T(1, w)E \le T(E, w) \le T(1, w), & as \quad E \le 1 \end{cases}$$

for any fixed $w > 0$. □

A more accurate estimate is possible when the maximum of $1 - g(u) - g\left(\frac{v}{w}\right)$ on the compact set $F(u, v) = E$ is obtained.

4.2.3 Dependence of T on w.

In the previous section, we discuss the dependence of the period function T on the energy and know that T is a monotone increasing function of energy. Because w will vary under the perturbation, it is also important to know how the period T depends on w. In this section, we will provide an estimate of the period in terms of w for fixed energy.

We already know that the period function can be written as

$$T(E, w) = \int_0^{2\pi} \frac{2E \sin\theta \cos\theta}{(v - w)(u - 1)} d\theta.$$

Now we define a Poincaré section

$$\Sigma = \{(u, v, w), u > 0, u \neq 1, v = w \geq \underline{w}\} = \Sigma_+ \cup \Sigma_-,$$

for some $\underline{w} > 0$ which will be determined later, where

$$\Sigma_+ = \{(u, v, w) \in \Sigma, u > 1\}, \qquad \Sigma_- = \{(u, v, w) \in \Sigma, 0 < u < 1\}.$$

Obviously the flow meets Σ transversely when the intersection is away from $u = 1$. Define

$$T_1(E, w) = \int_0^{\pi} \frac{2E \sin\theta \cos\theta}{(v - w)(u - 1)} d\theta, \qquad T_2(E, w) = \int_\pi^{2\pi} \frac{2E \sin\theta \cos\theta}{(v - w)(u - 1)} d\theta,$$

then T_1 is the first return time when starting from Σ_+, and T_2 is the first return time when starting from Σ_-. Apparently $T = T_1 + T_2$ when the return point for T_1 is the starting point for T_2.

Lemma 4.2.12. *For any fixed $E > 0$ and any $w > 0$, the period function T is monotonically decreasing in w. And T_1 and T_2 satisfy the following inequalities*

$$T_1(E, 1) \leq T_1(E, w) \leq \frac{T_1(E,1)}{\sqrt{w}}, \qquad \frac{T_2(E,1)}{\sqrt{w}} \leq T_2(E, w) \leq \frac{T_2(E,1)}{w}, \qquad as \quad 0 < w < 1$$

$$\frac{T_1(E,1)}{\sqrt{w}} \leq T_1(E, w) \leq T_1(E, 1), \qquad \frac{T_2(E,1)}{w} \leq T_2(E, w) \leq \frac{T_2(E,1)}{\sqrt{w}}, \qquad as \quad w > 1.$$

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Proof: Note that the dependence of T on w is explicit and also implicit through v. From (18), it follows that

$$\frac{\partial v}{\partial w} = -\frac{\ln \frac{w}{v}}{1 - \frac{w}{v}}.$$

Then we have that

$$T'_w = \int_0^{2\pi} \frac{-2E \sin\theta \cos\theta}{(v-w)^2(u-1)}\left(\frac{\partial v}{\partial w} - 1\right)d\theta = \int_0^{2\pi} \frac{2E \sin\theta \cos\theta}{(v-w)^2(u-1)}\left(\frac{1 - \frac{w}{v} + \ln\frac{w}{v}}{1 - \frac{w}{v}}\right)d\theta.$$

Note that, for all $x \in \mathbb{R}^+$, function

$$f(x) = \frac{x(1 - x + \ln x)}{(1-x)^2} \leq 0$$

hence

$$wT'_w = \int_0^{2\pi} \frac{2E \sin\theta \cos\theta}{(v-w)(u-1)} f\left(\frac{w}{v}\right)d\theta \leq 0,$$

that is, T is monotonically decreasing in w. In addition, f is also monotonically decreasing on $\mathbb{R}^+$, $-1 < f(x) \leq 0$ and $f(1) = -\frac{1}{2}$, then

$$wT'_{1w} = \int_0^{\pi} \frac{2E \sin\theta \cos\theta}{(v-w)(u-1)} f\left(\frac{w}{v}\right)d\theta \geq -\frac{1}{2}\int_0^{\pi} \frac{2E \sin\theta \cos\theta}{(v-w)(u-1)}d\theta = -\frac{T_1}{2},$$

because $\frac{w}{v} \leq 1$ as $\theta \in [0, \pi]$. Consequently it follows from the above differential inequality that

$$\int_w^1 d\ln T_1 \geq \int_w^1 -\frac{1}{2w}dw \Rightarrow \ln\left(\frac{T_1(E,1)}{T_1(E,w)}\right) \geq -\frac{1}{2}\ln\left(\frac{1}{w}\right) \Rightarrow T_1(E,w) \leq \frac{T_1(E,1)}{\sqrt{w}},$$

as $w < 1$ and $T_1(E,w) \geq \frac{T_1(E,1)}{\sqrt{w}}$ as $w > 1$. Plus the monotonicity of T in w, we have

$$T_1(E,1) \leq T_1(E,w) \leq \frac{T_1(E,1)}{\sqrt{w}}, \quad \text{as} \quad 0 < w < 1$$

$$\frac{T_1(E,1)}{w} \leq T_1(E,w) \leq T_1(E,1), \quad \text{as} \quad w > 1.$$

Similarly, as $\theta \in [\pi, 2\pi]$, $\frac{w}{v} \geq 1$ and $-1 < f\left(\frac{w}{v}\right) \leq -\frac{1}{2}$, thus we can obtain that

$$\frac{T_2(E,1)}{\sqrt{w}} \leq T_2(E,w) < \frac{T_2(E,1)}{w}, \quad \text{as} \quad 0 < w < 1$$

$$\frac{T_2(E,1)}{w} < T_2(E,w) \leq \frac{T_2(E,1)}{\sqrt{w}}, \quad \text{as} \quad w > 1$$

$\square$

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Lemma 4.2.13. *For $w > 0$ sufficiently small, $T_1 \leq -C \ln w$.*

Proof: Consider

$$T_1(E, w) = \int_0^\pi \frac{2E \sin \theta \cos \theta}{(v - w)(u - 1)} d\theta.$$

By the transformation (18) and series expansion given in Lemma 4.2.10, we have

$$\lim_{\theta \to k\pi} \frac{\sin \theta}{v - w} = \frac{1}{\sqrt{2Ew}}, \qquad \lim_{\theta \to k\pi + \frac{\pi}{2}} \frac{\cos \theta}{u - 1} = \frac{1}{\sqrt{2E}}.$$

Therefore $\frac{\cos \theta}{u-1}$ is continuous on $[0, \pi]$ and set $M = \max\limits_{\theta \in [0,\pi]} \left\{ \frac{\cos \theta}{u - 1} \right\}$. And it is also easy to see that when $w \ll 1$,

$$\frac{\sin \theta}{v - w} \leq \frac{1}{\sqrt{2Ew}}, \qquad \text{for} \quad \theta \in [0, \pi].$$

Consequently we can have the following estimate.

$$T_1(E, w) = I_1 + I_2 + I_3$$

where

$$I_1 = \int_0^{\sqrt{w}} \frac{2E \sin \theta \cos \theta}{(v - w)(u - 1)} d\theta \leq \frac{2EM}{\sqrt{2Ew}} \int_0^{\sqrt{w}} d\theta = M\sqrt{2E}$$

and similarly

$$I_3 = \int_{\pi - \sqrt{w}}^\pi \frac{2E \sin \theta \cos \theta}{(v - w)(u - 1)} d\theta \leq M\sqrt{2E},$$

and

$$I_2 = \int_{\sqrt{w}}^{\pi - \sqrt{w}} \frac{2E \sin \theta \cos \theta}{(v - w)(u - 1)} d\theta.$$

Note that as $\theta \in [0, \pi]$, $v \geq w$ and hence $v - w \geq E \sin^2 \theta$. Then

$$I_2 \leq M \int_{\sqrt{w}}^{\pi - \sqrt{w}} \frac{2E \sin \theta}{E \sin^2 \theta} d\theta = 2M \int_{\sqrt{w}}^{\pi - \sqrt{w}} \frac{1}{\sin \theta} d\theta = 2M \ln \left(\frac{\tan\left(\frac{\pi - \sqrt{w}}{2}\right)}{\tan\left(\frac{\sqrt{w}}{2}\right)} \right) \sim -4M \ln w.$$

Therefore there exists a constant C, which is independent of w, such that $T_1(E, w) \leq -C \ln w$ for w sufficiently small.

Lemma 4.2.14. *For $w > 0$ sufficiently small, $T_1 \geq -c \ln w$ for some $c > 0$.*

Proof: Because $\frac{\cos \theta}{u-1}$ is continuous and has no zero on $[0, \pi]$, set $m = \min\limits_{\theta \in [0,\pi]} \left\{ \frac{\cos \theta}{u - 1} \right\} > 0$, we have

$$T_1(E, w) \geq m \int_0^\pi \frac{2E \sin \theta}{v - w} d\theta.$$

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Note that

$$\int_0^{\frac{\pi}{2}} \frac{2E\sin\theta}{v-w}d\theta \;=\; \int_0^{\frac{\pi}{2}} \frac{2E\sin\theta}{(v-w)\frac{\partial v}{\partial\theta}}dv(\theta) = \int_0^{\frac{\pi}{2}} \frac{2E\sin\theta}{(v-w)\frac{2E\sin\theta\cos\theta}{1-\frac{w}{v}}}dv(\theta)$$

$$= \int_0^{\frac{\pi}{2}} \frac{1}{v\cos\theta}dv(\theta) \geq \int_w^{v_M} \frac{1}{v}dv = \ln\left(\frac{v_M}{w}\right),$$

and similarly

$$\int_{\frac{\pi}{2}}^{\pi} \frac{2E\sin\theta}{v-w}d\theta \;=\; \int_{\frac{\pi}{2}}^{\pi} \frac{1}{v\cos\theta}dv(\theta) = \int_{v_M}^{w} \frac{1}{v\cos\theta}dv \geq \int_w^{v_M} \frac{1}{v}dv = \ln\left(\frac{v_M}{w}\right).$$

On the other hand, since $v_M > w$ solves $v - w + w\ln\left(\frac{w}{v}\right) = E$, we have $v_M \geq E + w > E$,

therefore we may set $c = 2m\ln E$ and have

$$T_1(E, w) \geq -c\ln w.$$

Lemma 4.2.15. *Let $u_m < u_M$ be such that they solve $u - 1 - \ln u = E$. Then*

$$T_2(E, w) \geq \frac{\tilde{c}}{w}, \qquad \tilde{c} = max\left\{\frac{2(u_M - u_m)}{(u_M + u_m)}, \ln\left(\frac{u_M}{u_m}\right)\right\} = \ln\left(\frac{u_M}{u_m}\right).$$

Proof: It is obvious that

$$T_2 = \int_0^{T_2} dt = \int_0^{T_2} \frac{1}{\dot{u}}du = \int_{u_m}^{u_M} \frac{1}{u(w-v)}du.$$

Note that to calculate T_2, $v \leq w$, thus

$$T_2 \geq \int_{u_m}^{u_M} \frac{1}{uw}du = \ln\left(\frac{u_M}{u_m}\right)\frac{1}{w}.$$

And by Hölder inequality,

$$u_M - u_m \;=\; \int_{u_m}^{u_M} du \leq \left(\int_{u_m}^{u_M} u(w-v)du\right)^{\frac{1}{2}}\left(\int_{u_m}^{u_M} \frac{1}{u(w-v)}du\right)^{\frac{1}{2}}$$

$$\leq\; T_2^{\frac{1}{2}}\left(\int_{u_m}^{u_M} uwdu\right)^{\frac{1}{2}} = T_2^{\frac{1}{2}}\left[\frac{w}{2}(u_M^2 - u_m^2)\right]^{\frac{1}{2}},$$

from which it follows that

$$T_2 \geq \frac{2(u_M - u_m)}{w(u_M + u_m)}.$$

Note that $u_M - u_m = \ln\left(\frac{u_M}{u_m}\right)$ and $u_M + u_m \geq 2$, therefore

$$\frac{2(u_M - u_m)}{(u_M + u_m)} \leq \ln\left(\frac{u_M}{u_m}\right).$$

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Theorem 4.2.16. *As defined above, when w is sufficiently small, $T_1(E, w) \sim -\ln w$ and $T_2(E, w) \sim \dfrac{1}{w}$.*

Theorem 4.2.17. *When $w > 0$ is sufficiently small, $T_2(E, w) \sim \ln\left(\dfrac{u_M}{u_m}\right)\dfrac{1}{w}$.*

Proof: Consider

$$wT_2(E, w) = \int_{u_m}^{u_M} \frac{w}{u(w - v)} du \Rightarrow wT_2(E, w) - \ln\left(\frac{u_M}{u_m}\right) = \int_{u_m}^{u_M} \frac{v}{u(w - v)} du.$$

Under the polar-like transformation, it becomes

$$wT_2(E, w) = \int_{\pi}^{2\pi} \frac{-2Ev \sin\theta \cos\theta}{(w - v)(u - 1)} d\theta \leq 2ME \int_{\pi}^{2\pi} \frac{-v \sin\theta}{w - v} d\theta.$$

Set $g(\theta) = \frac{-v \sin\theta}{w - v}$ and it is easy to calculate

$$g'(\theta) = \frac{v \cos\theta \left[2wE \sin^2\theta - (w - v)^2\right]}{(w - v)^3}.$$

Because , by L'Hopital's rule,

$$\lim_{\theta \to k\pi} \frac{2wE \sin^2\theta - (w - v)^2}{(w - v)^3} = \lim_{\theta \to k\pi} \frac{4wE \sin\theta \cos\theta + 2(w - v)\frac{\partial v}{\partial \theta}}{-3(w - v)^2 \frac{\partial v}{\partial \theta}}$$

$$= \lim_{\theta \to k\pi} \frac{2w(\frac{w}{v} - 1) - 2(w - v)}{3(w - v)^2} = \frac{2}{3w},$$

we know that $g'(\theta) = 0$ only at $\theta = \frac{3\pi}{2}$. Then

$$\max_{\theta \in [\pi, 2\pi]} g(\theta) = \max\left\{g(\pi), g(2\pi), g\left(\frac{3\pi}{2}\right)\right\} = \max\left\{\sqrt{\frac{w}{2E}}, \frac{v_m}{w - v_m}\right\} = \sqrt{\frac{w}{2E}},$$

where $v_m = \min_{\theta \in [\pi, 2\pi]} v$ solves $v_m - w + w \ln\left(\frac{w}{v_m}\right) = E$ from which it follows that

$$w \ln\left(\frac{w}{v_m}\right) \geq E \Rightarrow v_m \leq we^{-\frac{E}{w}} \Rightarrow \frac{v_m}{w - v_m} \leq \frac{1}{e^{\frac{E}{w}} - 1} \leq \sqrt{\frac{w}{2E}}.$$

Therefore

$$wT_2(E, w) - \ln\left(\frac{u_M}{u_m}\right) \leq 2ME \int_{\pi}^{2\pi} \sqrt{\frac{w}{2E}} d\theta = 2\pi M \sqrt{2Ew}$$

which shows that

$$\lim_{w \to 0} wT_2(E, w) = \ln\left(\frac{u_M}{u_m}\right) \Rightarrow T_2(E, w) \sim \ln\left(\frac{u_M}{u_m}\right)\frac{1}{w}.$$

4.3 *Partially Perturbed System with $\sigma > 0$ and $\varepsilon = 0$.*

In the original 3D reversible Lotka-Volterra system in (11), the perturbation is introduced in the two different scales, $\varepsilon \ll \sigma$. Therefore, intuitively it is reasonable to consider the partially perturbed system in σ by dropping the higher order perturbation in ε. And the following discussion shows that this is a good strategy.

In this section, we will ignore the high order terms involving ε in (11) and mainly consider system

$$
\begin{cases}
\dot{u} &= u(w - v) \\
\dot{v} &= v(u - 1) \\
\dot{w} &= -\sigma w u
\end{cases}
\tag{22}
$$

which is called *partially perturbed system* in this paper.

4.3.1 Stable Invariant Manifold W_σ.

Note that when $\sigma = 0$, the unperturbed 3D system (12) admits a critical manifold

$$
W_0 = \{(u, v, w), u = 1, v = w > 0\}
\tag{23}
$$

which consists of all the centers of the two-dimensional version (17) of system (12) with w as parameters. Thus W_0 cannot survive under all the smooth perturbations. Indeed, Mané proved in [47] that a compact manifold is persistent if and only if it is normally hyperbolic. However the center type critical manifold W_0 produces all the eigenvalues with zero real parts and hence it is not normally hyperbolic.

Nevertheless, system (22) does have an invariant manifold close to W_0.

Lemma 4.3.1. *System (22) has an invariant manifold*

$$
W_\sigma = \{(u, v, w) | u = \mu_\sigma, \quad v = w > 0\}, \qquad \mu_\sigma = \frac{1}{1 + \sigma}.
\tag{24}
$$

which is close to W_0.

Proof: It is trivial by substitution. □

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Lemma 4.3.2. W_σ *is a stable invariant manifold.*

Proof: Consider function

$$E_\sigma(u, v, w) = (1 + \sigma)\left[(u - \mu_\sigma) + \mu_\sigma \ln\left(\frac{\mu_\sigma}{u}\right)\right] + \left[(v - w) + w \ln\left(\frac{w}{v}\right)\right].$$

Obviously E_σ is convex and attains the absolute minimum at (μ_σ, w, w) for any $w > 0$. Moreover,

$$
\begin{aligned}
\dot{E}_\sigma &= (1 + \sigma)\left(1 - \frac{\mu_\sigma}{u}\right)\dot{u} + \left(1 - \frac{w}{v}\right)\dot{v} + \ln\left(\frac{w}{v}\right)\dot{w} \\
&= (1 + \sigma)(u - \mu_\sigma)(w - v) + (v - w)(u - 1) - \sigma wu \ln\left(\frac{w}{v}\right) \\
&= [(1 + \sigma)u - 1](w - v) + (v - w)(u - 1) - \sigma wu \ln\left(\frac{w}{v}\right) \\
&= \sigma u(w - v) - \sigma wu \ln\left(\frac{w}{v}\right) = -\sigma uw\left[\left(\frac{v}{w}\right) - 1 - \ln\left(\frac{v}{w}\right)\right] \leq 0,
\end{aligned}
$$

which shows that E_σ plays the role of a Lyapunov function. Because

$$W_\sigma \subset \{\dot{E}_\sigma = 0\} = \{(u, v, w), v = w > 0\}$$

is invariant, by La'Salle's invariant set theorem, see [63], we can conclude that W_σ is a stable invariant set. $\square$

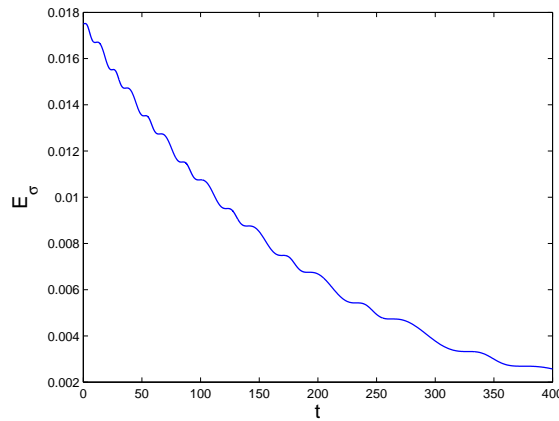The Lyapunov function along the trajectory of (22) is given in Figure 5.

Figure 5: Lyapunov function for the partially perturbed system.

Theorem 4.3.3. *The partially perturbed system (22) has a stable invariant manifold W_σ.*

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It is observed that when $\sigma = 0$, the Lyapunov function E_σ of the partially perturbed system becomes $E_0 = F$, which is exactly the first integral of the unperturbed system. And σ-perturbation changes the center type critical manifold W_0 to an invariant manifold W_σ on which the exponential decays occurs with exponent $\sigma\mu_\sigma$. Since the decay rate is small in σ order, it is natural to suspect that W_σ is approached in the oscillatory way even though the periodic orbits are all broken.

To see the oscillation, we will introduce the following transformation, which is similar to (18) for the unperturbed system,

$$(1 + \sigma)\left[(u - \mu_\sigma) + \mu_\sigma \ln\left(\tfrac{\mu_\sigma}{u}\right)\right] = E_\sigma \cos^2 \theta,$$
$$(v - w) + w \ln\left(\tfrac{w}{v}\right) = E_\sigma \sin^2 \theta,$$

under which, system (22) becomes

$$\begin{cases} \dot{E}_\sigma &= -\sigma u E_\sigma \sin^2 \theta, \\[2mm] \dot{\theta} &= \tfrac{(1+\sigma)}{2E_\sigma}\left(\tfrac{u-\mu_\sigma}{\cos\theta}\right)\left(\tfrac{v-w}{\sin\theta}\right) - \tfrac{\sigma u}{2} \sin\theta\cos\theta, \\[2mm] \dot{w} &= -\sigma u w. \end{cases} \qquad (25)$$

Obviously θ indicates the angle about the oscillation axis W_σ. The first equation in (25) shows that $E_\sigma = 0$ is a stable equilibrium, in other words, W_σ is stable. And the second equation shows that the oscillation takes place as $w > \underline{w} \sim \sigma^2$ because

$$\frac{(1 + \sigma)}{2E_\sigma}\left(\frac{u - \mu_\sigma}{\cos\theta}\right)\left(\frac{v - w}{\sin\theta}\right) - \frac{\sigma u}{2}\sin\theta\cos\theta > 0$$

which can be easily checked.

Also from equation (25), it follows that

$$\frac{dE_\sigma}{dw} = \frac{E_\sigma}{w}\sin^2\theta \le \frac{E_\sigma}{w}.$$

Thus the comparison lemma for ODEs [27] implies that

$$\frac{E_\sigma(t)}{E_\sigma(t_0)} \ge \frac{w(t)}{w(t_0)}, \qquad t \ge t_0.$$

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4.3.2 Lyapunov Type Numbers for W_σ.

In the previous section, we shows that W_σ is a stable invariant manifold in two different way, by constructing a Lyapunov function and by introducing a polar-like transformation. In this section, we will try to compute the Lyapunov type numbers which show not only the stability of W_σ, but also the persistence of W_σ under any smooth perturbation. And the latter will be very important for studying the existence of oscillation axis in the perturbed system (11).

Consider a general autonomous system with C^r vector field $V(x)$, that is,

$$\dot{x} = V(x), \qquad x \in \mathbb{R}^n. \tag{26}$$

Let $M \subset \mathbb{R}^n$ be a closed connected C^r manifold with boundary. Denote by $\phi_t(P)$, $P \in M$, the flow generated by (26).

Definition 4.3.4. *Manifold M is overflowing invariant under ϕ_t if $\phi_t(P) \in M$ for any $P \in \bar{M}$ and $t \leq 0$, and the vector field V is pointing strictly outward and is nonzero on the bounary ∂M of M.*

The definition of Lyapunov type numbers has several different versions, here we will use a more computable form as follows.

Definition 4.3.5. *The generalized Lyapunov type numbers are defined as*

$$\gamma_L(p) = \varlimsup_{t \to -\infty} \left\| \pi_p^N D\phi_t(p) \right\|^{\frac{1}{t}}, \qquad \sigma_L(p) = \varlimsup_{t \to -\infty} \frac{\log \left\| D\phi_t(p)\pi_p^T \right\|}{\log \left\| \pi_p^N D\phi_t(p) \right\|}, \quad if\ \gamma_L(p) < 1,$$

where $\| \cdot \|$ can be any matrix norm.

Theorem 4.3.6. *[18] Suppose that M is a C^r manifold with boundary, and overflowing invariant under ϕ_t with $\gamma_L(P) < 1$ and $\sigma_L(P) < \frac{1}{r}$ for all $P \in M$. Then, for any C^r vector field $\tilde{V}$ which is C^1-close to V, there exists a C^r manifold $\tilde{M}$ with boundary such that $\tilde{M}$ is C^r-close to M, has the same dimension as M, and is overflowing invariant under the flow induced by $\tilde{V}$.*

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Some useful properties of generalized Lyapunov type numbers and more details about normal hyperbolicity can also be found in [74, 76].

Theorem 4.3.7. *The portion of* W_σ,

$$W'_\sigma = \left\{ (u, v, w), \quad u = \mu_\sigma, \ v = w \geq \underline{w} = \frac{\sigma^2 \mu_\sigma^2}{4} > 0 \right\},$$

is overflowing invariant. And its Lyapunov type numbers are $\gamma_L < 1$ *and* $\sigma_L \geq 2$.

<u>Proof:</u> Because the solution on W_σ is given by $u = \mu_\sigma$ and $v = w = w_* e^{-\sigma \mu_\sigma t}$ for any $w_* > 0$, it is obvious that W'_σ is a C^∞ overflowing invariant manifold. Note that for any $p = (u_*, v_*, w_*) \in W'_\sigma$, the tangent space at p, $T_p W_\sigma$, is exactly the straight line on which W_σ is lying, and the normal space is

$$N_p W_\sigma = \{ X, \quad \langle X - p, \vec{n} \rangle = 0 \}, \qquad \vec{n} = [0, 1, 1]^T.$$

Denote by π_p^T and π_p^N the projection onto the tangent space and normal space, respectively, then they can be characterized by the matrices

$$\pi_p^T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \qquad \pi_p^N = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

Let ϕ_t be the flow induced by the vector field in (22), and ∇F is the Jacobian of this vector field, then we have the ajoint equation about $D\phi_t(p)$

$$\frac{d}{dt} [D\phi_t(p)] = \nabla F(p) [D\phi_t(p)].$$

where, precisely

$$\nabla F = \begin{bmatrix} w - v & -u & u \\ v & u - 1 & 0 \\ -\sigma w & 0 & -\sigma u \end{bmatrix} \Rightarrow \nabla F(p) = \begin{bmatrix} 0 & -\mu_\sigma & \mu_\sigma \\ w_* e^{-\sigma \mu_\sigma t} & -\sigma \mu_\sigma & 0 \\ -\sigma w_* e^{-\sigma \mu_\sigma t} & 0 & -\sigma \mu_\sigma \end{bmatrix}$$

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and consequently $D\phi_t(p) = e^{\int_0^t \nabla F(p)ds}$ with

$$P = \int_0^t \nabla F(p)ds = \begin{bmatrix} 0 & -\mu_\sigma t & \mu_\sigma t \\ \frac{w_*}{\sigma\mu_\sigma}(1 - e^{-\sigma\mu_\sigma t}) & -\sigma\mu_\sigma t & 0 \\ \frac{w_*}{\mu_\sigma}(e^{-\sigma\mu_\sigma t} - 1) & 0 & -\sigma\mu_\sigma t \end{bmatrix}.$$

Since $p \in W'_\sigma$, that is, $w_* \geq \underline{w}$, we can see that for any $t < 0$, A has three eigenvalues

$$\lambda_1 = \lambda_r = -\sigma\mu_\sigma t, \qquad \lambda_{2,3} = \frac{1}{2}(\lambda_r \pm i\lambda_i), \qquad \lambda_i = \sqrt{-\frac{4w_*t}{\sigma\mu_\sigma}(e^{\lambda_r} - 1) - \lambda_r^2}.$$

Note that $\lambda_{2,3}$ are complex. The associated eigenvectors are

$$\vec{v}_1 = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \qquad \vec{v}_{2,3} = \begin{bmatrix} \frac{2t(\lambda_r \mp i\lambda_i)}{\lambda_r^2 + \lambda_i^2} \\ -1 \\ \sigma \end{bmatrix}.$$

Define

$$Q = \begin{bmatrix} 0 & \frac{2t(\lambda_r - i\lambda_i)}{\lambda_r^2 + \lambda_i^2} & \frac{2t(\lambda_r + i\lambda_i)}{\lambda_r^2 + \lambda_i^2} \\ 1 & -1 & -1 \\ 1 & \sigma & \sigma \end{bmatrix} \Rightarrow Q^{-1} = \begin{bmatrix} 0 & \sigma\mu_\sigma & \mu_\sigma \\ \frac{i(\lambda_r^2 + \lambda_i^2)}{4\lambda_i t} & \frac{\mu_\sigma(\lambda_i - i\lambda_r)}{-2\lambda_i} & \frac{\mu_\sigma(\lambda_i - i\lambda_r)}{2\lambda_i} \\ \frac{i(\lambda_r^2 + \lambda_i^2)}{-4\lambda_i t} & \frac{\mu_\sigma(\lambda_i + i\lambda_r)}{-2\lambda_i} & \frac{\mu_\sigma(\lambda_i + i\lambda_r)}{2\lambda_i} \end{bmatrix}$$

and then we will have

$$Q^{-1}PQ = \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \Rightarrow e^\Lambda = \begin{bmatrix} e^{\lambda_r} & 0 & 0 \\ 0 & e^{\frac{1}{2}(\lambda_r + i\lambda_i)} & 0 \\ 0 & 0 & e^{\frac{1}{2}(\lambda_r - i\lambda_i)} \end{bmatrix}.$$

Therefore

$$e^P = Qe^\Lambda Q^{-1}$$

$$= \mu_\sigma e^{\frac{\lambda_r}{2}} \begin{bmatrix} \frac{\cos\frac{\lambda_i}{2} - \frac{\lambda_r}{\lambda_i}\sin\frac{\lambda_i}{2}}{\mu_\sigma} & -\frac{2t}{\lambda_i}\sin\frac{\lambda_i}{2} & \frac{2t}{\lambda_i}\sin\frac{\lambda_i}{2} \\ \frac{(\lambda_r^2 + \lambda_i^2)\sin\frac{\lambda_i}{2}}{2\mu_\sigma\lambda_i t} & \sigma e^{\frac{\lambda_r}{2}} + \frac{\lambda_r}{\lambda_i}\sin\frac{\lambda_i}{2} + \cos\frac{\lambda_i}{2} & e^{\frac{\lambda_r}{2}} - \frac{\lambda_r}{\lambda_i}\sin\frac{\lambda_i}{2} - \cos\frac{\lambda_i}{2} \\ \frac{\sigma(\lambda_r^2 + \lambda_i^2)\sin\frac{\lambda_i}{2}}{-2\mu_\sigma\lambda_i t} & \sigma\left(e^{\frac{\lambda_r}{2}} - \frac{\lambda_r}{\lambda_i}\sin\frac{\lambda_i}{2} - \cos\frac{\lambda_i}{2}\right) & e^{\frac{\lambda_r}{2}} + \sigma\frac{\lambda_r}{\lambda_i}\sin\frac{\lambda_i}{2} + \sigma\cos\frac{\lambda_i}{2} \end{bmatrix}$$

Now we can consider the generalized Lyapunov-type numbers as defined below

$$\gamma_L(p) = \overline{\lim_{t\to-\infty}} \left\|\pi_p^N D\phi_t(p)\right\|^{\frac{1}{t}}, \qquad \sigma_L(p) = \overline{\lim_{t\to-\infty}} \frac{\log\left\|D\phi_t(p)\pi_p^T\right\|}{\log\left\|\pi_p^N D\phi_t(p)\right\|}, \qquad \text{if } \gamma_L(p) < 1,$$

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where $\|\cdot\|$ is l_2 norm, that is, for any matrix A of $n \times n$, $\|A\|_2 = \left(\sum_{i,j=1}^{n} |a_{ij}|^2 \right)^{\frac{1}{2}}$.

Because

$$\pi_p^N D\phi_t(p) = e^{\frac{\lambda_r}{2}} \begin{bmatrix} \cos \frac{\lambda_i}{2} - \frac{\lambda_r}{\lambda_i} \sin \frac{\lambda_i}{2} & -\frac{2\mu_\sigma t}{\lambda_i} \sin \frac{\lambda_i}{2} & \frac{2\mu_\sigma t}{\lambda_i} \sin \frac{\lambda_i}{2} \\ \frac{(\lambda_r^2 + \lambda_i^2) \sin \frac{\lambda_i}{2}}{4\mu_\sigma \lambda_i t} & \frac{1}{2} \left(\frac{\lambda_r}{\lambda_i} \sin \frac{\lambda_i}{2} + \cos \frac{\lambda_i}{2} \right) & -\frac{1}{2} \left(\frac{\lambda_r}{\lambda_i} \sin \frac{\lambda_i}{2} + \cos \frac{\lambda_i}{2} \right) \\ \frac{(\lambda_r^2 + \lambda_i^2) \sin \frac{\lambda_i}{2}}{-4\mu_\sigma \lambda_i t} & -\frac{1}{2} \left(\frac{\lambda_r}{\lambda_i} \sin \frac{\lambda_i}{2} + \cos \frac{\lambda_i}{2} \right) & \frac{1}{2} \left(\frac{\lambda_r}{\lambda_i} \sin \frac{\lambda_i}{2} + \cos \frac{\lambda_i}{2} \right) \end{bmatrix}$$

and

$$D\phi_t(p)\pi_p^T = e^{\lambda_r} \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix} = e^{\lambda_r}\pi_p^T,$$

and as $w_* \geq \underline{w} > 0$ and t negatively large enough,

$$\left| \frac{\lambda_r}{\lambda_i} \right| < 1, \quad \left| \frac{t}{\lambda_i} \right| < 1, \quad \left| \frac{\lambda_r^2 + \lambda_i^2}{\lambda_i t} \right| = \frac{4w_*}{\sigma\mu_\sigma\lambda_i} \left(e^{\lambda_r} - 1 \right) \sim \frac{e^{\frac{\lambda_r}{2}}}{2\sqrt{-w_* t}},$$

we will have

$$\gamma_L(p) = \lim_{t \to -\infty} \left[\frac{e^{\lambda_r}}{(-t)^{\frac{1}{2}}} \right]^{\frac{1}{t}} = \lim_{t \to -\infty} e^{\frac{\lambda_r}{t}} = e^{-\sigma\mu_\sigma} < 1,$$

which implies that $\sigma_L(p)$ is well defined. And obviously $\|D\phi_t(p)\pi_p^T\| = e^{\lambda_r}$, thus

$$\sigma_L(p) \geq \lim_{t \to -\infty} \frac{\log e^{\lambda_r}}{\log e^{\frac{\lambda_r}{2}}} = 2.$$

$\square$

Remark 4.3.8. *In Theorem 4.3.7, $\gamma_L < 1$ infers the stability of W'_σ, that is, W'_σ is a stable overflowing invariant manifold. To apply Fenichel's result to show the persistence of W'_σ, we need the condition $\sigma_L < \frac{1}{r}$ if we suppose W'_σ is a C^r manifold. However Theorem 4.3.7 also shows that $\sigma_L \geq 2 > 1$, Fenichel's theorem is not applicable. Thus at this stage, we cannot draw any conclusion about the persistence of W'_σ. But the persistence of W'_σ under the perturbation given in (11) will be proven in section 4.4.1 by using the exponential dichotomy.*

4.3.3 Oscillation Time.

We already show that the oscillation remains in the partially perturbed system (12), but no periodic orbit exists because of the dissipation, which can be seen from $\dot{E}_\sigma \leq 0$. Thus we need a reference to study the oscillation time. Recall the Poincaré section Σ used for analyzing period function. Since the invariant manifolds W_0 and W_σ for the unperturbed and partially perturbed systems are all in Σ, and they all play the role of oscillation axis, we will still use Σ as the reference to consider the oscillation time. But , Σ_+ and Σ_- will be changed to

$$\Sigma_+^\sigma = \{(u, v, w) \in \Sigma, u > \mu_\sigma\}, \qquad \Sigma_-^\sigma = \{(u, v, w) \in \Sigma, u < \mu_\sigma\}.$$

Apparently the partially perturbed flow crosses Σ transversely when it is away from W_σ. This is also because the transversality is robust and persistent under the perturbation.

Lemma 4.3.9. *For any $E > 0$ and $w > 0$, the period function for system (17) has the following bounds*

$$\frac{\min\{E, 1\}}{\max\{w, 1\}} T(1, 1) \leq T(E, w) \leq \frac{\max\{E, 1\}}{\min\{w, 1\}} T(1, 1).$$

<u>Proof:</u> This is the direct consequence of Lemma 4.2.11 and Lemma 4.2.12. □

For any fixed $E^* > 0$ and $w_* > 0$ given in Theorem 4.3.7, define

$$K = \frac{\max\{E^*, 1\}}{\min\{w_*, 1\}} T(1, 1), \qquad \mathcal{T}_o = \{(u, v, w) \in \mathbb{R}^+, F(u, v; w) \leq E^*, w \geq w_*\}.$$

Clearly any periodic orbit in $\mathcal{T}_o$ is uniformly bounded above by K. The following theorem is a modified version of Proposition 2.1 in [75] for our system.

Theorem 4.3.10. *Let $X_0^{E,w}(t)$ be a periodic orbit of unperturbed system (12) with period $T(E, w) < K$. Then for sufficiently small $\sigma > 0$, there exists a perturbed solution $X_\sigma^{E,w}(t)$ such that*

$$X_\sigma^{E,w}(t) = X_0^{E,w}(t) + \sigma X_1^{E,w}(t) + o(\sigma)$$

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uniformly for $t \in [0, T(E, w)]$, where $X_1^{E,w}$ is the solution of the first variational equation of
(12).

It follows from Theorem 4.3.10 that the partial perturbation in σ is a regular perturbation in the oscillation zone. So is the complete perturbation in ε. And the first return time T_σ on Σ_+ is also close to the period T_0 of the unperturbed periodic solution.

To be more precise, let $P_{2k} = (u_{2k}, w_{2k}, w_{2k}) \in \Sigma_+$ and $P_{2k+1} \in \Sigma_-$ such that

$$P_{2k+1} = \phi_{t_{2k}}(P_{2k}), \qquad P_{2k+2} = \phi_{t_{2k+1}}(P_{2k+1}),$$

where ϕ_t is the flow induced by the partially perturbed system (22).

Lemma 4.3.11. *Suppose that P_n and t_n are as defined above, then*

$$t_{n+1} = \frac{1}{\sigma \mu_\sigma} (\ln w_n - \ln w_{n+1}).$$

Proof: Note that

$$\left[\ln(vw^{\frac{1}{\sigma}})\right]' = \frac{\dot{v}}{v} + \frac{1}{\sigma}\frac{\dot{w}}{w} = (u - 1) - u = -1$$

from which it follows that

$$t_{n+1} = \ln\left(v_n w_n^{\frac{1}{\sigma}}\right) - \ln\left(v_{n+1} w_{n+1}^{\frac{1}{\sigma}}\right).$$

Since $v_n = w_n$ and $v_{n+1} = w_{n+1}$, we finally have

$$t_{n+1} = \left(1 + \frac{1}{\sigma}\right)(\ln w_n - \ln w_{n+1}) = \frac{1}{\sigma \mu_\sigma}(\ln w_n - \ln w_{n+1}).$$

Theorem 4.3.12. *Suppose that E^*, w_*, K and $\mathcal{T}^o$ are as given above. Then for any initial P_0 with $w_0 > w_*$, there exists $n(\sigma) - 1$ complete oscillations as w decreasing from w_0 to w_* where*

$$n(\sigma) \geq \frac{\ln w_0 - \ln w_*}{2\sigma K}.$$

Proof: Because w is monotonically decreasing, there must exist n such that

$$\phi_{t_{2n-3}}^w(P_0) \geq w_*, \qquad \phi_{t_{2n-1}}^w(P_0) < w_*, \qquad n \geq 1$$

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where ϕ_t^w is the projection of the flow ϕ_t onto w and $t_{-k} = 0$ for $k > 0$. By Lemma 4.3.11, we know that

$$\sum_{k=0}^{n-1} (t_{2k} + t_{2k+1}) = \frac{1}{\sigma\mu_\sigma} \left(\ln w_0 - \ln \phi_{t_{2n}}^w (P_0) \right).$$

On the other hand, Theorem 4.3.10 implies that $t_{2k} + t_{2k+1} = T(\phi_{t_{2k-2}+t_{2k-1}}(P_0))[1 + O(\sigma)]$ with $T \leq K$. Therefore we have

$$\frac{1}{\sigma\mu_\sigma} \left(\ln w_0 - \ln \phi_{t_{2n-1}}^w (P_0) \right) \leq 2nK$$

and consequently

$$n(\sigma) \geq \frac{\ln w_0 - \ln w_*}{2\sigma K}.$$

Theorem 4.3.13. *Suppose that $P_0 \in \Sigma_+ \cap \mathcal{T}_o$ is the initial point in the oscillation zone. Then the time T^o spent in the oscillation zone is given by*

$$T^o \sim \frac{1}{\sigma\mu_\sigma} \ln\left(\frac{4w_0}{\sigma^2\mu_\sigma^2} \right).$$

Proof: It follows directly from Lemma 4.3.11 that

$$T^o = \frac{1}{\sigma\mu_\sigma} (\ln w_0 - \ln w_n)$$

where $w_n \geq \underline{w} = \frac{\sigma^2\mu_\sigma^2}{4}$ and $w_{n+1} < \underline{w}$. Therefore

$$T^o \sim \frac{1}{\sigma\mu_\sigma} \ln\left(\frac{4w_0}{\sigma^2\mu_\sigma^2} \right).$$

Remark 4.3.14. *By Theorem 4.3.12, we know that the number n of complete oscillation in the oscillation zone is in the algebraic order of σ^{-1}, that is, the smaller σ will produce more oscillations. And Theorem 4.3.13 shows that the oscillation time T^o spent in the oscillation zone is finite but also in the algebraic order of σ^{-1}, thus smaller σ results in the oscillation lasting in a longer time. Moreover, from the discussion in the following section, we will see that in the perturbed system (11), ε introduces a regular perturbation in the oscillation zone. Therefore all the discussion in this section is also valid in the oscillation zone of the perturbed system.*

4.4 Perturbed Lotka-Volterra System.

In this section, we will study the perturbed Lotka-Volterra system. The discussion consists mainly in two parts. One is about the oscillation, the other is about the dynamical transition from oscillation into a non-oscillation zone.

4.4.1 Existence of Oscillation Axis

In this section, we will consider the oscillation zone by showing the existence of oscillation axis for the perturbed Lotka-Volterra system (11).

Recall that the partially perturbed system admits an overflowing invariant manifold

$$W'_\sigma = \left\{ (u, v, w), \quad u = \mu_\sigma,\ v = w \geq \underline{w} \right\},$$

which plays the role of the oscillation axis for that system. Thus it is natural to ask if there is an oscillation axis for the perturbed system.

Since W'_σ is the oscillation axis in the partially perturbed system (22), it is a natural idea to show the existence of oscillation axis in the perturbed system by studying the persistence of W'_σ. However, Theorem 4.3.7 shows that $\sigma_L \geq 2 > 1$, thus Fenichel's theorem cannot be applied directly. In other word, it is not ensured that W_σ can persist under any small smooth perturbation. Nevertheless, it is enough to show the persistence under the specific perturbation we study. And indeed this is true. Inspired by the idea of Sakamoto in [61], I will prove the persistence by considering the exponential dichotomy of the invariant manifold W'_σ. But the difference from Sakamoto's proof is that we will only consider the bounded portion of W'_σ in the reaction zone and in the finite time interval. The first restriction will provide boundedness of the vector field on the right hand side of (11), and second one will ensure that the portion of central axis, which is entering the transition layer, approaching the equilibrium and resulting in singular perturbation, is excluded. Indeed, it must be a regular perturbation in the oscillation zone.

In the following, we will prove the existence of such an oscillation axis. Before doing that, we will first review some results on exponential dichotomy.

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Lemma 4.4.1. *[29] Suppose that for some integer k with $0 \leq k \leq n$ and some real number $v > 0$, matrix A has k eigenvalues with real part $\Re(\lambda) < -2v$ and $n - k$ eigenvalues with $\Re(\lambda) > 2v$. Then there exist projection operators P and Q and constant $K > 0$ such that $P + Q = I$ and*

$$|\Phi(t, s) \circ P| \leq K e^{-v(t-s)}, \qquad t \geq s$$

$$|\Phi(t, s) \circ Q| \leq K e^{v(t-s)}, \qquad t \leq s,$$

where Φ is the fundamental matrix solution of system $\dot{x} = A(t)x$. And an operator satisfying the above equalities is called to have **exponential dichotomy**.

For any $\rho \geq 0$ and a normed space $(\mathbb{R}^m, |\cdot|)$, define

$$|\psi|_\rho = \sup_{t \in \mathbb{R}^+} e^{-\rho t} |\psi(t)|$$

for any $\psi : \mathbb{R} \to \mathbb{R}^m$, and

$$BC^\rho(\mathbb{R}^m) = \left\{ \psi \in C^0(\mathbb{R}^m), \quad |\psi|_\rho < \infty \right\}.$$

Lemma 4.4.2. *[58] (a) For $\rho > 0$ and $w \in BC^\rho(\mathbb{R}^m)$, define $w_r(t, s) = \int_s^t w(\tau)e^{r\tau}d\tau$ for $s, t \in \mathbb{R}^+$ and $s \leq t$. Then $w_0(t, 0) \in BC^\rho(\mathbb{R}^m)$ and $|w_0(t, 0)|_\rho \leq \frac{1}{\rho}|w|_\rho$.*

(b) For any $\psi_1 \in BC^{\rho_2}(\mathbb{R}^n)$, the solution ψ of $\psi' = A(w(t))\psi + \psi_1(s)$ is given by

$$\psi(t) = \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, w)\psi_1(s)ds, \qquad t \in \mathbb{R}^+$$

and $|\psi|_{\rho_2} \leq \frac{2K|\psi_1|_{\rho_1}}{v + \sigma\rho_1}$ for any $0 < \rho_1 < \rho_2$, where $\Phi^\sigma(t, s, w)$ is the fundamental solution matrix of the linear system $X' = A(w(t))X$ for any given $w(t)$.

Proof: (a) Note that

$$|w_r(t, s)| = \left| \int_s^t w(\tau)e^{r\tau}d\tau \right| \leq |w|_\rho \int_s^t e^{(\rho+r)\tau}d\tau = \frac{|w|_\rho}{\rho + r}(e^{(\rho+r)t} - e^{(\rho+r)s}).$$

Thus

$$|w_0(t, 0)|_\rho \leq \frac{|w|_\rho}{\rho} \sup_{t \in \mathbb{R}^+} \{(e^{\rho t} - 1)e^{-\rho t}\} \leq \frac{|w|_\rho}{\rho}.$$

(b)

$$
\begin{aligned}
|\psi(t)| &= |\psi_1|_{\rho_2} \frac{1}{\sigma} \int_0^t |\Phi^\sigma(t, s, w)|\, e^{\rho_2 s}ds \leq \frac{K|\psi_1|_{\rho_2}}{\sigma} \int_0^t e^{-\frac{v}{\sigma}(t-s)}e^{\rho_2 s}ds \\
&= \frac{K|\psi_1|_\rho e^{-\frac{v}{\sigma}t}}{\sigma(\frac{v}{\sigma} + \rho_2)} e^{(\frac{v}{\sigma}+\rho_2)s}\Big|_{s=0}^{s=t} = \frac{K|\psi_1|_{\rho_2}}{v + \sigma\rho_2} \left(e^{\rho_2 t} - e^{-\frac{v}{\sigma}t} \right)
\end{aligned}
$$

which implies that

$$|\psi(t)|_{\rho_2} \leq \frac{K|\psi_1|_{\rho_2}}{\nu + \sigma\rho_2} \leq \frac{K|\psi_1|_{\rho_1}}{\nu + \sigma\rho_1}$$

because $|\psi_1|_{\rho_2} \leq |\psi_1|_{\rho_1}$ as $\rho_2 \geq \rho_1$. $\qquad\square$

Let $a, b > 0$ be such that $a(\sigma), b(\sigma) \to 0$ as $\sigma \to 0$. By the following transformation

$$u \to x + 1 - a, \qquad v \to y + w + b, \qquad w \to w,$$

system (11) can be rewritten as

$$\begin{cases} \sigma X' & = & A(w)X + G(X, w, \sigma) \\ w' & = & F(X, w, \sigma) \end{cases} \qquad (27)$$

where $X = (x, y)^T$ and

$$F(X, w, \sigma) = -(x + 1 - a)[w - \varepsilon\sigma(x + 1 - a)]$$

$$G(X, w, \sigma) = \begin{bmatrix} -xy - \varepsilon(\sigma x^2 - y^2) + (1-a)b + \varepsilon(w+b)^2 - \varepsilon\sigma(1-a)^2 \\ xy - (a+\varepsilon)(w+b) + (\sigma w - \varepsilon)(1-a) - \varepsilon\left[\sigma^2 x^2 + y^2 + (w+b)^2 - \xi + \frac{w}{\sigma} + \sigma^2(1-a)^2\right] \end{bmatrix}$$

$$A(w) = \begin{bmatrix} -b - 2\varepsilon\sigma(1-a) & 2\varepsilon(w+b) - (1-a) \\ (1+\sigma)w + b - \varepsilon - 2\varepsilon\sigma^2(1-a) & -a - 2\varepsilon(w+b) - \varepsilon \end{bmatrix}.$$

Then

$$A'(w) = \begin{bmatrix} 0 & 2\varepsilon \\ (1+\sigma) & -2\varepsilon \end{bmatrix}, \quad \nabla_X F = \begin{bmatrix} 2\varepsilon\sigma(x + 1 - a) - w \\ 0 \end{bmatrix}, \quad D_w F = x + 1 - a,$$

$$D_X G = \begin{bmatrix} -y - 2\varepsilon\sigma x & 2\varepsilon y - x \\ y - 2\varepsilon\sigma^2 x & x - 2\varepsilon y \end{bmatrix}, \quad D_w G = \begin{bmatrix} 2\varepsilon(w+b) \\ \sigma(1-a) - (a+\varepsilon) - 2\varepsilon(w+b) - \frac{\varepsilon}{\sigma} \end{bmatrix},$$

Lemma 4.4.3. *For $\sigma > 0$ sufficiently small and $w(t) \in C^0(\mathbb{R}^+)$ satisfying $w(t) \geq \underline{w} \sim \frac{\sigma^2\mu_\sigma^2}{4}$, system $\sigma X' = A(w(t))X$ has uniform exponential dichotomy with exponent $\nu = \frac{a+b}{4}$.*

Proof: Note that

$$\text{tr}(A) = -a - b - \varepsilon[1 + 2\sigma(1-a) + 2(w+b)] < -a - b$$

and

$$\Delta = \text{tr}(A)^2 - 4\det(A) = c_1 w^2 + c_2 w + c_3$$

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where

$$c_1 = 4\varepsilon(2 + 2\sigma + \varepsilon),$$

$$c_2 = -4\left[1 + \sigma + \varepsilon^2(1 + 2\sigma + 4\sigma^2) - b\varepsilon(3 + 2\varepsilon + 2\sigma) - a(1 + \varepsilon + \sigma + 2\varepsilon^2\sigma(1 + 2\sigma))\right]$$

$$c_3 = b^2(1 + 2\varepsilon)^2 + \varepsilon[4 + \varepsilon(1 - 2\sigma)^2 + 8\sigma^2] + a^2[(1 + 2\varepsilon\sigma)^2 + 8\varepsilon\sigma^2]$$

$$-2b[2 + \varepsilon - 2\varepsilon\sigma + \varepsilon^2(2 + 4\sigma + 8\sigma^2)] - 2a\varepsilon[1 + 2\sigma(1 - \varepsilon) + 4\sigma^2(2 + \varepsilon)]$$

$$+2ab[1 + 2\varepsilon(1 - \sigma) + 4\varepsilon^2\sigma(1 + 2\sigma)].$$

Note that

$$c_1 \sim 4\varepsilon, \qquad c_2 \sim -4, \qquad c_3 \sim \max\{4b, a^2, 4\varepsilon\},$$

we will see that $\Delta < 0$ as $\frac{c_3}{4} \sim \underline{w} \leq w \leq \sigma\xi$. Therefore A will have two complex eigenvalues whose real parts are exactly $\frac{\mathrm{tr}(A)}{2}$. Denote by $\Phi^\sigma(t, s)$ the fundamental matrix solution of $\sigma X' = A(w(t))X$ and set $v = \frac{a+b}{4}$, then $\mathrm{tr}(A) < -4v$. Because all the eigenvalues have negative real parts, there exists constant $K > 0$ such that

$$|\Phi^\sigma(t, s, w))| \leq K e^{-\frac{v}{\sigma}(t-s)}, \qquad t \geq s.$$

Note that v is independent of $w \geq \underline{w}$, thus the exponential dichotomy is uniform. $\qquad\square$

Since system (11) is positively stable and we are interested only in its forward dynamics, the following discussion is for $t \in \mathbb{R}^+$. And it can be verified that for any initial $\eta = w(t_0)$ at fixed initial time $t_0 > 0$, the solution of (27) can be written as

$$X(t) = \frac{1}{\sigma}\int_0^t \Phi^\sigma(t, s, w(s))G(X(s), w(s), \sigma)ds$$

$$w(t) = \eta + \int_{t_0}^t F(X(s), w(s), \sigma)ds$$

see [58, 61] for the general setup for $t \in \mathbb{R}$.

Denote by ϕ_t the flow of system (11), then $\tilde{\mathcal{T}} = \phi_{t_0}(\mathcal{T}) \subset \mathcal{T}$ is compact because $\mathcal{T}$ is compact and positively invariant under the continuous flow ϕ_t. Set

$$\bar{u} = \max\left\{u, (u, v, w) \in \tilde{\mathcal{T}}\right\}, \quad \bar{v} = \max\left\{v, (u, v, w) \in \tilde{\mathcal{T}}\right\}, \quad \bar{w} = \max\left\{w, (u, v, w) \in \tilde{\mathcal{T}}\right\}$$

$$\underline{u} = \min\left\{u, (u, v, w) \in \tilde{\mathcal{T}}\right\}, \quad \underline{v} = \min\left\{v, (u, v, w) \in \tilde{\mathcal{T}}\right\},$$

then functions F and G are C^r bounded for any $r > 0$ on $\tilde{\mathcal{T}}$.

On the other hand, for any given function $X(t)$ and initial $w(t_0) = \eta \in [\underline{w}, \bar{w}]$, the second equation in (27) has a unique solution, denoted by $H_\sigma(\eta, X)(t)$. More precisely, we have

$$H_\sigma(\eta, X)(t) = \eta e^{-\int_{t_0}^t (x(s)+1-a)ds} + \varepsilon\sigma \int_{t_0}^t (x(s) + 1 - a)^2 e^{-\int_s^t (x(\tau)+1-a)d\tau} ds.$$

Lemma 4.4.4. *For fixed $t_0 > 0$, $\eta \in (\underline{w}, \bar{w})$ and $a, \delta > 0$ sufficiently small, if $|X| < \delta$, then there exists $t_1(\eta) > 0$ such that*

$$\underline{w} \le H(\eta, X)(t) \le e^{\mu_+ t_0} (\eta + \varepsilon\sigma\mu_+),$$

for $t \in [0, t_1(\eta)]$, where $\mu_\pm = 1 - a \pm \delta$.

Proof: Suppose $|X| < \delta$. For $t \in [0, t_0]$,

$$H_\sigma(\eta, X)(t) \le \eta e^{\mu_+(t_0-t)} + \varepsilon\sigma \int_t^{t_0} \mu_+^2 e^{\mu_+(s-t)} ds \le \eta e^{\mu_+ t_0} + \varepsilon\sigma\mu_+ \left(e^{\mu_+(t_0-t)} - 1 \right).$$

$$H_\sigma(\eta, X)(t) \ge \eta e^{\mu_-(t_0-t)} - \varepsilon\sigma\mu_+^2 \int_t^{t_0} e^{\mu_+(s-t)} ds = \eta e^{\mu_-(t_0-t)} - \varepsilon\sigma\mu_+ \left(e^{\mu_+(t_0-t)} - 1 \right) \ge \eta$$

because $\varepsilon \ll \sigma$ and $\eta > \underline{w} \sim \sigma^2$. And for $t > t_0$, we have

$$H_\sigma(\eta, X)(t) \le \eta e^{-\mu_-(t-t_0)} + \varepsilon\sigma \int_{t_0}^t \mu_+^2 e^{-\mu_-(t-s)} ds = \eta e^{-\mu_-(t-t_0)} + \varepsilon\sigma\frac{\mu_+^2}{\mu_-} \left(1 - e^{-\mu_-(t-t_0)} \right),$$

which implies that $H_\sigma(\eta, X)(t) < \underline{w} \sim \sigma^2$ for t sufficiently large. On the other hand, we know that $H(\eta, X)(0) = \eta > \underline{w}$, thus

$$t_1(\eta) = \min\{t > 0, \ H(\eta, X)(t) \le \underline{w} \text{ for all } |X| < \delta\} > t_0$$

is well defined. Precisely $t_1(\eta) \ge t_0 + \frac{1}{\mu_+} \left(\ln \eta - \ln \underline{w} \right)$ for all $\eta \in (\underline{w}, \bar{w})$. Then it follows immediately that, for any $\eta \in (\underline{w}, \bar{w})$ and $|X| < \delta$,

$$\underline{w} \le H_\sigma(\eta, X)(t) \le e^{\mu_+ t_0} (\eta + \varepsilon\sigma\mu_+), \qquad t \in [0, t_1(\eta)].$$

$\square$

Denote by $|\psi|_{\rho,\eta} = \sup_{t \in [0, t_1(\eta)]} e^{-\rho t} |\psi|$ the weighted norm on the finite time interval $[0, t_1(\eta)]$.

Lemma 4.4.5. *With $t_0, \eta, a, \delta > 0$ and $t_1(\eta)$ as given in Lemma 4.4.4, if $|X|, |X_0| < \delta$, then*

$$|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)|_{\rho,\eta} \le \left[\frac{\eta}{\rho} e^{(\rho+2\delta)t_0} + \frac{2\varepsilon\sigma\mu_+}{\mu_- - \rho} + \frac{\varepsilon\sigma\mu_+^2}{(\mu_- - 2\delta)(\mu_- - 2\delta - \rho)} \right] |X - X_0|_{\rho,\eta}.$$

for $\rho \in (0, \mu_- - 2\delta)$.

Proof: Define $h(x) = \frac{e^x - 1}{x}$. For any X, X_0 such that $|X|, |X_0| < \delta$, and

$$u_0 = x_0 + 1 - a, \quad u = x + 1 - a \in [\mu_-, \mu_+] \subset [\underline{u}, \bar{u}]$$

Let $\psi_1 = x - x_0 = u - u_0$ and $\psi^s(t) = \int_s^t \psi_1 d\tau$ for $s, t \in [0, t_1(\eta)]$, then $|\psi_1| \leq 2\delta$ and $|\psi^s| \leq 2\delta|t - s|$. Thus,

$$
\begin{aligned}
&|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)| \\
\leq{}& \eta e^{-\int_{t_0}^t u_0 ds} \left| e^{-\int_{t_0}^t (u-u_0) ds} - 1 \right| + \varepsilon\sigma \left| \int_{t_0}^t \left(|u^2 - u_0^2| e^{-\int_s^t u d\tau} + u_0^2 e^{-\int_s^t u_0 d\tau} \left| e^{-\int_s^t (u-u_0) d\tau} - 1 \right| \right) ds \right| \\
\leq{}& \eta e^{-\mu_- t} \left| \sum_{k=1}^\infty \frac{(\psi^{t_0})^k}{k!} \right| + \varepsilon\sigma \left| \int_{t_0}^t \left(2\mu_+ |\psi_1| e^{-\mu_-|t-s|} + \mu_+^2 e^{-\mu_-|t-s|} \left| \sum_{k=1}^\infty \frac{(\psi^s)^k}{k!} \right| \right) ds \right| \\
\leq{}& \eta e^{-\mu_- t} |\psi^{t_0}| h(|\psi^{t_0}|) + \varepsilon\sigma \left| \int_{t_0}^t \left(2\mu_+ |\psi_1| e^{-\mu_-|t-s|} + \mu_+^2 e^{-\mu_-|t-s|} |\psi^s| h(|\psi^s|) \right) ds \right| \\
\leq{}& \eta e^{-\mu_- t} h(2\delta|t - t_0|) |\psi^{t_0}| + \varepsilon\sigma \left| \int_{t_0}^t \left(2\mu_+ |\psi_1| e^{-\mu_-|t-s|} + \mu_+^2 e^{-\mu_-|t-s|} h(2\delta|t - s|) |\psi^s| \right) ds \right| \\
\leq{}& \eta e^{-\mu_- t} e^{2\delta|t - t_0|} |\psi^{t_0}| + \varepsilon\sigma \left| \int_{t_0}^t \left(2\mu_+ |\psi_1| e^{-\mu_-|t-s|} + \mu_+^2 e^{-(\mu_- - 2\delta)|t-s|} |\psi^s| \right) ds \right|
\end{aligned}
$$

because $h(x) \leq e^x$ for $x \geq 0$. Then, for $t \in [t_0, t_1(\eta)]$,

$$
\begin{aligned}
&|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)| \\
\leq{}& \eta e^{-(\mu_- - 2\delta)t} e^{-2\delta t_0} |\psi^{t_0}| + \varepsilon\sigma \int_{t_0}^t \left(2\mu_+ |\psi_1| e^{-\mu_-(t-s)} + \mu_+^2 e^{-(\mu_- - 2\delta)(t-s)} |\psi^s| \right) ds \\
\leq{}& \frac{\eta}{\rho} e^{-(\mu_- - 2\delta)t} e^{-2\delta t_0} |\psi_1|_{\rho,\eta} (e^{\rho t} - e^{\rho t_0}) + 2\varepsilon\sigma\mu_+ e^{-\mu_- t} \frac{|\psi_1|_{\rho,\eta}}{\mu_- + \rho} \left(e^{(\mu_- + \rho)t} - e^{(\mu_- + \rho)t_0} \right) \\
&+ \varepsilon\sigma\mu_+^2 \int_{t_0}^t e^{-(\mu_- - 2\delta)(t-s)} \frac{|\psi_1|_{\rho,\eta}}{\rho} (e^{\rho t} - e^{\rho s}) ds \\
\leq{}& |\psi_1|_{\rho,\eta} \left[\frac{\eta}{\rho} e^{-(\mu_- - 2\delta)t} e^{-2\delta t_0} (e^{\rho t} - e^{\rho t_0}) + \frac{2\varepsilon\sigma\mu_+}{\mu_- + \rho} \left(e^{\rho t} - e^{(\mu_- + \rho)t_0 - \mu_- t} \right) \right. \\
&\left. + \frac{\varepsilon\sigma\mu_+^2}{\rho} \left(\frac{e^{\rho t}(1 - e^{-(\mu_- - 2\delta)(t-t_0)})}{\mu_- - 2\delta} - \frac{e^{\rho t}(1 - e^{-(\mu_- - 2\delta + \rho)(t-t_0)})}{\mu_- - 2\delta + \rho} \right) \right] \\
\leq{}& |\psi_1|_{\rho,\eta} e^{\rho t} \left[\frac{\eta}{\rho} e^{-(\mu_- - 2\delta)t} e^{-2\delta t_0} (1 - e^{-\rho(t - t_0)}) + \frac{2\varepsilon\sigma\mu_+}{\mu_- + \rho} \left(1 - e^{-(\mu_- + \rho)(t - t_0)} \right) \right. \\
&\left. + \frac{\varepsilon\sigma\mu_+^2}{\rho} \left(\frac{1 - e^{-(\mu_- - 2\delta)(t-t_0)}}{\mu_- - 2\delta} - \frac{1 - e^{-(\mu_- - 2\delta + \rho)(t-t_0)}}{\mu_- - 2\delta + \rho} \right) \right] \\
\leq{}& |\psi_1|_{\rho,\eta} e^{\rho t} \left[\frac{\eta}{\rho} e^{-(\mu_- - 2\delta)t} \left(1 - e^{-\rho(t - t_0)} \right) + \frac{2\varepsilon\sigma\mu_+}{\mu_- + \rho} + \frac{\varepsilon\sigma\mu_+^2 \left(1 - e^{-(\mu_- - 2\delta)(t - t_0)} \right)}{(\mu_- - 2\delta)(\mu_- - 2\delta + \rho)} \right]
\end{aligned}
$$

that is, for any $\rho > 0$,

$$
|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)|_{\rho,\eta} \leq |\psi_1|_{\rho,\eta} \left[\frac{\eta}{\rho} + \frac{2\varepsilon\sigma\mu_+}{\mu_- + \rho} + \frac{\varepsilon\sigma\mu_+^2}{(\mu_- - 2\delta)(\mu_- - 2\delta + \rho)} \right].
$$

And for $t \in [0, t_0]$ and $\rho < \mu_- - 2\delta$,

$$
\begin{aligned}
&|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)| \\
&\leq \quad \eta e^{-(\mu_-+2\delta)t} e^{2\delta t_0} |\psi^{t_0}| + \varepsilon\sigma \int_t^{t_0} \left(2\mu_+ |\psi_1| e^{\mu_-(t-s)} + \mu_+^2 e^{(\mu_--2\delta)(t-s)} |\psi^s| \right) ds \\
&\leq \quad \frac{\eta}{\rho} e^{-(\mu_-+2\delta)t} e^{2\delta t_0} |\psi_1|_{\rho,\eta} (e^{\rho t_0} - e^{\rho t}) + 2\varepsilon\sigma\mu_+ e^{\mu_- t} \frac{|\psi_1|_{\rho,\eta}}{\rho - \mu_-} \left(e^{(\rho-\mu_-)t_0} - e^{(\rho-\mu_-)t} \right) \\
&\qquad + \varepsilon\sigma\mu_+^2 \int_t^{t_0} e^{(\mu_--2\delta)(t-s)} \frac{|\psi_1|_{\rho,\eta}}{\rho} \left(e^{\rho s} - e^{\rho t} \right) ds \\
&\leq \quad |\psi_1|_{\rho,\eta} \left[\frac{\eta}{\rho} e^{-(\mu_-+2\delta)t} e^{2\delta t_0} (e^{\rho t_0} - e^{\rho t}) + \frac{2\varepsilon\sigma\mu_+}{\rho - \mu_-} \left(e^{(\rho-\mu_-)t_0 + \mu_- t} - e^{\rho t} \right) \right. \\
&\qquad + \left. \frac{\varepsilon\sigma\mu_+^2}{\rho} \left(\frac{e^{\rho t}(1 - e^{(\mu_--2\delta-\rho)(t-t_0)})}{\mu_- - 2\delta - \rho} - \frac{e^{\rho t}(1 - e^{(\mu_--2\delta)(t-t_0)})}{\mu_- - 2\delta} \right) \right] \\
&\leq \quad |\psi_1|_{\rho,\eta} e^{\rho t} \left[\frac{\eta}{\rho} e^{-(\mu_-+2\delta)t} e^{2\delta t_0} (e^{\rho(t_0-t)} - 1) + \frac{2\varepsilon\sigma\mu_+}{\rho - \mu_-} \left(e^{(\rho-\mu_-)(t_0-t)} - 1 \right) \right. \\
&\qquad + \left. \frac{\varepsilon\sigma\mu_+^2}{\rho} \left(\frac{1 - e^{(\mu_--2\delta-\rho)(t-t_0)}}{\mu_- - 2\delta - \rho} - \frac{1 - e^{(\mu_--2\delta)(t-t_0)}}{\mu_- - 2\delta} \right) \right] \\
&\leq \quad |\psi_1|_{\rho,\eta} e^{\rho t} \left[\frac{\eta}{\rho} e^{-(\mu_-+2\delta)t} e^{2\delta t_0} \left(e^{\rho(t_0-t)} - 1 \right) + \frac{2\varepsilon\sigma\mu_+}{\mu_- - \rho} + \frac{\varepsilon\sigma\mu_+^2 \left(1 - e^{(\mu_--2\delta)(t-t_0)} \right)}{(\mu_- - 2\delta)(\mu_- - 2\delta - \rho)} \right]
\end{aligned}
$$

that is,

$$
|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)|_{\rho,\eta} \leq |\psi_1|_{\rho,\eta} \left[\frac{\eta}{\rho} e^{(\rho+2\delta)t_0} + \frac{2\varepsilon\sigma\mu_+}{\mu_- - \rho} + \frac{\varepsilon\sigma\mu_+^2}{(\mu_- - 2\delta)(\mu_- - 2\delta - \rho)} \right].
$$

Therefore

$$
|H_\sigma(\eta, X) - H_\sigma(\eta, X_0)|_{\rho,\eta} \leq \left[\frac{\eta}{\rho} e^{(\rho+2\delta)t_0} + \frac{2\varepsilon\sigma\mu_+}{\mu_- - \rho} + \frac{\varepsilon\sigma\mu_+^2}{(\mu_- - 2\delta)(\mu_- - 2\delta - \rho)} \right] |\psi_1|_{\rho,\eta}.
$$

$\square$

Define

$$
\mathcal{F}(X)(t) \;=\; \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, H(\eta, X(s))) G(X(s), H(\eta, X(s)), \sigma) ds,
$$

and

$$
\mathcal{B}_\eta = \left\{ X \in C([0, t_1(\eta)], \mathbb{R}^2), \ |X|_0 \leq \delta \right\}.
$$

Lemma 4.4.6. *[58]. Let σ be sufficiently small, $\psi \in BC^\rho(\mathbb{R}^2)$ and $\rho < \frac{\nu}{\sigma}$. Suppose that $w, w_0 \in C^1 \left([0, t_1(\eta)], (\underline{w}, \bar{w}) \right)$ and*

$$
\tilde{\psi} = \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, w(s)) \psi(s) ds,
$$

then

$$\tilde{\psi} = \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, w_0(s)) \left[(A(w(s)) - A(w_0(s)))\tilde{\psi}(s) + \psi(s) \right] ds.$$

Proof: Note that if

$$\tilde{\psi} = \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, w(s))\psi(s)ds,$$

then $\tilde{\psi}$ solves the following equation

$$\sigma\dot{\tilde{\psi}} = A(w)\tilde{\psi} + \psi. \tag{28}$$

We can also rewrite equation (28) as

$$\sigma\dot{\tilde{\psi}} = A(w_0)\tilde{\psi} + \left[(A(w) - A(w_0))\tilde{\psi} + \psi \right]$$

whose solution can also be written as

$$\tilde{\psi} = \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, w_0(s)) \left[(A(w(s)) - A(w_0(s)))\tilde{\psi}(s) + \psi(s) \right] ds.$$

$\square$

Lemma 4.4.7. $\mathcal{F}$ *is Lipschitz in* $X \in C([0, t_1(\eta)], \mathbb{R}^2)$.

Proof: From Lemma 4.4.6, we know that

$$\frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, H(\eta, X))G(X, H(\eta, X), \sigma)ds$$
$$= \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, H(\eta, X_0)) \left[(A(H(\eta, X)) - A(H(\eta, X_0)))\mathcal{F}(X) + G(X, H(\eta, X), \sigma) \right] ds.$$

Therefore

$$\mathcal{F}(X) - \mathcal{F}(X_0) = \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, H(\eta, X_0)) \left[A(H(\eta, X)) - A(H(\eta, X_0)) \right] \mathcal{F}(X)ds$$
$$+ \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, H(\eta, X_0)) \left[G(X, H(\eta, X), \sigma) - G(X_0, H(\eta, X_0), \sigma) \right] ds.$$

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Consequently, by Lemma 4.4.2, we have the following estimate

$$|\mathcal{F}(X) - \mathcal{F}(X_0)|_{\rho,\eta}$$

$$\leq \frac{K}{\nu + \sigma\rho} |A(H(\eta, X)) - A(H(\eta, X_0))|_{\rho,\eta} |\mathcal{F}(X)|_0$$

$$+ \frac{K}{\nu + \sigma\rho} |G(X, H(\eta, X), \sigma) - G(X_0, H(\eta, X_0), \sigma)|_{\rho,\eta}$$

$$\leq \frac{K}{\nu + \sigma\rho} \left[|\mathcal{F}(X)|_0 |A'(w)|_0 |H(\eta, X) - H(\eta, X)|_{\rho,\eta} \right.$$

$$+ \frac{K}{\nu + \sigma\rho} \left(|D_X G|_0 |X - X_0|_{\rho,\eta} + |D_w G(X)|_0 |H(\eta, X) - H(\eta, X_0)|_{\rho,\eta} \right)$$

$$\leq \frac{K}{\nu + \sigma\rho} (c_1 |\mathcal{F}(X)|_0 |A'(w)|_0 + |D_X G|_0 + c_1 |D_w G(X)|_0) |X - X_0|_{\rho,\eta},$$

where c_1 is the Lipschitz constant of $H(\eta, X)$ given in Lemma 4.4.5. $\qquad\square$

Lemma 4.4.8. *Let $a = -\sigma\mu_\sigma$ and $b = 0$ and hence $\nu = \frac{\sigma\mu_\sigma}{4}$. If δ is such that*

$$(H1) \qquad \frac{K}{\nu}(c_2\delta^2 + c_3\tfrac{\varepsilon}{\sigma}) \leq \delta,$$

$$(H2) \qquad c_1\delta(1 + 2\sigma) + 2\delta(1 + 2\sigma\varepsilon) + \frac{2c_1\varepsilon}{\sigma} < \frac{\nu + \sigma\rho}{K},$$

where c_1, c_2, c_3 are some constants independent of σ, ε, then $\mathcal{F}$ is a self contraction mapping onto $\mathcal{B}_\eta$ for any fixed $\eta \in (\underline{w}, \bar{w})$.

Proof: Note that,

$$|A'(w)|_0 = \sup_{H(\eta, \mathcal{B}_\eta)} |A'(w)| \leq 1 + 2\sigma, \qquad \sup_{\mathcal{B}_\eta} |D_X G| \leq 2(1 + 2\sigma\varepsilon)\delta.$$

And if $a = \sigma\mu_\sigma$ and $b = 0$, then $\nu = \frac{\sigma\mu_\sigma}{4}$ and

$$G(X, w, \sigma) = \begin{bmatrix} -xy - \varepsilon\left(\sigma x^2 - y^2 - w^2 + \sigma\mu_\sigma^2\right) \\ xy - \varepsilon\left(y^2 + w^2 + \sigma^2 x^2 - \xi + \mu_\sigma + w + \frac{w}{\sigma}\right) \end{bmatrix}, \qquad D_w G = \begin{bmatrix} 2\varepsilon w \\ \varepsilon - 2\varepsilon w - \frac{\varepsilon}{\sigma} \end{bmatrix}$$

and hence

$$|G|_0 = \sup_{\mathcal{B}_\eta} |G| \leq c_2\delta^2 + c_3\frac{\varepsilon}{\sigma}, \qquad |D_w G|_0 = \sup_{H(\eta, \mathcal{B}_\eta)} |D_X G| \leq \frac{2\varepsilon}{\sigma}.$$

Therefore

$$|\mathcal{F}|_0 \leq \frac{|G|_0}{\sigma} \int_0^t K e^{-\frac{\nu}{\sigma}(t-s)} ds = \frac{K|G|_0}{\nu}\left(1 - e^{-\frac{\nu}{\sigma}t}\right) \leq \frac{K|G|_0}{\nu},$$

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and $|\mathcal{F}|_0 \le \delta$ only if (H1) holds

$$\frac{K}{\nu}(c_2\delta^2 + c_3\frac{\varepsilon}{\sigma}) \le \delta.$$

In addition, by Lemma 4.4.5, we know that

$$|H(\eta, X) - H(\eta, X_0)|_{\rho,\eta} \le c_1|X - X_0|_{\rho,\eta}$$

where $c_1 < \infty$ is independent of σ because $\rho \sim \frac{\nu}{\sigma} = \frac{\mu_\sigma}{4}$. It follows from Lemma 4.4.7 that

$$|\mathcal{F}(X) - \mathcal{F}(X_0)|_{\rho,\eta} \le L|X - X_0|_{\rho,\eta}, \qquad L < 1$$

if (H2) holds

$$\frac{K}{\nu + \sigma\rho}\left(c_1\delta(1 + 2\sigma) + 2\delta(1 + 2\sigma\varepsilon) + \frac{2c_1\varepsilon}{\sigma}\right) < 1.$$

Thus $\mathcal{F} : \mathcal{B}_\eta \to \mathcal{B}_\eta$ is a contraction mapping under conditions (H1-H2). $\qquad\square$

Lemma 4.4.9. *For sufficiently small $\sigma > 0$, let $\varepsilon = o(\sigma^n)$ with $n > 3$. Then for any $\eta \in (\underline{w}, \bar{w})$, there exists a unique $Y_\eta = (X_\eta, w_\eta)$ such that*

$$\begin{aligned}
X_\eta(t) &= \frac{1}{\sigma}\int_0^t \Phi^\sigma(t, s, w_\eta(s))G(X_\eta(s), w_\eta(s), \sigma)ds \\
w_\eta(t) &= \eta + \int_{t_0}^t F(X_\eta, w_\eta, \sigma)ds.
\end{aligned}$$

Moreover, $\eta \to X_\eta$ defines a Lipschitz map.

Proof: When $\varepsilon = o(\sigma^n)$ with $n \ge 3$, there exists $\delta > 0$ such that conditions (H1-H2) hold and thus $\mathcal{F}$ is a contraction mapping on $\mathcal{B}_\eta$. Define $X_{k+1} = \mathcal{F}(X_k)$, $k \ge 0$, with $X_0 \in \mathcal{B}$. For any positive integer $k, m > 0$, obviously

$$|X_{k+m} - X_k|_{\rho,\eta} \le L^m|X_k - X_0|_{\rho,\eta} < 2\delta L^m \to 0$$

as $m \to \infty$, thus $\{X_k\}$ is a Cauchy sequence. Note that if the normed space $(\mathbb{R}^2, |\cdot|)$ is complete, then $(\mathbb{R}^2, |\cdot|_{\rho,\eta})$ is also complete for $\rho > 0$. By the same argument in [58], we know that there exists an X_η such that $\lim_{k\to\infty} X_k = X_\eta$ in the $|\cdot|_{\rho,\eta}$-norm. Therefore

$\lim_{k \to \infty} X_k(t) = X_\eta(t)$ uniformly in $[0, t_1(\eta)]$. Consequently, for any $t \in [0, t_1]$, $X_\eta(t) = \mathcal{F}(X_\eta)(t)$ which implies that $|X_\eta(t)| \leq \delta$ when $t \in [0, t_1]$. Apparently

$$w_\eta(t) = H(\eta, X_\eta)(t), \qquad t \in [0, t_1(\eta)]$$

is uniquely determined, and $Y_\eta = (X_\eta, w_\eta)$ satisfies

$$
\begin{aligned}
X_\eta(t) &= \frac{1}{\sigma} \int_0^t \Phi^\sigma(t, s, w_\eta(s)) G(X_\eta(s), w_\eta(s), \sigma) ds \\
w_\eta(t) &= \eta + \int_{t_0}^t F(X_\eta, w_\eta, \sigma) ds.
\end{aligned}
\tag{29}
$$

for $t \in [0, t_1(\eta)]$. It follows, from the fact that $\mathcal{F}$ is a contraction mapping, that X_η is unique and hence w_η is unique. Thus Y_η is unique.

Lemma 4.4.10. *There exists $\bar{t} > t_0$ such that $\eta \to Y_\eta$ defines a Lipschitz mapping from $(2\underline{w}, \bar{w})$ to $BC^\rho(\mathbb{R}^3)$.*

Proof: By Lemma 4.4.4, set $\bar{t} = t_0 + \frac{2}{\mu_+} > t_0$, then $H(\eta, X) \geq 2\underline{w}$ for all $\eta \in (2\underline{w}, \bar{w})$ and $X \in \mathcal{B} = \{X \in C([0, \bar{t}], \mathbb{R}^2), \ |X| \leq \delta\}$. Denote by ϕ_t the flow induced by (29). By the same argument in [61], we know that η_t is a Lipschitz mapping from $(2\underline{w}, \bar{w})$ to $BC^\rho(\mathbb{R}^3)$ for t fixed.

Theorem 4.4.11. *For sufficiently small $\sigma > 0$, $\varepsilon = o(\sigma^n)$ with $n > 3$, and $0 < \underline{w} < \bar{w}$, there exists a function $h(w, \sigma)$ such that $W_{\sigma, \varepsilon} = \{(w, h(w, \varepsilon)), \ w \in (2\underline{w}, \bar{w})\}$ is invariant and as $\sigma \to 0$,*

$$\sup\{|h(w, \sigma) - h(w)|, \ w \in (2\underline{w}, \bar{w})\} \to 0.$$

Proof: The same as in [61], it suffices to show that $h(w, \sigma) = h(w) + \phi_{t_0}(w)$ with $w \in (2\underline{w}, \bar{w})$ is invariant, where $h(w) = (1, w)^T$. To indicate the explicit dependence of $\mathcal{F}$ on η, we replace $\mathcal{F}(\cdot)$ by $\mathcal{F}(\eta, \cdot)$ in the proof.

First we claim that $X_{H(\eta, X_\eta(s+t_0))}(t_0) = X_\eta(s+t_0)$ for any $s \in [0, t_1-t_0)$ if $X_\eta(t) = \mathcal{F}(\eta, X_\eta)(t)$ for $t \in [0, t_1]$. For any fixed $s \in [0, t_1 - t_0)$, define

$$X^s(t) = X_\eta(s + t), \qquad w^s(t) = H(\eta, X_\eta)(s + t), \qquad t \in [0, t_1 - s].$$

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Because X_η is the unique fixed point of $\mathcal{F}(\eta, X)$ and $(X_\eta, H(\eta, X_\eta))(t)$ solves equation (27) for $t \in [0, t_1]$, we know that $(X_\eta, H(\eta, X_\eta))(s+t)$ also solves (27) for $t \in [0, t_1 - s]$. Therefore X^s is the unique fixed point of $\mathcal{F}(w^s(t_0), \cdot)$. And note that the fixed point of $\mathcal{F}(w^s(t_0), \cdot)$ is given by $X_{w^s(t_0)}$, the uniqueness of fixed point of $\mathcal{F}$ implies that

$$X^s(t) = X_{w^s(t_0)}(t), \qquad t \in [0, t_1 - s].$$

In particular, we have

$$X_\eta(s + t_0) = X^s(t_0) = X_{w^s(t_0)}(t_0) = X_{H(\eta, X_\eta)(s+t_0)}(t_0), \qquad s \in [0, t_1 - t_0).$$

For any $(Z_0, w_0) \in W_{\sigma, \varepsilon}$, let $w(t) = H(w_0, X_{w_0}(t))$ and $Z(t) = h(w(t)) + X_{w_0}(t)$. Then $(Z(t), w(t))$ solves equation (11) with initial conditions $Z(t_0) = h(w_0, \sigma) = Z_0$ and $w(t_0) = w_0$. Thus, for $t \in [t_0, t_1]$,

$$Z(t) = h(w(t)) + X_{w_0}(t) = h(w(t)) + X_{H(w_0, X_{w_0})(t)}(t_0) = h(w(t)) + X_{w(t)}(t_0) = h(w(t), \sigma),$$

that is, $(Z(t), w(t))$ remains on $W_{\sigma, \varepsilon}$ in $[t_0, t_1]$ when $(Z(t_0), w(t_0)) \in W_{\sigma, \varepsilon}$. Therefore we can conclude that $W_{\sigma, \varepsilon}$ is the portion of the invariant manifold of equation (11). And $|X_{w_0}(t)| \leq \delta$ infers that, as $\sigma \to 0$,

$$\sup\{|h(w, \sigma) - h(w)|, \ w \in (2\underline{w}, \bar{w})\} \leq a + \delta = \sigma\mu_\sigma + \delta \to 0.$$

since $\delta \to 0$ as $\sigma \to 0$, see conditions (H1-H2).

This completes the proof. $\qquad\qquad\square$

Corollary 4.4.12. *Suppose that $\varepsilon = o(\sigma^n)$ with $n > 3$, then*

$$\sup\left\{|W_{\sigma, \varepsilon} - W_\sigma|, \ w \in [\underline{w}, \bar{w}]\right\} \sim \frac{\varepsilon}{\sigma}.$$

<u>Proof:</u> This is trivially from the fact that $a = \sigma\mu_\sigma$ and δ can be taken to the order of $\frac{\varepsilon}{\sigma}$ to make conditions (H1-H2) still satisfied. $\qquad\qquad\square$

Remark 4.4.13. *Corollary 4.4.12 shows that the oscillation axis of the perturbed system is very close to the oscillation axis of the partially perturbed system. Therefore, in the oscillation zone, it is enough to approximate $W_{\sigma,\varepsilon}$ by W_σ. And also the oscillation time with respect to the Poincaré section Σ can also be approximated by the counterpart of the partially perturbed system.*

4.4.2 Approximation of Oscillation Axis.

After having the existence of the oscillation axis $W_{\sigma,\varepsilon}$, in this section, we will study the approximation to $W_{\sigma,\varepsilon}$. Even though W_σ is already a good approximation in the oscillation zone $\mathcal{T}^o$, especially in the upper level(w large) of $\mathcal{T}^o$, it is not so clear how good it is in the lower level(w small). By finding a better approximation, we may see the location of the passage, from the oscillation zone into the transition zone $\mathcal{T}^t$, where the convergence of approximation fails, and how the oscillation is driven into the transition zone $\mathcal{T}^t$.

Because the computation involved in this section relies on the Bessel function, we will first provide a brief review on the Bessel functions.

The Bessel differential equation is given by

$$x^2 \frac{dy^2}{dx^2} + x\frac{dy}{dx} + (x^2 - v^2)y = 0 \tag{30}$$

and its solutions of first and second kinds, $J_v(x)$ and $Y_v(x)$, are given by

$$J_v(x) = \frac{(-1)^k \left(\frac{x}{2}\right)^{v+2k}}{k!\Gamma(v + k + 1)}, \qquad Y_v(x) = \frac{(\cos v\pi)J_v(x) - J_{-v}(x)}{\sin v\pi}.$$

And the Wronskian of J_v and Y_v is

$$J_v(x)Y_v'(x) - Y_v(x)J_v'(x) = \frac{2}{\pi x} \tag{31}$$

For any given constants α, β, γ, under the following two transformations

$$x \to \beta x^\gamma \qquad \text{and} \qquad y \to x^\alpha f,$$

the Bessel equation (30) can be modified into the following form

$$x^2\frac{df^2}{dx^2} + (2\alpha + 1)x\frac{df}{dx} + (\beta^2\gamma^2 x^{2\gamma} + \alpha^2 - n^2\gamma^2)f = 0. \tag{32}$$

In particular, set

$$n = 1, \qquad \alpha = -\frac{1}{2}, \qquad \gamma = \frac{1}{2},$$

equation (32) becomes

$$x^2 \frac{df^2}{dx^2} + \frac{\beta^2}{4} xf = 0, \tag{33}$$

whose solutions are $\sqrt{x} J_1(\beta \sqrt{x})$ and $\sqrt{x} Y_1(\beta \sqrt{x})$. Please refer to [66] for the details about this modified Bessel equation.

Let $\sigma > 0$ be fixed. Suppose that $W_{\sigma,\varepsilon}$ has a series expansion representation in terms of ε, that is,

$$u = \mu_\sigma + \sum_{k=1}^{\infty} f_k(w)\varepsilon^k, \qquad v = w + \sum_{k=1}^{\infty} g_k(w)\varepsilon^k.$$

By substitution into (11), we can obtain

$$-\sigma(\varepsilon f_1' + \varepsilon^2 f_2' + \dots)(\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)\left[w - \varepsilon\sigma(\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)\right]$$

$$= -\varepsilon\left[\sigma(\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)^2 - (w + \varepsilon g_1 + \varepsilon^2 g_2 + \dots)^2\right]$$

$$-(\varepsilon g_1 + \varepsilon^2 g_2 + \varepsilon^3 g_3 + \dots)(\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)$$

and

$$-\sigma(1 + \varepsilon g_1' + \varepsilon^2 g_2' + \dots)(\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)\left[w - \varepsilon\sigma(\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)\right]$$

$$= \left[-\sigma\mu_\sigma + (\varepsilon f_1 + \varepsilon^2 f_2 + \dots)\right](w + \varepsilon g_1 + \varepsilon^2 g_2 + \dots) - \varepsilon(w + \varepsilon f_1 + \varepsilon^2 f_2 + \dots)^2$$

$$+\varepsilon\left[\xi - (\mu_\sigma + \varepsilon f_1 + \varepsilon^2 f_2 + \dots) - (w + \varepsilon g_1 + \varepsilon^2 g_2 + \dots) - \frac{w}{\sigma}\right].$$

Comparing the coefficients of the first order terms yield the following two equations

$$\sigma\mu_\sigma w f_1' - \mu_\sigma g_1 = \sigma\mu_\sigma^2 - w^2$$

$$\sigma\mu_\sigma w g_1' - \sigma\mu_\sigma g_1 + (1 + \sigma)w f_1 = \sigma^2\mu_\sigma^2 + w^2 + \left[\xi - \mu_\sigma - \left(1 + \tfrac{1}{\sigma}\right)w\right]$$

from which we can obtain an equation of second order about f_1 as follows

$$w^2 f_1'' + c_1 w f_1 = c_2 w^2 + c_3 w + c_4 \tag{34}$$

where

$$c_1 = \left(\frac{1 + \sigma}{\sigma}\right)^2, \qquad c_2 = \frac{1 - \sigma^2}{\sigma^2}, \qquad c_3 = \frac{(1 + \sigma)^2}{\sigma^3}, \qquad c_4 = \frac{1 + \sigma}{\sigma^2}(\xi - \mu_\sigma).$$

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Theorem 4.4.14. *Let* $w = O(\sigma^k)$ *for* $k \geq 0$ *and* $n_0 = \max\{k + 3, 2k + 2\}$. *If* $\varepsilon \sim \sigma^n$ *with* $n > n_0$, *then*

$$W_{\sigma,\varepsilon} = \{(u, v, w), u = \mu_\sigma + \varepsilon f_1(w) + o(\sigma^{n-n_0}), \quad v = w + \varepsilon g_1(w) + o(\sigma^{n-n_0})\},$$

where f_1 *and* g_1 *are given by*

$$
\begin{aligned}
f_1 &= \pi\left[-f_{11} \int f_{12}(w)p(w)dw + f_{12} \int f_{11}(w)p(w)dw\right], \\
g_1 &= \sigma\pi w\left[-f_{11}' \int f_{12}(w)p(w)dw + f_{12}' \int f_{11}(w)p(w)dw\right] - \sigma\mu_\sigma + \frac{w^2}{\mu_\sigma}.
\end{aligned}
\tag{35}
$$

and

$$f_{11} = \sqrt{w}J_1(2\sqrt{c_1 w}), \qquad and \qquad f_{12} = \sqrt{w}Y_1(2\sqrt{c_1 w}).$$

Proof: Note that the corresponding homogeneous equation of (34)

$$w^2 f_1'' + c_1 w f_1 = 0. \tag{36}$$

is exactly a modified Bessel function with $\beta = 2\sqrt{c_1}$, and it admits two linearly independent solutions, $f_{11} = \sqrt{w}J_1(2\sqrt{c_1 w})$ and $f_{12} = \sqrt{w}Y_1(2\sqrt{c_1 w})$. To find a particular solution to equation (34), the following formula for variation of parameters(see [15]) will be used

$$f_{1p} = -f_{11} \int \frac{f_{12}(w)p(w)}{W(w)}dw + f_{12} \int \frac{f_{11}(w)p(w)}{W(w)}dw$$

where $p(w) = c_2 + \frac{c_3}{w} + \frac{c_4}{w^2}$ and $W = f_{11}'f_{12} - f_{12}'f_{11}$ is the Wronskian determinant of f_{11} and f_{12}. By the property (31), we can attain

$$W = \sqrt{c_1 w}\left[J_1\left(2\sqrt{c_1 w}\right)Y_1'\left(2\sqrt{c_1 w}\right) - Y_1\left(2\sqrt{c_1 w}\right)J_1'\left(2\sqrt{c_1 w}\right)\right] = \frac{1}{\pi}$$

and consequently

$$f_{1p} = \pi\left[-f_{11} \int f_{12}(w)p(w)dw + f_{12} \int f_{11}(w)p(w)dw\right].$$

Because

$$g_1 = \sigma w f_1' + \frac{w^2}{\mu_\sigma} - \sigma\mu_\sigma,$$

it immediately follows that

$$g_1 = \sigma \pi w \left[-f'_{11} \int f_{12}(w)p(w)dw + f'_{12} \int f_{11}(w)p(w)dw \right] - \sigma \mu_\sigma + \frac{w^2}{\mu_\sigma}.$$

Note that as $\varepsilon \sim \sigma^n$ with $n > 3$, $\varepsilon p(w) \sim \sigma^{n-3}$ because $\varepsilon c_3 \sim \sigma^{n-3}$. Furthermore, we may also write out the equations for (f_2, g_2), (f_3, g_3) up to any order m, and we will have similar equations with coefficients of the same order in σ. Therefore

$$u = \mu_\sigma + \varepsilon f_{1p} + o(\sigma^{n-3}), \qquad v = w + \varepsilon g_{1p} + o(\sigma^{n-3}).$$

Remark 4.4.15. *Theorem 4.4.14 shows that as $w \sim \sigma$, the perturbed system allows oscillation approximately around the axis $\{u = \mu_\sigma, v = w\}$ because the high order εf_{11} can be neglected. However, because f_{11} is given in terms of Bessel's function Y_1 of the second kind, when w is decreasing to the higher order in σ, i.e. $o(\sigma)$ or $O(\varepsilon)$, εf_{11} is not negligible any more, and the asymptotic expansion becomes invalid. Consequently the dynamics is forced to be driven away from the oscillation into the transition layer.*

By doing the series expansion to approximate the oscillation axis, we encounter the Bessel's function which make the series convergence a big problem. In the rest of this section, we will redo the approximation in a different way. This may not be rigorous, however we may show that the results we will obtain is a good approximation indeed.

The idea traces back to Corollary 4.4.12. Because $W_{\sigma,\varepsilon}$ is very close to W_σ in the order of $\frac{\varepsilon}{\sigma}$ and W_σ is a straight line and hence its curvature is zero. Intuitively we may suspect that the curvature of $W_{\sigma,\varepsilon}$ is also very small, and it is the only one solution has such a property because other solutions show oscillation around it. Therefore we may solve equation $\kappa = 0$ along the trajectories of (11) to find an approximate curve and then show it is close to $W_{\sigma,\varepsilon}$ by showing that it almost solves (11).

Consider a smooth vector field $F(X)$ which determines a curve satisfying $X' = F(X)$. Let $\vec{T}$ be the tangent vector to this curve, then $\vec{T} = \frac{X'}{\|X'\|} = \frac{F(X)}{\|F(X)\|}$. And its curvature is

$$\kappa = \left\| \frac{d\vec{T}}{ds} \right\| = \left\| \frac{\vec{T}'}{\|X'\|} \right\| = \frac{\|\vec{T}'\|}{\|X'\|}.$$

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Note that

$$\vec{T}' = \frac{X''}{\|X'\|} - \frac{\langle X', X''\rangle X'}{\|X'\|^3}, \qquad X'' = \mathscr{F}X' = \mathscr{F}F(X)$$

where $\mathscr{F}$ is the Jacobian matrix of F, thus we have a formula for the curvature

$$\kappa = \frac{\left\|\|F\|^2 \mathscr{F}F - \langle F, \mathscr{F}F\rangle F\right\|}{\|F\|^4}.$$

and at any nonequilibrium point of F,

$$\kappa = 0 \iff \|F\|^2 \mathscr{F}F - \langle F, \mathscr{F}F\rangle F \iff \mathscr{F}F = \frac{\langle F, \mathscr{F}F\rangle}{\|F\|^2}F.$$

In other word, if $\kappa = 0$ at some point X such that $F(X) \neq 0$, then $F(X)$ must be an eigenvector of $\mathscr{F}(X)$ associated to eigenvalue $\lambda = \langle T(X), \mathscr{F}(X)T(X)\rangle$.

Now we will consider the vector field F given in the following equation

$$\begin{cases} \dfrac{du}{d\tau} &= u(w - v) \\ \dfrac{dv}{d\tau} &= v(u - 1) - \varepsilon\left(\xi - \frac{w}{\sigma}\right) \\ \dfrac{dw}{d\tau} &= -\sigma wu. \end{cases} \tag{37}$$

which is obtained by dropping some terms of order ε in (11). Then

$$F = \begin{bmatrix} u(w - v) \\ v(u - 1) - \varepsilon\left(\xi - \frac{w}{\sigma}\right) \\ -\sigma wu \end{bmatrix}, \qquad \mathscr{F} = \begin{bmatrix} w - v & -u & u \\ v & u - 1 & -\frac{\varepsilon}{\sigma} \\ -\sigma w & 0 & -\sigma u \end{bmatrix}.$$

It follows from $\mathscr{F}F = \lambda F$ that

$$v = g(w) = \frac{1}{2}\left(w + \sqrt{w^2 + 4\sigma\varepsilon\mu_\sigma\xi}\right), \qquad u = f(w) = \mu_\sigma\left(1 - \frac{\varepsilon(\xi - \frac{w}{\sigma})}{g(w)}\right).$$

And the simple calculation shows that

$$u' - f'(w)w' = -\frac{2\sigma^2\varepsilon^2\mu_\sigma^2\xi u}{g^2(2g - w)}, \qquad v' - g'(w)w' = \frac{2\sigma^2\varepsilon u\mu_\sigma\xi}{2g - w}.$$

Because $(f(w), g(w))$ is an approximation of the central axis of (37), and (11) is the regular ε-perturbation of (37) when σ is fixed, we have the following approximation

$$W_{\sigma,\varepsilon}^o \sim \left\{(u, v, w), u = \mu_\sigma\left(1 - \frac{\varepsilon(\xi - \frac{w}{\sigma})}{v}\right), \ v = \frac{1}{2}\left(w + \sqrt{w^2 + 4\sigma\varepsilon\mu_\sigma\xi}\right), w \in [\underline{w}, \bar{w}]\right\}. \tag{38}$$

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4.4.3 Transition of Dynamics

From the previous sections, we already know that the reaction starts with oscillation around $W_{\sigma,\varepsilon}$ and ends at the equilibrium state $P_3 = (u^*, v^*, w^*)$. However, the distance from W_σ to the point P_3 is significantly large, thus, there must exist a stage in between to transit the dynamics from oscillation to asymptotic approach P_3. Note that the oscillation disappears when w is of order σ^2, which implies that the transition layer is a very thin layer. To study the transition dynamics, somehow we need to zoom in this very thin layer. The spatial rescaling is naturally a simple way to do it.

Even though the oscillation will disappear when $w \sim \sigma^2$ for the partially perturbed system, it may not work for the perturbed system because ε-perturbation deform the oscillation axis and oscillation can still proceed around the deformed axis but not W_σ. Thus the natural rescaling $w \to \sigma^2 w$ is not good enough for amplifying the transition layer. This does not seem to be a trivial job.

To choose an appropriate scale, let's recall Theorem 3.0.4 which says that the minimum w in the oscillation zone of 2D open system satisfies $\dfrac{\delta}{2} \leq \min_D w \leq \dfrac{\delta}{1+\delta}$ where $\delta = \varepsilon\sigma$. Because 2D open system can be thought of as an approximation of 3D closed system, and $\min_D w$ is a critical value of w through which the dynamics transits from oscillation to non-oscillation, it is reasonable to take the following rescaling

$$u \to u, \qquad v \to \varepsilon v, \qquad w \to \sigma\varepsilon w.$$

And the following discussion shows that this is correct choice. By above rescaling, equation (11) becomes

$$\begin{cases} \dfrac{du}{d\tau} &= \varepsilon\left[u(\sigma w - v) - (\sigma u^2 - \varepsilon^2 v^2)\right] \\ \dfrac{dv}{d\tau} &= v(u-1) - \varepsilon^2 v^2 + (\xi - u - \varepsilon v - \varepsilon w) \\ \dfrac{dw}{d\tau} &= -\sigma u(w-u). \end{cases} \tag{39}$$

Now we have another singular perturbation problem. A well known theory for studying this system is the geometric singular perturbation theory developed by Fenichel in [21], which

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is based on a series of his previous work about the invariant manifold theorem [18, 19, 20]. Mainly it says that a normally hyperbolic invariant manifold is persistent under any smooth perturbation. In [47], it was proved that normal hyperbolicity is not only sufficient but also necessary for the persistence. Roughly speaking, an invariant manifold is normally hyperbolic if the growth rate of the linearized flow in its normal direction of the manifold dominates the growth rate along the tangent direction of the manifold.

However, because there are three different time scales in system (40) when $0 < \varepsilon \ll \sigma \ll 1$, that is, v is the fast variable, u the slow variable and w in between. Fenichel's theorem cannot be applied directly. But this difficulty can be overcome simply by applying the singular perturbation twice as shown below.

Theorem 4.4.16. *For some* $0 < \eta < 1$ *and* $\sigma_0 > 0$*, system (39) has a two-dimensional stable manifold*

$$M_\sigma^\eta = \left\{ (u, v, w), \quad v = \frac{\xi - u}{1 - u} + O(\sigma), \ u, w \in [0, \eta] \right\}.$$

for all $\sigma \in [0, \sigma_0]$.

Proof: When $\sigma = 0$ and so $\varepsilon = 0$, system (39) has a two-dimensional critical manifold

$$M_0 = \left\{ (u, v, w), \quad v = h_0(u) = \frac{\xi - u}{1 - u}, u \neq 1 \right\}.$$

For any $u < 1$ fixed, $v = h_0(u)$ is asymptotically stable. Hence, for certain $0 < \eta < 1$,

$$M_0^\eta = \{(u, v, w), \quad v = h_0(u), \quad u, w \in [0, \eta]\}$$

is normally hyperbolically stable and positively invariant with respect to (39) as $\sigma = 0$. More precisely, we know that M_0^η is a collection of equilibria and can be parametrized by $s = (u, h_0(u), w)$, thus it is invariant and has normal direction

$$\vec{n} = \frac{s_u \times s_w}{\|s_u \times s_w\|} = \frac{1}{\sqrt{1 - a^2}} (a, -1, 0)^T, \qquad a = h_0'(u) = \frac{\xi - 1}{(1 - u)^2}.$$

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Therefore for any $p \in M_0^\eta$, the projection onto the tangent space and normal spaces at p are characterized by the matrices

$$\pi_p^N = \frac{1}{1-a^2} \begin{bmatrix} a^2 & -a & 0 \\ -a & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \pi_p^T = I - \pi_p^N = \frac{1}{1-a^2} \begin{bmatrix} 1 & a & 0 \\ a & a^2 & 0 \\ 0 & 0 & 1-a^2 \end{bmatrix},$$

respectively. Let ϕ_t be the flow induced by the vector field in (39) as $\sigma = 0$ and ∇F is the Jacobian of this vector field, then we have the equation about $D\phi_t(p)$

$$\frac{d}{dt}[D\phi_t(p)] = \nabla F(p)[D\phi_t(p)],$$

where, precisely

$$\nabla F = \begin{bmatrix} 0 & 0 & 0 \\ v-1 & u-1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \Rightarrow \nabla F(p) = \begin{bmatrix} 0 & 0 & 0 \\ \frac{\xi-1}{1-u} & u-1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = (u-1) \begin{bmatrix} 0 & 0 & 0 \\ -a & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and consequently $D\phi_t(p) = e^{\int_0^t \nabla F(p)ds}$ with

$$\int_0^t \nabla F(p)ds = \begin{bmatrix} 1 & 0 & 0 \\ -a(e^{(u-1)t}-1) & e^{(u-1)t} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Now we can consider the generalized Lyapunov-type numbers [74, 76] as defined below

$$\gamma_L(p) = \overline{\lim_{t\to\infty}} \left\| \pi_p^N D\phi_t(p) \right\|^{\frac{1}{t}}, \qquad \sigma_L(p) = \overline{\lim_{t\to\infty}} \frac{\log \left\| D\phi_t(p)\pi_p^T \right\|}{\log \left\| \pi_p^N D\phi_t(p) \right\|}, \quad \text{if } \gamma_L(p) < 1,$$

where $\| \cdot \|$ is the l_2 matrix norm. Because

$$\pi_p^N D\phi_t(p) = \frac{e^{(u-1)t}}{1-a^2} \begin{bmatrix} a^2 & -a & 0 \\ -a & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = e^{(u-1)t}\pi_p^N$$

and

$$D\phi_t(p)\pi_p^T = \frac{1}{1-a^2} \begin{bmatrix} 1 & a & 0 \\ a & a^2 & 0 \\ 0 & 0 & 1-a^2 \end{bmatrix} = \pi_p^T,$$

we will have

$$\gamma_L(p) = \lim_{t \to \infty} \left[e^{(u-1)t} \right]^{\frac{1}{t}} = \lim_{t \to \infty} e^{u-1} < 1,$$

and

$$\sigma_L(p) = \lim_{t \to \infty} \frac{\log \sqrt{2}}{\log e^{(u-1)t}} = \lim_{t \to \infty} \frac{\log \sqrt{2}}{(u-1)t} = 0,$$

which implies M_0^η is normally hyperbolic. It follows, from Fenichel's invariant manifold theorem, that M_0^η will be persistent under sufficiently small smooth perturbation, that is, there exists $\sigma_0 > 0$ such that for any $\sigma \in [0, \sigma_0]$, system (39) admits a normally hyperbolically stable invariant manifold

$$M_\sigma^\eta = \{(u, v, w), \quad v = h_0(u) + O(\sigma), \ u, w \in [0, \eta]\} \, .$$

$\square$

Under the time rescaling $\tau' = \sigma\tau$, we have the slow system associated with (39)

$$\begin{cases} \dfrac{du}{d\tau'} & = \ \dfrac{\varepsilon}{\sigma} \left[u(\sigma w - v) - (\sigma u^2 - \varepsilon^2 v^2) \right] \\ \sigma \dfrac{dv}{d\tau'} & = \ v(u - 1) - \varepsilon^2 v^2 + (\xi - u - \varepsilon v - \varepsilon w) \\ \dfrac{dw}{d\tau'} & = \ -u(w - u). \end{cases} \tag{40}$$

As $\sigma = 0$, we have the slow manifold M_0^η. And Theorem 4.4.16 ensures that M_0^η is persistent under perturbation, that is, there exists M_σ^η such that it is an invariant manifold of system (39) and close to M_0^η. Indeed, M_σ^η is a slow manifold of (39). Now we can consider system (39) restricted on the slow manifold M_σ^η, then we reduce (39) into a two-dimensional system on M_σ^η, which is written as

$$\begin{cases} \dfrac{du}{d\tau'} & = \ \delta \left[u(\sigma w - h(u, w, \sigma)) - (\sigma u^2 - \varepsilon^2 h^2(u, w, \sigma)) \right] \\ \dfrac{dw}{d\tau'} & = \ -u(w - u), \end{cases} \tag{41}$$

where $\delta = \delta(\sigma) = \dfrac{\varepsilon}{\sigma} \ll 1$.

Theorem 4.4.17. *For $\eta < 1$ and $\delta_0 > 0$, system (41) has a one-dimensional stable manifold*

$$W_\delta^\eta = \{(u, w), \quad w = u + O(\delta), u \in [0, \eta]\},$$

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for all $\delta \in [0, \delta_0]$.

Proof: The slow system with $t = \delta\tau'$ of (41) is given by

$$\begin{cases} \dfrac{du}{dt} & = & u(\sigma w - h(u, w, \sigma)) - (\sigma u^2 - \varepsilon^2 h^2(u, w, \sigma)) \\ \delta\dfrac{dw}{dt} & = & -u(w - u). \end{cases} \qquad (42)$$

Thus as $\delta = 0$, system (41) has a critical manifold

$$W_0^\eta = \{(u, w), \quad w = u \in [0, \eta]\}.$$

Under the same argument as in Theorem 4.4.16, W_0^η is normally hyperbolic invariant manifold and hence is persistent. Namely, there exists $\delta_0 > 0$ such that there exists an invariant manifold

$$W_\delta^\eta = \{(u, w), \quad w = h_1(u, \sigma) = u + O(\delta), u \in [0, \eta]\}.$$

diffeomorphic and close to W_0^η for any $\delta \in [0, \delta_0]$. $\qquad \square$

When we use the original variables (u, v, w) without spatial rescaling, we will have

Corollary 4.4.18. *For some $0 < \eta < 1$, system (11) has a two-dimensional strongly stable manifold*

$$M_{\sigma,\varepsilon}^\eta = \left\{(u, v, w), \quad \frac{v}{\varepsilon} = \frac{\xi - u}{1 - u} + O(\sigma), \ u, \frac{w}{\sigma\varepsilon} \in [0, \eta]\right\},$$

and a one-dimensional stable invariant manifold

$$W_{\sigma,\varepsilon}^t = \left\{(u, v, w), \quad \frac{v}{\varepsilon} = \frac{\xi - u}{1 - u} + O(\sigma), \ \frac{w}{\sigma\varepsilon} = u + \frac{\varepsilon(\xi - u)}{\sigma(1 - u)} + O(\frac{\varepsilon}{\sigma}), \ u \in [0, \eta]\right\} \quad (43)$$

on it, that it, $W_{\sigma,\varepsilon}^t \subset M_{\sigma,\varepsilon}^\eta$.

Proof: This follows immediately from Theorem 4.4.16 and Theorem 4.4.17. For the better approximation to $W_{\varepsilon,\sigma}^t$ as given in (43), the series expansion can be used as in Theorem 4.4.14 for central axis in the oscillation zone. $\qquad \square$

Note that along the stable invariant manifold $W_{\sigma,\varepsilon}^t$, the solution will first reach the vicinity of the equilibrium P_3 and then approach P_3 along the eigendirection associated to eigenvalue of the smallest modulus. Thus we may estimate the time T^t spent on the transition

along $W_{\sigma,\varepsilon}^t$ into the vicinity of P_3. By equation (42) with $\sigma = 0$, we approximately have

$$\frac{du}{dt} \sim -uh_0(u) = -\frac{u(\xi - u)}{1 - u} \Rightarrow T^t \sim \frac{1}{\varepsilon\xi}\left[\ln\left(\frac{u(0)}{u(T^t)}\right) + (\xi - 1)\ln\left(\frac{\xi - u(0)}{\xi - u(T^t)}\right)\right].$$

Since $u(0) < \mu_\sigma < 1$ and $u(T^t) \sim \varepsilon^2\xi$, we have

Theorem 4.4.19. *The transition time T^t into the vicinity of the equilibrium point P_3 along $W_{\sigma,\varepsilon}^t$ is approximately given by*

$$T^t \sim -\frac{\ln\varepsilon}{\varepsilon}.$$

Theorem 4.4.16 shows that in the transition layer, all the orbits are attracted onto the two-dimensional strongly stable invariant manifold $M_{\sigma,\varepsilon}^\eta$. And furthermore, Theorem 4.4.17 shows that on $M_{\sigma,\varepsilon}^\eta$, the orbits are attracted onto a one-dimensional stable invariant manifold $W_{\sigma,\varepsilon}^t \subset M_{\sigma,\varepsilon}^\eta$. Therefore, before the time rescaling, system (11) also has a two-dimensional stable invariant manifold which is a slightly curved strip of very tiny width and thus not seen in the numerical simulation for (11). And Theorem 4.4.19 says that it will take a longer time of order $-\frac{\ln\varepsilon}{\varepsilon}$ to get really "close" to the equilibrium point P_3.

4.4.4 Numerical Simulation

Recall that if initial w_0 and energy E are relatively large, Theorem 4.3.12 states that there will be $n \sim \frac{1}{\sigma}$ oscillations in the oscillation zone. As showed in Figure 6 where large ξ allows large w_0 and thus many oscillation can be observed. In contrast, if ξ is small and hence w_0 must be small, then the number of complete oscillations is much less than the case for large ξ, as in Figure 7.

On the other hand, if the energy E is large, then each complete oscillation will sweep a large area because it is away from the central axis $W_{\sigma,\varepsilon}^o$. While if E is small, that is, the initial point is chosen to be very close to $W_{\sigma,\varepsilon}^o$, then the oscillation will be proceeding very closely around $W_{\sigma,\varepsilon}^o$, which can be observed from the following figures 8 and 9.

The transition layer is as in Figure 10, where the analytical curve of the central axis is drawn by using the the approximation of $W_{\sigma,\varepsilon}^t$ given in (43). Figure 10 shows that all the numerical solutions are eventually attracted onto the analytical curve.
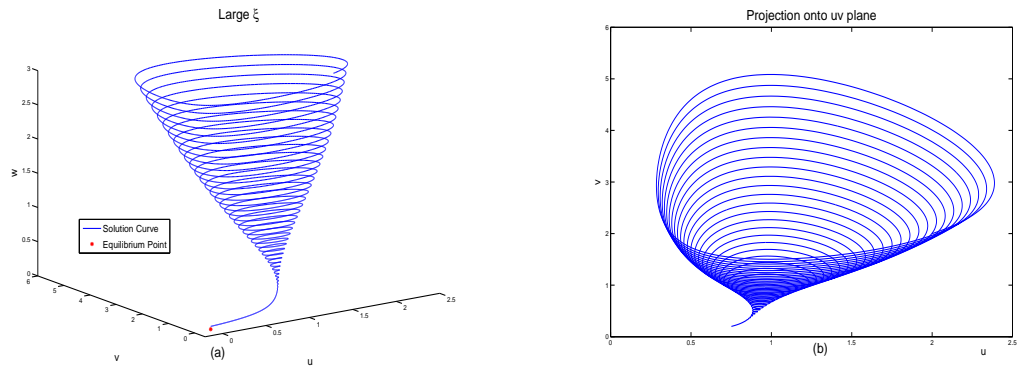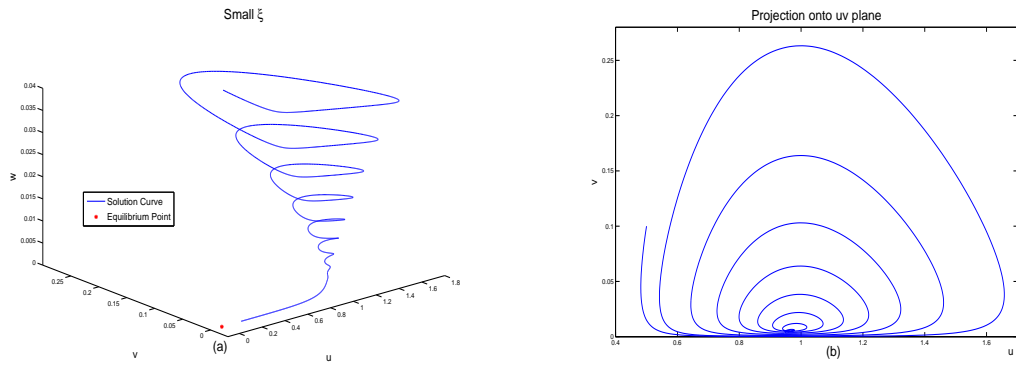
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Figure 6: Oscillation for ξ large.

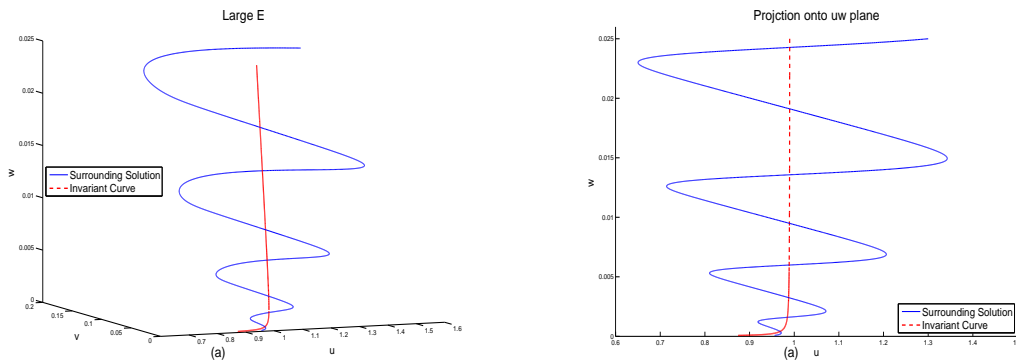**Figure 7:** Oscillation for ξ small.
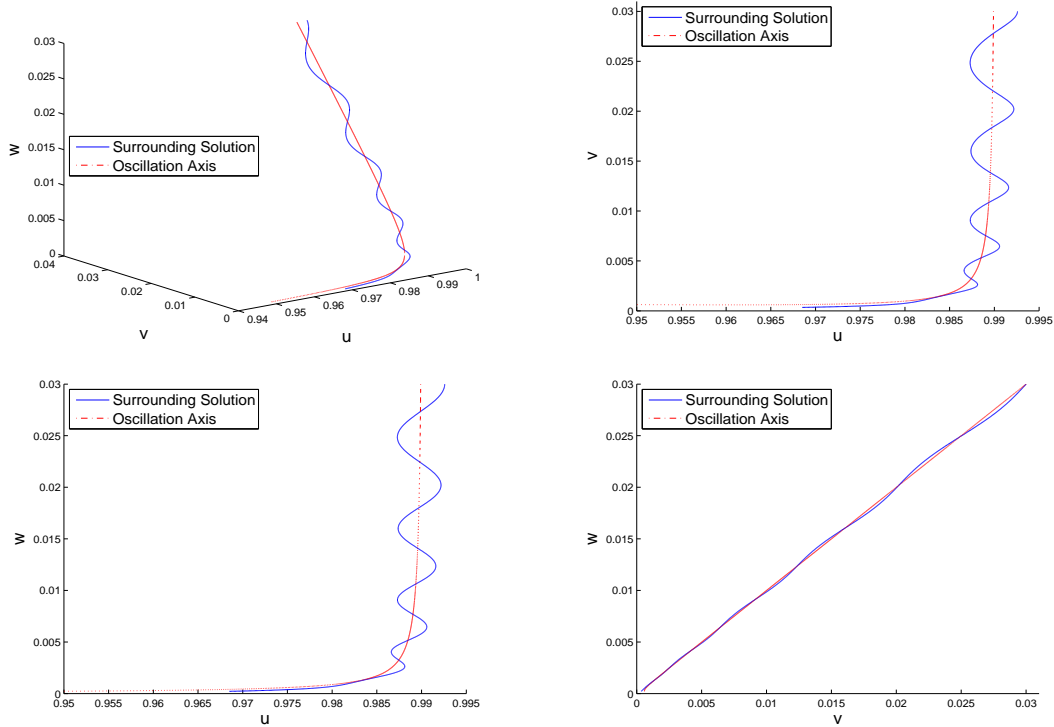

Figure 8: Oscillation for E large.

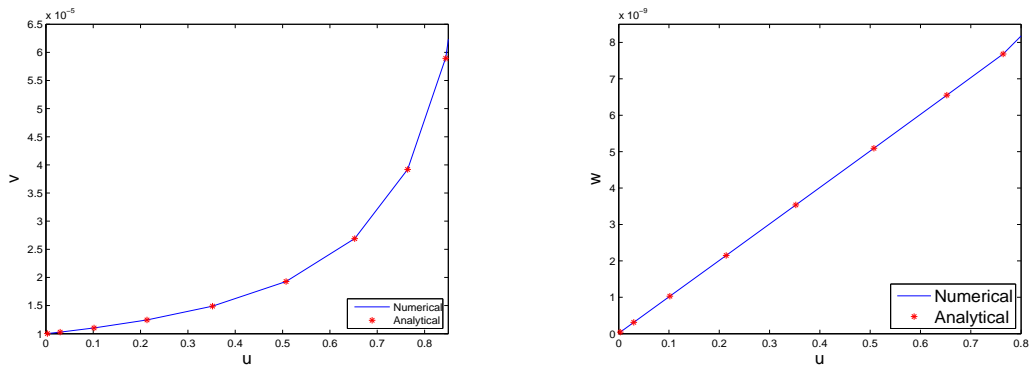**Figure 9:** Oscillation for *E* small.

Figure 10: Transition Layer.

Figure 11 provides a closer look of the dynamical transition from oscillatory to monotonic behavior.

4.5 *Analysis in Terms of Action-Action-Angle Variables*

In the previous sections, we already studied the three-dimensional reversible Lotka-Volterra system by the method of geometric singular perturbation. Now if we reconsider this system
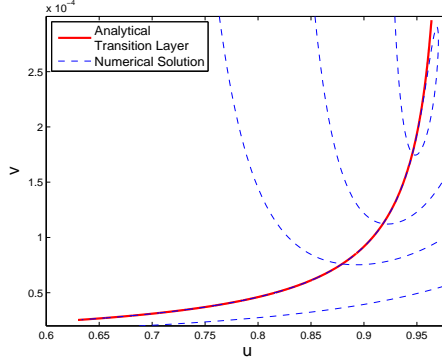
Figure 11: Transition Layer.

in the oscillation zone, we notice that the unperturbed system is a standard LV system which has Hamiltonian structure. The application of Hamilton-Jacobi theory to an integrable LV system can be found in [14]. In this section, we will study the reversible LV system by tools of Hamiltonian system, mainly in terms of action-action-angle variables.

4.5.1 Action-Action-Angle Variables.

Consider the unperturbed LV system (17). Under the following transformation

$$x = \ln u, \qquad y = \ln v - \ln z, \qquad z = w,$$

system (17) becomes

$$\begin{cases} \dfrac{dx}{d\tau} &= z(1 - e^y) = -\dfrac{\partial H}{\partial y} \\ \dfrac{dy}{d\tau} &= e^x - 1 = \dfrac{\partial H}{\partial x} \end{cases} \tag{44}$$

with the Hamiltonian

$$H(x, y; z) = (e^x - x - 1) + z\,(e^y - y - 1) \geq 0.$$

Note that the level set of the Hamiltonian H is a closed plane curve, by Arnold-Liouville's theorem [2], there exists a canonical transformation

$$x = x(I_1, \theta; z), \qquad y = y(I_1, \theta; z)$$

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such that under this transformation, the unperturbed Hamiltonian system (44) can be rep-resented in terms of action-angle variable as

$$\begin{cases} \dot{I}_1 & = & 0 \\ \dot{\theta} & = & \Omega(I_1; z). \end{cases}$$

where $\Omega(I_1, z) = \frac{\partial H}{\partial I_1}$ is the frequency and $H(x(I_1, \theta; z), y(I_1, \theta; z); z) = H(I_1; z)$.

For the partially perturbed system (22), we may rewrite it as

$$\begin{cases} \dot{u} & = & u(w - v) \\ \dot{v} & = & (1 + \sigma)v(u - \mu_\sigma) - \sigma uv \\ \dot{w} & = & -\sigma uw. \end{cases} \qquad (45)$$

Consider

$$\begin{cases} \dot{u} & = & u(w - v) \\ \dot{v} & = & (1 + \sigma)v(u - \mu_\sigma) \end{cases} \qquad (46)$$

whose first integral is exactly

$$E^\sigma(u, v, w) = (1 + \sigma)\left[(u - \mu_\sigma) + \mu_\sigma \ln\left(\frac{\mu_\sigma}{u}\right)\right] + \left[(v - w) + w \ln\left(\frac{w}{v}\right)\right].$$

By the similar transform

$$x = \ln u - \ln \mu_\sigma, \qquad y = \ln v - \ln z, \qquad z = w,$$

(46) becomes a Hamiltonian system

$$\begin{cases} \dfrac{dx}{d\tau} & = & z(1 - e^y) \\ \dfrac{dy}{d\tau} & = & e^x - 1 \end{cases} \qquad (47)$$

with

$$\begin{aligned} H(x, y; z) & = & E^\sigma(u, v, w) = (1 + \sigma)\mu_\sigma\,(e^x - x - 1) + z\,(e^y - y - 1) \\ & = & (e^x - x - 1) + z\,(e^y - y - 1) \geq 0. \end{aligned}$$

Then (45) becomes a perturbed Hamiltonian system

$$\begin{cases} \dfrac{dx}{d\tau} & = & z(1 - e^y) \\ \dfrac{dy}{d\tau} & = & e^x - 1 \\ \dfrac{dz}{d\tau} & = & -\sigma\mu_\sigma z e^x \end{cases} \qquad (48)$$

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and

$$\dot{H} = -\sigma\mu_\sigma z e^x (e^y - y - 1) \le 0.$$

By applying the canonical transform $x = x(I_1, \theta; z)$, $y = y(I_1, \theta, z)$ of action-angle variable to (48) and treating $z = I_2$ as the second action variable, we will have the action-action-angle form of equation (45)

$$\begin{cases} \dot{I}_1 &=& -\sigma f_1(I_1, I_2, \theta) \\ \dot{I}_2 &=& -\sigma f_2(I_1, I_2, \theta) \\ \dot{\theta} &=& \Omega(I_1; I_2) - \sigma f_3(I_1, I_2, \theta) \end{cases} \tag{49}$$

where

$$f_1(I_1, I_2, \theta) = \mu_\sigma e^x I_2 \det\left|\frac{\partial(x, y)}{\partial(I_2, \theta)}\right|, \qquad f_2(I_1, I_2, \theta) = \mu_\sigma I_2 e^x$$

$$f_3(I_1, I_2, \theta) = \mu_\sigma e^x I_2 \det\left|\frac{\partial(x, y)}{\partial(I_1, I_2)}\right|,$$

and $H(x(I_1, I_2, \theta), y(I_1, I_2, \theta); z = I_2) = H(I_1; I_2)$ and $\Omega(I_1, I_2) = \frac{\partial H}{\partial I_1}$. Note that

$$1 = \det\left|\frac{\partial(x, y)}{\partial(I_1, \theta)}\right| = \frac{\partial x}{\partial I_1}\frac{\partial y}{\partial \theta} - \frac{\partial x}{\partial \theta}\frac{\partial y}{\partial I_1}, \qquad 0 = \frac{\partial H}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial H}{\partial y}\frac{\partial y}{\partial \theta}$$

imply that

$$\frac{\partial x}{\partial \theta} = -\frac{1}{\Omega}\frac{\partial H}{\partial y}, \qquad \frac{\partial y}{\partial \theta} = \frac{1}{\Omega}\frac{\partial H}{\partial x}$$

Therefore

$$\det\left|\frac{\partial(x, y)}{\partial(I_2, \theta)}\right| = \frac{I_2}{\Omega}\left(\frac{\partial H}{\partial I_2} - \frac{\partial H}{\partial z}\right).$$

Now by averaging principle [28], we will consider the averaged equation

$$\begin{cases} \dot{J}_1 &=& -\sigma \bar{f}_1(J_1, J_2) \\ \dot{J}_2 &=& -\sigma \bar{f}_2(J_1, J_2) \end{cases}$$

To this end, we need

$$I_i = J_i + \sigma g_i(J_1, J_2, \theta).$$

Thus we can obtain that

$$\begin{cases} \dot{J}_1 &=& -\sigma\left[f_1(J_1, J_2, \theta) - \frac{\partial g_1}{\partial \theta}\Omega(J_1, J_2)\right] + o(\sigma) \\ \dot{J}_2 &=& -\sigma\left[f_2(J_1, J_2, \theta) - \frac{\partial g_2}{\partial \theta}\Omega(J_1, J_2)\right] + o(\sigma) \end{cases}$$

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To eliminate the the oscillation of $\tilde{f}(J_1, J_2, \theta) = f(J_1, J_2, \theta) - \bar{f}(J_1, J_2)$, we need averaging by setting

$$\tilde{f}_i(J_1, J_2, \theta) = \frac{\partial g_i}{\partial \theta} \Omega(J_1, J_2), \qquad i = 1, 2.$$

Note that

$$\bar{f}_2(I_1, I_2) = \frac{1}{2\pi} \int_0^{2\pi} f_2(I_1, I_2, \theta) d\theta = -\frac{\mu_\sigma I_2}{2\pi} \int_0^{2\pi} e^x d\theta.$$

By the following facts,

$$\frac{\partial H}{\partial x} = e^x - 1, \qquad \frac{\partial H}{\partial y} = z(e^y - 1), \qquad \frac{\partial H}{\partial z} = e^y - y - 1,$$

we notice that

$$\int_0^{2\pi} e^x d\theta = \int_0^{2\pi} \left(\frac{\partial H}{\partial x} + 1 \right) d\theta = \int_0^{2\pi} \left(\Omega \frac{\partial y}{\partial \theta} + 1 \right) d\theta = 2\pi,$$

because Ω is independent of θ. Hence

$$\bar{f}_2(I_1, I_2) = -\mu_\sigma I_2.$$

Consequently

$$\dot{J}_2 = -\sigma \mu_\sigma J_2 \Rightarrow J_2 = J_2(0) e^{-\sigma \mu_\sigma t}.$$

In addition,

$$\det \left| \frac{\partial(x, y)}{\partial(I_2, \theta)} \right| = \frac{\partial x}{\partial I_2} \frac{\partial y}{\partial \theta} - \frac{\partial x}{\partial \theta} \frac{\partial y}{\partial I_2} = \frac{1}{\Omega} \frac{\partial H}{\partial x} \frac{\partial x}{\partial I_2} - (-\frac{1}{\Omega}) \frac{\partial H}{\partial y} \frac{\partial y}{\partial I_2}$$

$$= \frac{1}{\Omega} \left[\frac{\partial H}{\partial x} \frac{\partial x}{\partial I_2} + \frac{\partial H}{\partial y} \frac{\partial y}{\partial I_2} \right] = \frac{1}{\Omega} \left[\frac{\partial H}{\partial I_2} - \frac{\partial H}{\partial z} \right] = \frac{1}{\Omega} \left[\frac{\partial H}{\partial I_2} - (e^y - y - 1) \right],$$

then

$$\bar{f}_1(I_1, I_2) = -\frac{\mu_\sigma I_2}{2\pi\Omega} \int_0^{2\pi} \left[\frac{\partial H}{\partial I_2} - (e^y - y - 1) \right] e^x d\theta.$$

Because

$$\int_0^{2\pi} e^x (e^y - y - 1) d\theta = \int_0^{2\pi} \left(\frac{\partial H}{\partial x} + 1 \right) (e^y - y - 1) d\theta$$

$$= \int_0^{2\pi} \left(\Omega \frac{\partial y}{\partial \theta} + 1 \right) (e^y - y - 1) d\theta = \int_0^{2\pi} (e^y - y - 1) d\theta$$

$$= \int_0^{2\pi} \frac{1}{I_2} \frac{\partial H}{\partial y} d\theta - \int_0^{2\pi} y d\theta = -\int_0^{2\pi} \frac{\Omega}{I_2} \frac{\partial x}{\partial \theta} d\theta - \int_0^{2\pi} y d\theta = -2\pi\bar{y},$$

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where

$$\bar{y} = \frac{1}{2\pi} \int_0^{2\pi} y d\theta.$$

We finally have

$$\bar{f}_1(I_1, I_2) = -\frac{\mu_\sigma I_2}{2\pi\Omega} \left(2\pi \frac{\partial H}{\partial I_2} + 2\pi \bar{y} \right) = -\frac{\mu_\sigma I_2}{\Omega} \left(\frac{\partial H}{\partial I_2} + \bar{y} \right).$$

On the other hand, because H is independent of θ, we can see that

$$
\begin{aligned}
H &= \frac{1}{2\pi} \int_0^{2\pi} H d\theta = \frac{1}{2\pi} \int_0^{2\pi} \left[(e^x - x - 1) + I_2(e^y - y - 1) \right] d\theta \\
&= \frac{1}{2\pi} \int_0^{2\pi} (-x - I_2 y) \, d\theta = -\bar{x} - I_2 \bar{y}.
\end{aligned}
$$

from which it follows that

$$\frac{\partial H}{\partial I_2} + \bar{y} = -\frac{\partial \bar{x}}{\partial I_2} - I_2 \frac{\partial \bar{y}}{\partial I_2}$$

And by Jessen's inequality, we have

$$
\begin{aligned}
\bar{x} &= \frac{1}{2\pi} \int_0^{2\pi} x d\theta \le \ln \left[\frac{1}{2\pi} \int_0^{2\pi} e^x d\theta \right] = \ln 1 = 0 \\
\bar{y} &= \frac{1}{2\pi} \int_0^{2\pi} y d\theta \le \ln \left[\frac{1}{2\pi} \int_0^{2\pi} e^y d\theta \right] = \ln 1 = 0.
\end{aligned}
$$

Now we have the averaged equation

$$
\begin{cases}
\dot{J}_1 &= \sigma \mu_\sigma \frac{J_2}{\Omega} \left(\frac{\partial \bar{x}}{\partial I_2} + J_2 \frac{\partial \bar{y}}{I_2} \right) \\
\dot{J}_2 &= -\sigma \mu_\sigma J_2.
\end{cases}
\tag{50}
$$

The averaged equation shows that the second action variable J_2 has exponentially decay. However it is not so obvious how the first action variable changes. But we have the numerical simulation as in Figure 12. (In the top two figures in Figure 12, the colored closed curves correspond to the first action variable at that time, and the area of each enclosed region is exactly equal to the action I_1.)

Remark 4.5.1. *By using the same canonical transform, the completely perturbed system can also be rewritten in terms of action-action-angle variables to find the corresponding averaged equation. And as $\varepsilon \ll \sigma$, we will have the similar averaged equation.*
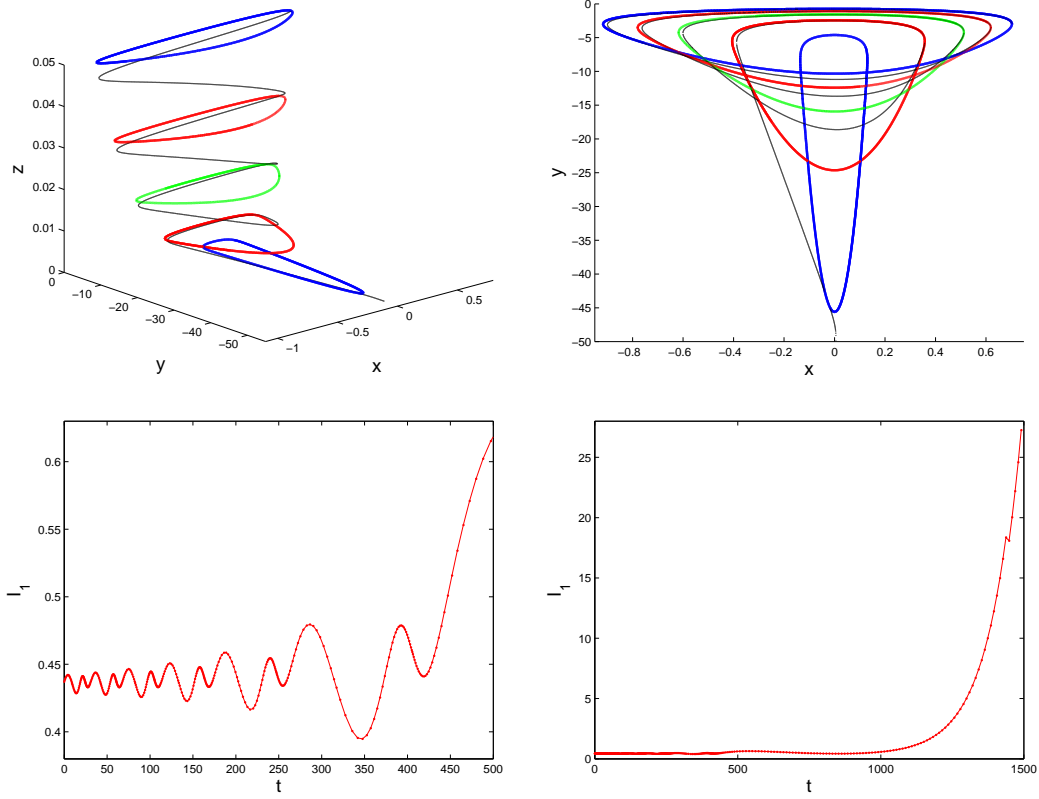
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Figure 12: Change of the First Action Variable I_1 of System (47) in Time.

4.5.2 Action Variable from Geometric Viewpoint

Note that the geometric meaning of the first action variable is the area of the region enclosed by the level curve of the Hamiltonian H. In this section, we will study $\dot{I}_1$ in the geometric way. Suppose that $H(X; z)$ is C^2 differentiable in (X, z) and convex in X for any z. And suppose that for any z, there exists $X_0(z)$ such that

$$H(X; z) \geq H(X_0(z); z) = 0, \qquad \forall X.$$

For any fixed $h > 0$ and appropriate z, $H(X; z) = h$ determines a closed curve and denote by $A(h, z)$ the area of its enclosed region.

Proposition 4.5.2. *Suppose that H is the convex, then $\dfrac{\partial A}{\partial h} \geq 0$. Additionally, if H is the Hamiltonian of system (44), then $\dfrac{\partial A_H}{\partial z} \leq 0$; and if $H = F(u, v; w)$ is the first integral of system (17), then $\dfrac{\partial A_F}{\partial w} \geq 0$.*

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Proof: Consider the transform

$$X = X_0(z) + R(\alpha; h, z)\vec{n}, \qquad \vec{n} = \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix},$$

where $R(\alpha, h; z)$ is the distance from $X_0(z)$ to the level curve $H = h$ in the direction $\vec{n}$. (actually $X_0(z)$ above can be replace by any interior point in $H \leq h$), then

$$A(h; z) = \frac{1}{2} \int_0^{2\pi} R^2 d\alpha.$$

As a matter of fact, this area plays the role of action variable of Hamiltonian system in the action-variable setup. And

$$\frac{\partial A}{\partial h} = \int_0^{2\pi} R\frac{\partial R}{\partial h} d\alpha, \qquad \frac{\partial A}{\partial z} = \int_0^{2\pi} R\frac{\partial R}{\partial z} d\alpha$$

And it follows from $H(X_0(z) + R\vec{n}, z) = h$ that

$$\langle \nabla H, \vec{n} \rangle \frac{\partial R}{\partial h} = 1, \qquad \langle \nabla H, X_0'(z) + \frac{\partial R}{\partial z}\vec{n} \rangle + \frac{\partial H}{\partial z} = 0$$

or furthermore

$$\frac{\partial R}{\partial z} = -\frac{\partial R}{\partial h}\left(\frac{\partial H}{\partial z} + \langle \nabla H, X_0'(z) \rangle\right).$$

Because H is convex, we know that $\langle \nabla H, \vec{n} \rangle > 0$ and thus $\frac{\partial R}{\partial h} > 0$. Therefore $\frac{\partial A}{\partial h} > 0$.

When H is given by

$$H(x, y; z) = (e^x - x - 1) + z(e^y - y - 1),$$

then

$$X_0(z) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad \nabla H = \begin{bmatrix} e^x - 1 \\ z(e^y - 1) \end{bmatrix}, \qquad H_z = e^y - y - 1,$$

and consequently

$$\frac{\partial H}{\partial z} + \langle \nabla H, X_0' \rangle = \frac{\partial H}{\partial z} = e^y - y - 1 \geq 0,$$

which implies that $\frac{\partial R}{\partial z} \leq 0$ and thus $\frac{\partial A}{\partial z} \leq 0$. While if H is the first integral of system (17), that is,

$$H = F(u, v; w) = (u - 1 - \ln u) + \left[v - w + w\ln\left(\frac{w}{v}\right)\right].$$

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with w as the parameter, then

$$X_0(w) = \begin{bmatrix} \mu \\ w \end{bmatrix} \Rightarrow X_0' = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad \nabla F = \begin{bmatrix} 1 - \dfrac{1}{u} \\ 1 - \dfrac{w}{v} \end{bmatrix}, \qquad \frac{\partial F}{\partial w} = \ln \frac{w}{v}$$

and consequently

$$F_w + \langle \nabla F, X_0' \rangle = \ln \frac{w}{v} + 1 - \frac{w}{v} \leq 0$$

which implies that $\frac{\partial R}{\partial w} = -\frac{\partial R}{\partial h}\left(\frac{\partial F}{\partial w} + \langle \nabla F, X_0' \rangle \right) \geq 0$ and thus $\frac{\partial A}{\partial w} \geq 0$.

Proposition 4.5.3. *In system (22), the enclosed area A is decreasing in time.*

Proof: Obviously, $\dot{A} = \frac{\partial A}{\partial E_\sigma}\dot{E}^\sigma + \frac{\partial A}{\partial w}\dot{w}$. And Under the same discussion as that in section 4.5.2, we will have $\frac{\partial A}{\partial E_\sigma} \geq 0$ and $\frac{\partial A}{\partial w} \geq 0$. Because $\dot{E}_\sigma \leq 0$ and $\dot{w} \leq 0$ for system (22), it is easy to see that $\dot{A} \leq 0$. $\qquad\qquad\square$

Remark 4.5.4. *Proposition 4.5.3 indicates that, in the situation of partial perturbation, the area swept by a complete 2π unperturbed oscillation around (μ_σ, w) is decreasing in time, that is, the oscillation is shrinking to the oscillation axis. This is also verified by the numerical simulation in Figure 13, where the red line denotes the partially perturbed trajectory, and the blue closed curves denote the unperturbed periodic orbits in the corresponding level of w.*
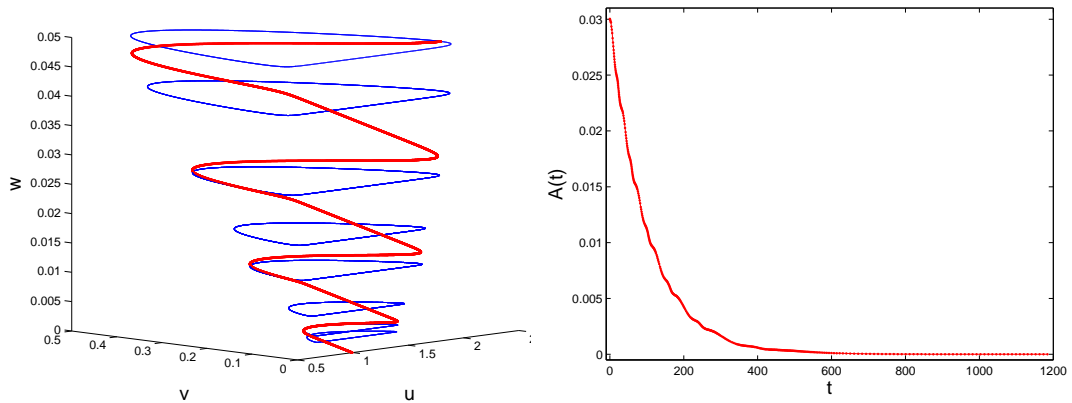

Figure 13: Change of Action Variable of System (22) in Time.

CHAPTER V

MRC CONTROL OF BZ CHEMICAL REACTION

Model reference control(MRC) is a mature engineering control technique applied to many different plants and has a broad application such as controlling robot's [26, 41], flight vehicles [37, 38, 39, 40, 68], mechanical oscillators [32] and so on. Because it works directly with the input-output data to identify the unknown system(plant), no mathematical model determined by a system of equations(differential equations or difference equations) is required.

On the other hand, biological system is a complex system. Because there is no first principle, like Newton's law in mechanics, available in biology, it is hard to set up a mathematical model in terms of equations even though people still do it in this way by the limited knowledge. Without a good model, it becomes even harder to control such a system.

Motivated by these two facts, we think it reasonable to borrow the idea of MRC to control a biological system. By the numerical simulation, the MRC control for SIRS disease models shows the validity of this new biological control method, see[6].

In this chapter, we will briefly provide a mathematical framework for MRC and neural network(NN) structure in which MRC can be manipulated. Then we will consider the MRC control for the reversible BZ reaction described in (11) to eliminate the oscillation exhibiting during the reaction.

5.1   Model Reference Control.

There are two important processes involved in the MRC control. One is the system identification in which the plant can be identified in the sense that the identified system and the real plant have almost the same response to the same input signal. The other is the controller

generation in which a controller can be trained and generated to drive the plant to behave in the desired manner described by the reference model.

5.1.1 System Identification.

Let X and Y be two spaces and $F : X \rightarrow Y$ be an operator. Then F can be regarded as a plant, X and Y as input and output spaces. Any $(x, y) \in X \times Y$, an input-output pair of (x, y) with $y = F(x)$, is called a pattern. The collection of patterns is called a training set.

For a real plant, if we can embed the input signal into $\mathbb{R}^m$ and the output signal into $\mathbb{R}^n$, and also assume that vector-valued function $F : D \rightarrow \mathbb{R}^n$ is continuous, where $D \subset \mathbb{R}^m$ is compact, then the system identification is simply to find an approximation of F on D. With these notations, the training set can be represented by $U = \{(x, y), y = F(x), x \in D\}$.

Theorem 5.1.1. *(Stone-Weierstrass) [10]: Let domain $D \subset \mathbb{R}^m$ be compact and let $\mathscr{F} \subset C(D)$ satisfy the following criteria:*

1. *Identity Function: The constant function $f(x) = 1$ is in $\mathscr{F}$.*

2. *Separability: For any $x_1 \neq x_2 \in D$, there is an $f \in \mathscr{F}$ such that $f(x_1) \neq f(x_2)$.*

3. *Algebraic Closure: If $f, g \in \mathscr{F}$, then $fg, af + bg \in \mathscr{F}$ for any $a, b \in \mathbb{R}$.*

Then $cl(\mathscr{F})= C(D)$, the set of continuous real-valued functions on D.

Indeed, Stone-Weierstrass theorem ensures that F can be always approximated by some functions in the prescribed function set $\mathscr{F}$. For example, $\mathscr{F}$ may be chosen to be the set consisting of all the polynomials. However, the structure of $\mathscr{F}$ is not unique, and what is preferred is the one easy to be generated. To have a simple way to construct $\mathscr{F}$ and to take into account the manipulation of MRS by neural network which will be introduced later, the following theorem is useful.

Definition 5.1.2. *A function σ is **discriminatory** if for a measure $\mu \in M(I_m)$,*

$$\int_{I_m} \sigma\left(y^T x + \beta\right) d\mu(x) = 0 \tag{51}$$

*for all $y \in \mathbb{R}^m$ and $\beta \in \mathbb{R}$, implies that $\mu = 0$. And σ is **sigmoidal** if $\sigma(-\infty) = 0$, $\sigma(+\infty) = 1$.*

Say $\sigma(t) = \frac{1}{1+e^{-t}}$.

Theorem 5.1.3. *(Cybenko, [11]) Suppose that σ is a continuous discriminatory sigmoidal function. Then finite sums of the form*

$$G(x) = \sum_{j=1}^{k} c_j \sigma \left(w_j^T x + \beta_j \right)$$

is dense in $C(I_m)$, where I_m is a unit cube of m-dimension. In other words, given $F \in C(I_m)$ and $\varepsilon > 0$, there is a sum $G(x)$ of the above form, such that $|G(x) - F(x)| < \varepsilon$ for all $x \in I_m$.

Remark 5.1.4. *Theorem 5.1.3 makes it possible to approximate a continuous multi-variate function by functions of one variable function(sigmoidal function) composed with affine functions. Since both sigmoidal function and affine functions have simple forms, this type of approximation will have a relatively simple representation. Moreover, the result in Theorem 5.1.3 can be strengthened by restricting the components of w and β to be integers, see [8], or by kth-degree sigmoidal functions satisfying*

$$\lim_{x \to -\infty} x^{-k}\sigma(x) = 0, \qquad \lim_{x \to \infty} x^{-k}\sigma(x) = 1, \tag{52}$$

Note that Theorem 5.1.3 says that F can be approximated by

$$G_1(x; c, w, \beta) = \sum_{j=1}^{k} c_j \sigma \left(w_j^T x + \beta_j \right) \tag{53}$$

on a compact set D for certain c, w and β, which, however, depends on F and the approximation accuracy and are unknown. Set $\vec{W}_1 = (c, w, \beta)$, we can define the identification error

$$e_I(\vec{W}_1) = \max_{x \in D} \left\{ \text{dist}(G_1(x, \vec{W}_1), F(x)) \right\}. \tag{54}$$

In the mathematical literature, system identification can be formulated to the following minimization problem

$$\min_{\vec{W}_1} \left\{ e_I(\vec{W}_1) \right\}. \tag{55}$$

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And in the control theory, $e_I(\vec{W}_1)$ should be the feedback signal sent back to the identification system to modify the parameter $\vec{W}_1$ accordingly, see the following block diagram for system identification.
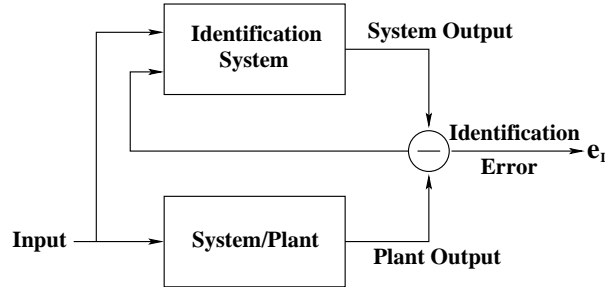

Figure 14: Block Diagram of System Identification.

5.1.2 Controller Generation.

Once the plant is identified, we are ready to consider the control on it. Now the reference model plays an important role. Roughly speaking, reference model is a model whose output is what the plant is expected to have. The controller generator will produce a controller according to the reference output such that such a controller can drive the plant to follow the reference output. See Figure 15.
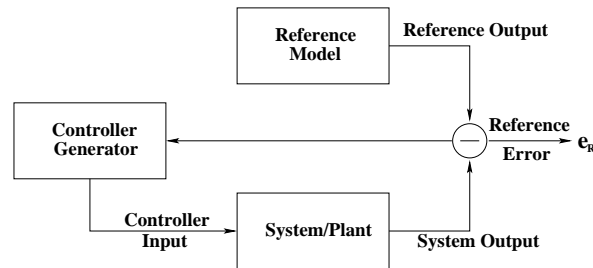

Figure 15: Block Diagram of Controller Generation.

Note that the controller should be designed to be capable of producing all the admissible control for the plant. Suppose that the controller generator has a similar structure to the system identification and is given by

$$u = G_2(y; \vec{W}_2), \qquad y = G_1(x, u; \vec{W}_1) \tag{56}$$

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where $\vec{W}_2$ collects all the parameters in the construction of controller generator. Here we abuse notation and replace x in (53) by (x, u) and instead, D will denote the set of plant input and control input. This is because the complete input to the plant consists of the genuine plant input and the control input in MRC control, and the identification process will be based on both of them.

Then the reference error will be defined as

$$e_R(\vec{W}_1, \vec{W}_2) = \max_{x \in D} \left\{ \text{dist}(G_1(x, u; \vec{W}_1), r(x)) \right\}, \qquad u = G_2(y; \vec{W}_2) \qquad (57)$$

where $r(x)$ is the reference signal. Note that e_R depends not only on $\vec{W}_1$ directly, but also on $\vec{W}_2$ indirectly through control u. And the controller generation is to search $(\vec{W}_1, \vec{W}_2)$ such that e_R is minimized.

If we reconsider the controller generation by treating the reference model as a plant, this procedure will be same as system identification, but what needs to be identified is not the real plant but the reference signal. Therefore, from this point of view, system identification and controller generation are essentially the same. And the difference between them occurs in two aspects. One is that the roles they play in MRC are different, which is a trivial fact. The other is the algorithm to complete these two processes are very different, as shown in the following section.

5.1.3 Learning and Training in MRC.

By gluing the two block diagrams for system identification and controller generation, we will have a complete picture for the model reference control as a whole, see Figure 16. And MRC is mathematically to minimize both the identification error e_I and reference error e_R simultaneously.

In a word, MRC becomes a minimization problem. The algorithm by which the optimal solution can be achieved is called learning and training algorithm. A well known approach for minimization is the gradient method. However, we must be careful to apply gradient method to these two processes.
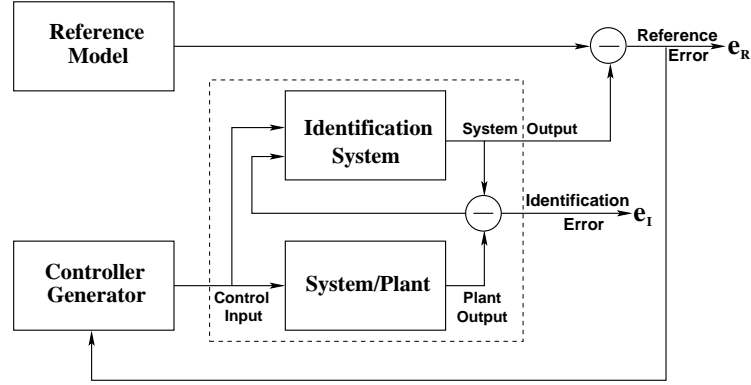
Figure 16: Block Diagram of Model Reference Control.

First, even though u depends on $\vec{W}_2$, e_I is independent of $\vec{W}_2$ because the identification is according to (x, u) by thinking u as the part of the plant input, but not only x. Due to the explicit dependence of e_I on $\vec{W}_1$, the gradient method reads

$$\vec{W}_1^{k+1} = \vec{W}_1^k - \varepsilon \frac{\partial e_I}{\partial \vec{W}_1}$$

where ε is called learning rate. This generates a feedforward network and relatively easy to be trained.

Second, in (56), we can see that u and y are strongly coupled. When the second equation on y is substituted into the first one in (56) and repeat this process, it will be an composition of infinitely many times. In other words, due to the indirect dependence of e_R on $\vec{W}_1$ through u, the gradient methods will induce a recurrent or feedback network which makes training harder than identification. A detailed discussion in terms of neural network will be provided in the next section.

Since the delay occurs only at the network input, and the network contains no feedback loops, the network plant model can be trained using the backpropagation for feedforward networks, which will be discussed with neural network. This algorithm is called offline.

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5.2   NN Structure of MRC

Cybenko's Theorem 5.1.3 provides a mathematical foundation to construct artificial neural network and make it capable of universal approximation. Thus neural network is a good choice to implement MRC. In this section, we will mainly introduce the neural network structure of MRC.

5.2.1   Neural Network

In [3], J.P. Aubin studied neural network in the mathematical framework and brought up some mathematical description about neural network in the different viewpoint. The following is a brief introduction of the neural network by Aubin's notation in [3].

A **neural network** is a collection of "formal neurons" linked in certain way. The node of network is called **synapse** and its strength the synaptic weight. Each individual neuron is a function φ_i which receives input signal x from the presynaptic neuron $i - 1$, processes the afferent signal and releases an output signal to the postsynaptic neuron $i + 1$. Precisely, it can be written as

$$\varphi_i : x = (x_k)_{k=1}^n \mapsto \varphi_i(x). \tag{58}$$

Suppose that the jth neuron is linked with other n presynaptic neurons, then it is excited by

$$\sum_{k=1}^n w_j^k \varphi_k(x) - \beta_j \tag{59}$$

if the threshold β_j is taken into account, where w_j is the synaptic weight. The sign of w_j indicates the excitation for $w_j > 0$ and inhibition for $w_j < 0$, and its modulus the strength. Consequently the output of the j-th neuron is a function of the neuron potential as

$$y_j = g_j \left(\sum_{k=1}^n w_j^k \varphi_k(x) - \beta_j \right), \tag{60}$$

where g_j is the nonlinear function in SW theorem, or precisely a sigmoidal function σ in Cybenko's theorem. Figure 17 shows the general structure of a neuron.

When $\varphi_k(x) = x$, a one-layer network can be represented by

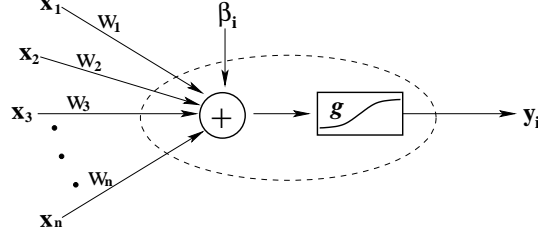$$y = g(Wx - \beta), \qquad x \in X, \quad y, \beta \in Y, \quad W \in \mathcal{L}(X, Y), \tag{61}$$

Figure 17: Structure of a neuron.

where $\mathcal{L}(X, Y)$ denotes the space of linear operators W from X to Y. For simplicity, we will use W to represent all the parameters involved in one neuron, including synaptic weights w_j and threshold β.

If there are $L > 1$ layers in the network, the sequence of signals is represented by

$$x_i = g_i(W_i x_{i-1}), \qquad x_i \in X_i, \quad W_i \in \mathcal{L}(X_{i-1}, X_i), \quad i = 1, \ldots, L \tag{62}$$

where $X_0 = X$ and $X_L = Y$ are the input and output spaces, and other X_i's are the spaces of "hidden layers". Then the input and output are related in the following way

$$x_L = g_L \left(W_L g_{L-1} \left(\ldots \left(g_1 \left(W_1 x_0 \right) \right) \ldots \right) \right). \tag{63}$$

Note that the sequence of superposition implies the concatenation of several layers of neurons. Denote by $\vec{W} = (W_i)_{i=1,\ldots,L}$, then it shows that a multilayer neural network can be regarded as a one-layer network controlled by $\vec{W}$, as shown below

$$y = x_L = \Phi(x_0, \vec{W}) = \Phi(x_0, W_1, \ldots, W_L). \tag{64}$$

The following theorem is useful for choosing the number of layers of neurons.

Theorem 5.2.1. *Let g be a bounded, increasing real function, $\Omega \subset \mathbb{R}^d$ is compact and $f : \Omega \to \mathbb{R}^d$ is continuous. Then for any $\varepsilon > 0$, there exist some $n \in \mathbb{N}$ and $w_i, w_{ij}, \beta_j \in \mathbb{R}$, such that*

$$\max_{x \in \Omega} |y(x) - f(x)| < \varepsilon, \quad where \quad y(x) = \sum_{i=1}^{n} w_i g \left(\sum_{j=1}^{d} w_{ij} x_j - \beta_j \right).$$

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It follows from this theorem that the feedforward neural network of two layers is capable of universal approximation to any continuous functions on a compact set. By convention, neural network of finite layers is called **synchronous** and governed by a discrete dynamical system (64). In contrast, the network of infinite layers is called **asynchronous** and given by a differential equation

$$x'(t) = f(x(t), W(t)), \tag{65}$$

which maps the initial input $x_0 \in X$ to the output signal

$$\Phi(x_0, W(\cdot)) = x_{W(\cdot)}(T) \tag{66}$$

where $x(\cdot)$ is the solution of equation (65) controlled by $t \mapsto W(t)$.

5.2.2 Learning Algorithm via NN

Following the notation in [3], we set

$$\vec{W} \in \mathcal{W} = \prod_{i=1}^{L} \mathcal{L}(X_{i-1}, X_i), \qquad y = \Phi(x, \vec{W}). \tag{67}$$

In control theory, the system governed by $\Phi : X \times \mathcal{W} \to Y$ can be regarded as an adaptive system with input x, output y and control $\vec{W} \in \mathcal{W}$. For a given training set $\mathcal{K} \in X \times Y$, a pattern (x^p, y^p) is recognized by the adaptive system programmed by such a control $\vec{W}$ if $y^p = \Phi(x^p, \vec{W})$. And the choice of such a control is made by *learning* the patterns in $\mathcal{K}$. Namely one should find a control $\vec{W}$ satisfying

$$y^p = \Phi(x^p, \vec{W}), \qquad (x^p, y^p) \in \mathcal{K}. \tag{68}$$

Then the learning process can be formulated by the minimization problem

$$0 = \inf_{\vec{W}} \left\{ \sum_{(x^p, y^p) \in \mathcal{K}} E\left(\Phi(x^p, \vec{W}), y^p\right)^\alpha \right\}^{\frac{1}{\alpha}}, \tag{69}$$

where $\alpha \in [1, \infty]$ and E is a distance on Y. Suppose that the linear operator $p \otimes y \in \mathcal{L}(X, Y)$ is defined by

$$p \otimes y : x \mapsto (p \otimes y)(x) = \langle p, x \rangle y, \qquad p \in X^\star, y \in Y, x \in X \tag{70}$$

where $X^\star$ is the dual space of X and $\langle p, x \rangle = p(x)$. Let E, g and hence Φ be differentiable and $\vec{W}$ be a solution of $\Phi_L(a, \vec{W}) = b$ for $\mathcal{K} = \{(a, b)\}$, then one may start with an initial synaptic matrix $\vec{W}^0$, define $\vec{W}^{n+1}$ as

$$W_i^{n+1} - W_i^n = -\varepsilon_n x_{i-1}^n \otimes g_i'(W_i^n x_i^n)^\star p_i^n \tag{71}$$

where ε_n is the learning rate, $x_i^n = g_i(W_i^n x_{i-1}^n)$ (starting at $x_0^n = a$) and

$$p_i^n = W_{i+1}^{n\star} g_{i+1}'(x_{i+1}^n)^\star \cdots W_L^{n\star} g_L'(x_L^n)^\star E'(x_L^n - b) \tag{72}$$

We start with modifying the synaptic weights of the last layer L by computing

$$p_L^n = W_L^{n\star} g_L'(x_L^n)^\star E'(x_L^n - b), \tag{73}$$

and W_L^{n+1} from (71), then all the synaptic matrices W_i^n in each layer can be obtained from the last one back to the first one. Thus this algorithm is called backpropagation.

In particular, if $\mathcal{K} = \{(a^q, b^q) | q = 1, \ldots, Q\}$, then (71) becomes

$$W_i^{n+1} - W_i^n = -\varepsilon_n \sum_{q=1}^{Q} x_{i-1}^{n,q} \otimes g_i'(W_i^n x_i^{n,q})^\star p_i^{n,q} \tag{71$'$}$$

where $x_i^{n,q} = g_i(W_i^n x_{i-1}^{n,q})$ (starting at $x_0^{n,q} = a^q$) and

$$p_i^{n,q} = W_{i+1}^{n\star} g_{i+1}'(x_{i+1}^{n,q})^\star \cdots W_L^{n\star} g_L'(x_L^{n,q})^\star E'(x_L^{n,q} - b^q). \tag{74}$$

Certainly the solution of $\Phi_L(a, \vec{W}) = b$ may not exist for $(a, b) \in \mathcal{K}$ when $\mathcal{K}$ is of large size. In this situation, we can reconsider to search for its least square solution. Please refer to [3] for details.

5.3   MRC Control of BZ Reaction

Model reference control has a wide application in engineering but not in biological systems. Few examples about MRC control of SIRS disease models are given in [6]. In this section, we will apply MRC to the BZ reaction determined by the reversible Lotka-Volterra system (11). By the analysis in Section 4.4.1, we know that the reaction exhibits nonlinear

oscillation far away from the equilibrium point. Our goal is to eliminate the oscillation, or lower the oscillation amplitude by applying some control.

First, we need to choose the control variable. It is reasonable to have each reactant of (u, v, w) as the controller by adding the corresponding reactant to increase its concentration. For instance, suppose that u is the control variable, then the system with control is given below

$$\begin{cases} \dfrac{du}{d\tau} &= u(w - v) - \varepsilon(\sigma u^2 - v^2) + x'(\tau) \\ \dfrac{dv}{d\tau} &= v(u - 1) - \varepsilon v^2 + \varepsilon\left(\xi + x(\tau) - u - v - \frac{w}{\sigma}\right) \\ \dfrac{dw}{d\tau} &= -\sigma(wu - \varepsilon\sigma u^2). \end{cases} \tag{75}$$

Second, we need to have a measure about the oscillation amplitude. Since we know that there exists an oscillation axis $W^o_{\sigma,\varepsilon}$ in the oscillation zone, we can calculate the distance from the surrounding solution to $W^o_{\sigma,\varepsilon}$ in the same level of w. Here, we use the version given in (38) to approximate $W^o_{\sigma,\varepsilon}$. Define

$$L(t) = \sqrt{[u(t) - h_1(w(t), \sigma)]^2 + [v(t) - h_2(w(t), \sigma)]^2}.$$

where

$$h_1(w, \sigma) = \mu_\sigma\left(1 - \frac{\varepsilon(\xi - \frac{w}{\sigma})}{h_2(w, \sigma)}\right), \qquad h_2(w, \sigma) = \frac{1}{2}\left(w + \sqrt{w^2 + 4\sigma\varepsilon\mu_\sigma\xi}\right).$$

Then we may think that there is no oscillation when $L(t)$ is small. Therefore our target is to find a control to minimize $L(t)$.

Third, we need to find a reference model. Actually there are many options for the reference model as long as it can have the desired output. For example, to control the robot's arm determined by

$$\frac{d^2\phi}{dt^2} = -10\sin\phi - \frac{d\phi}{dt} + u, \tag{76}$$

the reference model can be chosen as

$$\frac{d^2 y_r}{dt^2} = -9y_r - 6\frac{dy_r}{dt} + 9r, \tag{77}$$

and the numerical simulation is shown in Figure 18, see [26]. We may notice that the
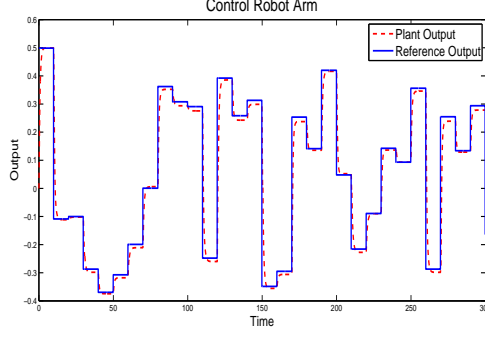
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Figure 18: MRC control of robot arm.

reference output smooths out its piecewise constant input which allows the robots arm can move in any angle. However, generically speaking, it is impossible to make the biological system behave in any way we want because of its self-organization and robustness. But since we care only about the long time behavior of L, getting smaller with time evolution, we will simply choose the reference model as

$$\dot{r} = -r \tag{78}$$

which gives the exponential decay to zero.

In this example, we will assume that the plant given by (75) is unknown. Mainly we will use (75) to generate input-output data set, namely the training set $\mathcal{K}$, for the learning purpose in the system identification and controller generation.

We will consider both the plant and reference model in the time interval $[0, \bar{t}]$ with $\bar{t}$ given. For any partition of this time interval

$$0 = t_0 < t_1 < \ldots, < t_N = \bar{t}$$

where N is the number of the sample data, define , for $1 \leq i \leq N$,

$$x(t) = x_i, \qquad \text{as} \qquad t \in [t_{i-1}, t_i),$$

where x_i's are randomly picked in the range $[0, 0.1]$. With $x(t)$ as the input signal to the plant, let $L(t)$ be the corresponding output of (75) which is sampled at time t_i and defined by $L_P^i = L_P(t_i)$. Denote $\mathbf{x} = (x_1, \ldots, x_N)$ and $\mathbf{L}_P = (L_P^1, \ldots, L_P^N)$, then we can generate

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the training set for the system identification as $\mathcal{K}_1 = (\mathbf{x}, \mathbf{L}_P)$. For the given NN plant, let $\mathbf{L}_N(\vec{\mathbf{W}}_1) = (L_N(t_i))_{1 \leq i \leq N}$ be the corresponding NN plant output to the input $\mathbf{x}$, where $\vec{\mathbf{W}}_1$ collects all the weights involved in the network of NN plant. Now we are ready to define, respectively, the identification error and cost functional for identification by

$$e_I(\vec{\mathbf{W}}_1) = |\mathbf{L}_P - \mathbf{L}_N(\vec{\mathbf{W}}_1)|, \qquad \hat{\mathbf{F}}_I(\vec{\mathbf{W}}_1) = e_I^2(\vec{\mathbf{W}}_1).$$

The system identification is to minimize the functional $\hat{\mathbf{F}}_I(\vec{\mathbf{W}}_1)$ over the parameters $\vec{\mathbf{W}}_1$.

Next, similar to the random input $\mathbf{x}$ for identification, under a time partition $0 = s_0 < s_1 < \cdots < s_M = \bar{t}$, for a random reference input $\mathbf{x}_r = (x_{r1}, \ldots, x_{rM})$ where M is the number of samples, let $\mathbf{r} = (r_1, \ldots, r_M)$ be the reference output of (78). Then the training set for the controller is given by $\mathcal{K}_c = (\mathbf{x}_r, \mathbf{r})$. And the reference error and the associated cost functional are defined similarly as follows

$$e_R(\vec{\mathbf{W}}_2) = |\mathbf{L}_P - \mathbf{r}|, \qquad \hat{\mathbf{F}}_R(\vec{\mathbf{W}}_2) = e_R^2(\vec{\mathbf{W}}_2).$$

where $\vec{\mathbf{W}}_2$ contains all the weights and biases in the NN controller.

In the numerical simulation, set

$$\sigma = 0.01, \qquad \varepsilon = \sigma^3, \qquad \xi = 500.$$

The network of system identification is trained under the admissible control in $u \in [0.0, 0.1]$, that is, the plant input is $\mathbf{x} = (x_i)_i$ with $x_i \in [0, 0.1]$.

By the backpropagation, all the parameters in the NN plant will be justified for the best performance of the NN plant, that is, for the NN plant outputs being as close to the plant output as possible. Here the Levenberg-Marquardt algorithm is employed for backpropagation. This algorithm is a variation of Newton's method and is designed for minimizing functions which are in terms of the square sums of other functions(see [25]), like $\hat{\mathbf{F}}_I$ and $\hat{\mathbf{F}}_R$. The built-in function for this algorithm in the SIMULINK is called trainlm.

Usually the network processes one pattern in the training set $\mathcal{K}_1$ at a time, feed the input into the network, processes with the weights and functions in the layers and then

compare the resulting output with the desired output. Then the errors are propagated back to the network so that the weights can be adjusted correspondingly and carried into the processing of the next pattern. One sweep through all the patterns in $\mathcal{K}_2$ is called an epoch, that is, the number of the iteration of NN plant training to be performed. In the simulation, we use 300 training epochs for the system identification.

With the well-trained network of NN plant which provides a good approximation to the plant (75), the system identification is complete. Now we are ready to train the controller. It will always take much more time to train a controller than to identify a plant because the dynamic backpropagation is needed for the recurrent network of controller. Therefore, instead of processing the entire training set $\mathcal{K}_2$ in one epoch, first we will divide $\mathcal{K}_1$ into several segments, and then process them one by one in the same way as for identification until all the segments are presented to the network. Here we will choose, for the controller training, 30 segments for the training set $\mathcal{K}_2$ and 10 epochs for the processing of each segment.

The network for controller is trained under the random reference inputs in [0, 10], that is, the reference input is $\mathbf{r} = (r_i)_i$ with $r_i \in [0, 10]$. After the controller is trained, we can start the simulation, see the following figures.

As shown in Figure 19, without control, the plant output $L(t)$ oscillates in the relatively large amplitudes, and the oscillation lasts in a relatively long time around $t = 200$. But when the control is imposed, the oscillation amplitude decreases dramatically and becomes very small after $t = 30$. We can also compare the (u, v) output with and without control given in Figure 20. We may observe that without control, u and v oscillates with large amplitudes and small frequencies because they are far away from the oscillation axis. While after the control is turned on, we can see that they all oscillates with much smaller amplitudes and high frequencies because they are driven to be close to the oscillation axis.
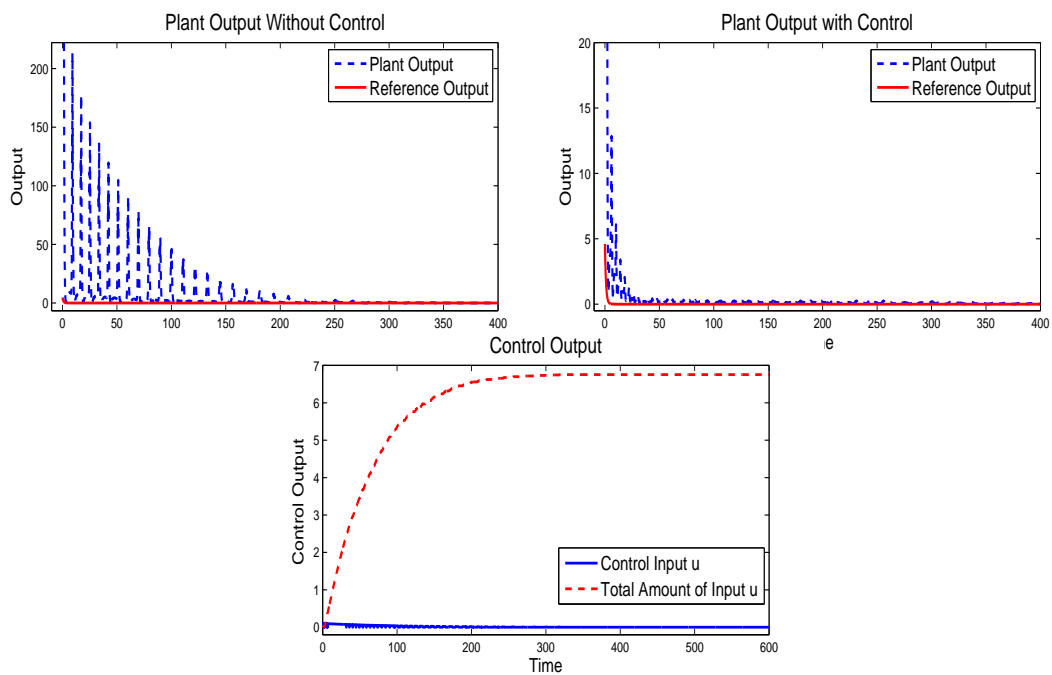
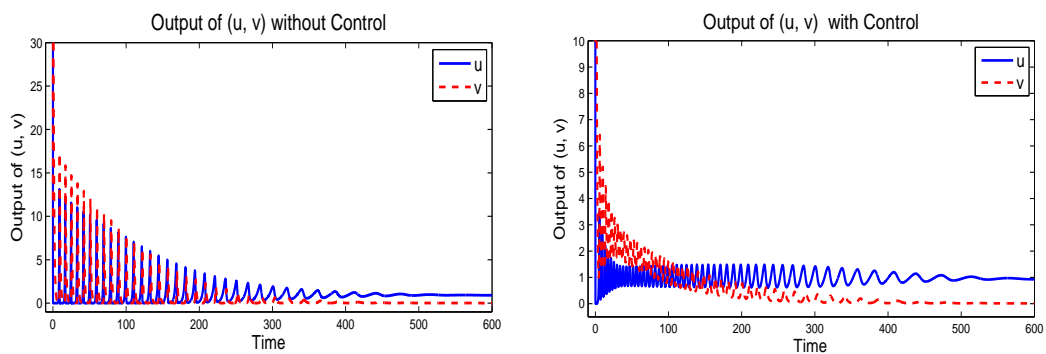**Figure 19:** MRC of BZ reaction given by reversible LV Model.

Figure 20: Output of (u, v) with and without control.

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