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Center Bifurcation for the Smallest Bimolecular Mass-Action System

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Abstract. This paper investigates the center bifurcation of the smallest bimolecular mass-action system. A three-dimensional reaction network, consisting of three species and four reactions, governed by mass-action kinetics with a positive equilibrium point, is considered. In addition to the stability analysis of the equilibrium point, the dynamic directions of the model in its planes are examined. It has been previously shown that the equilibrium point is classified as a center when the reaction rate constants satisfy a specific condition, leading to a vertical Andronov-Hopf bifurcation. Furthermore, it is demonstrated that only one limit cycle can bifurcate from the center equilibrium point using a bifurcation technique.

2020 Mathematics Subject Classifications: 37G10, 37G15, 34C23

Key Words and Phrases: Bimolecular mass-action system, Hopf bifurcation, limit cycle, center bifurcation

1. Introduction

Chemical reaction networks are fascinating for both practical and theoretical reasons. They are essential components of various biological models and significantly impact other fields of science and engineering. Numerous important findings, both traditional and contemporary, provide insights into the dynamics of a chemical reaction network based on its combinatorial structure [1].

Wilhelm described a bimolecular chemical reaction network with three species and four reactions, having rank three, that exhibits Hopf bifurcation due to mass action dynamics [2]. His example demonstrated that the set of bimolecular networks with Hopf bifurcation is not empty. However, there are, up to isomorphism, 14670 bimolecular networks (with three species and four reactions of rank three) that permit positive equilibria [3]. The main question: is how many of these networks allow for Hopf bifurcation due to mass action dynamics?

To answer this question, a scientific study by Banaji and Boros investigated the smallest

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bimolecular chemical reaction networks with Hopf bifurcation [3]. This means that these networks have the fewest species and reactions. The results show that the smallest bimolecular mass-action network allowing Hopf bifurcation must have at least three species and at least four reactions. They found that 138 non-isomorphic bimolecular networks allow for Andronov-Hopf bifurcation. These networks can be dynamically divided into 87 non-equivalent classes. Of these classes, 86 admit non-degenerate Andronov-Hopf bifurcations, leading to isolated limit cycles. However, in the remaining class, Andronov-Hopf bifurcations can only be degenerate. The three-dimensional system corresponding to the last class of the reaction network is

$$\begin{aligned} \dot{x}_1 &= x_1(k_1x_3 - k_2x_2), \\ \dot{x}_2 &= x_2(k_2x_1 - k_3x_3). \\ \dot{x}_3 &= -x_3(k_1x_1 + k_3x_2) + 2k_4, \end{aligned} \tag{1}$$

where $k_i, i = 1, 2, 3, 4$ are real positive parameters called the reaction rate constants and $x_i \geq 0$. System (1) has a unique positive equilibrium point, which is of type center when the parameters satisfy $k_1 = k_2 + k_3$ [4]. It is proven by finding a constant of motion. They also proved the existence of a global center manifold that attracts all positive solutions. To gain information about bimolecular networks with Hopf bifurcation, the reader should consult the references [5–10].

An important question arises: If we perturb the parameters in system (1), how many periodic orbits can bifurcate from the positive equilibrium point? To address this, a technique is applied to system (1) to estimate the cyclicity bifurcating from the center. This method was first employed in three dimensions by Salih [11]. It has since been utilized in various scientific studies. Salih demonstrated that four limit cycles can bifurcate from the center of the 3D Lotka-Volterra system [11]. Additionally, Salih *et al.* [12] applied the technique to two differential systems, showing that one and five limit cycles can bifurcate from the quadratic polynomial system and the Lü system, respectively. Salih *et al.* [13] examined a specific type of the Jerk system, revealing that three and four limit cycles can bifurcate from the center equilibrium point under two different sets of conditions.

This paper is organized as follows: Section 2 focuses on identifying the existence of equilibrium points in system (1) and studying their stability. The trajectory directions in the planes are investigated in Section 3. The next section is dedicated to the study of both Hopf and center bifurcations. Lastly, the conclusions are presented.

2. Equilibrium Point and Its Stability

Equilibrium points are fundamental to understanding various aspects of dynamical systems. To identify the equilibrium points of system (1), the right-hand sides of the equations are set to zero. It is found that there is one positive equilibrium point, given by $E = \left(\sqrt{\frac{k_3k_4}{k_1k_2}}, \sqrt{\frac{k_1k_4}{k_2k_3}}, \sqrt{\frac{k_2k_4}{k_1k_3}}\right)$. Through simple analysis, one can easily derive the following conclusion.

Proposition 1. *For system (1), the stability of the equilibrium point E is determined as follows:*

i. It is asymptotically stable if and only if $k_1 > k_2 + k_3$.

ii. It is a center when $k_1 = k_2 + k_3$.

iii. It is unstable when $k_1 < k_2 + k_3$.

Proof. The Jacobian matrix of system (1) at the equilibrium points E is given by

$$\begin{bmatrix} 0 & -\sqrt{\frac{k_2k_3k_4}{k_1}} & \sqrt{\frac{k_1k_3k_4}{k_2}} \\ \sqrt{\frac{k_1k_2k_4}{k_3}} & 0 & -\sqrt{\frac{k_1k_3k_4}{k_2}} \\ -\sqrt{\frac{k_1k_2k_4}{k_3}} & -\sqrt{\frac{k_2k_3k_4}{k_1}} & -2\sqrt{\frac{k_1k_3k_4}{k_2}} \end{bmatrix} \tag{2}$$

its characteristic equation is

$$\lambda^3 - T\lambda^2 - K\lambda - D = 0, \tag{3}$$

where

- T is the trace of (2) and $T = -2\sqrt{\frac{k_1k_3k_4}{k_2}}$,
- K is the sum of the diagonal minors of (2) and $K = k_4\,(k_3 - k_1 - k_2)$,
- D is the determinant of (2) and $D = -4k_4\sqrt{k_1k_2k_3k_4}$.

Since D is negative, Eq. (3) has one negative real root and two other roots that have the same sign. As T is negative, the sign of $TK + D$ is determined by $(k_1 - k_2 - k_3)$. The sign of $(k_1 - k_2 - k_3)$ plays an important role in determining the stability of the equilibrium point. Thus,

i. When $k_1 > k_2 + k_3$, it implies that $TK + D > 0$. According to the Routh-Hurwitz criterion, the real parts of the eigenvalues are negative. Therefore, the equilibrium point E is asymptotically stable if and only if $k_1 > k_2 + k_3$, see Fig.1-a.

ii. When $k_1 = k_2 + k_3$, Eq. (3) has one real negative root and a pair of purely imaginary roots. In reference [4], it has been proven that the equilibrium point E is of center type, see Fig.1-b.

iii. When $k_1 < k_2 + k_3$, it implies that $TK + D < 0$. In this case, Eq. (3) has two roots with positive real parts, making the equilibrium point E unstable, see Fig.1-c.

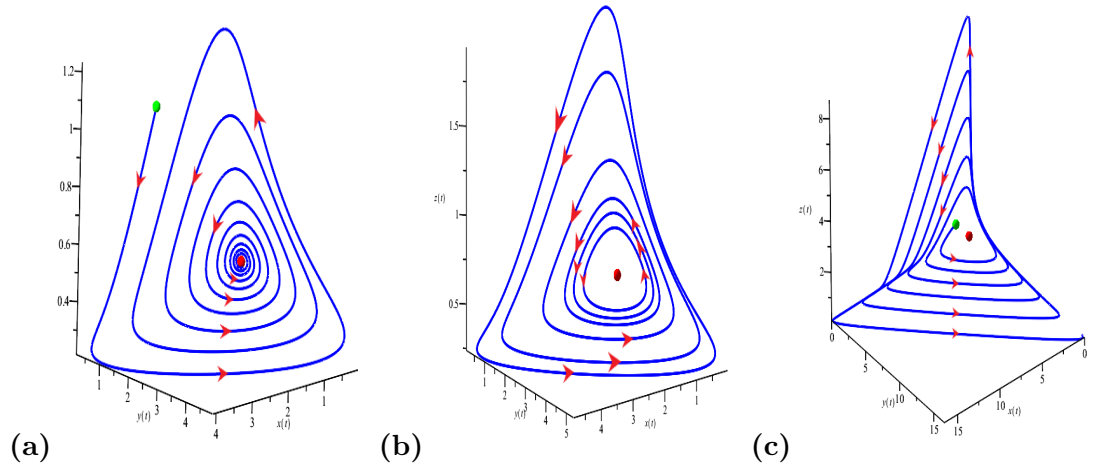

Figure 1: The phase portrait of system (1) is shown and the parameters $k_2 = \frac{1}{2}, k_3 = k_4 = 1$ are fixed. **(a)** when $k_1 = 2$, E is asymptotically stable. **(b)** when $k_1 = \frac{3}{2}$, E is a center. **(c)** when $k_1 = 1$, E is unstable. The green and red balls indicate the equilibrium and initial points, respectively.

3. Trajectories in Planes

This section focuses on the study of the dynamics of system (1) in the planes. To understand the dynamics of the system, the trajectories and their evolution on the planes are investigated individually. Two of the planes, namely the x_1x_3-plane and the x_2x_3-plane, are invariant, meaning that the trajectories remain confined to them as time approaches infinity. Moreover, along all three coordinate axes, $\dot{x}_3$ is always positive.
On the x_2x_3-plane, $\dot{x}_2$ is always negative. The horizontal isocline, $x_2x_3 = \frac{2k_4}{k_3}$, is used to determine the sign of $\dot{x}_3$. A point (x_2, x_3) is chosen on one side of the isocline. First, a point on the left side is selected and $x_2x_3 = \frac{2k_4}{k_3} - \epsilon$, where $\epsilon > 0$ is set. This implies that $\dot{x}_3 = k_3\epsilon > 0$. However, if a point on the other side is chosen, $x_2x_3 = \frac{2k_4}{k_3} + \epsilon$, $\epsilon > 0$, then $\dot{x}_3 = -k_3\epsilon < 0$. The x_3-axis is always invariant and on the x_2-axis, $\dot{x}_3 > 0$. Now, sufficient information has been gathered to sketch the trajectory directions of the system, as depicted in Fig. 2-a.

On the x_1x_3-plane, $\dot{x}_1$ is always positive and a horizontal isocline, $x_1x_3 = \frac{2k_4}{k_1}$, is present, which determines the sign of $\dot{x}_3$. It can be easily shown that $\dot{x}_3 > 0$ on the left side, while $\dot{x}_3 < 0$ on the other side of the isocline. The x_3-axis is found to be invariant and $\dot{x}_3$ is positive on the x_1-axis. By combining these observations, sufficient conditions for sketching the trajectory directions are derived and illustrated in Fig. 2-b.

On the x_1x_2-plane, it is noted that $\dot{x}_1$ is always negative, while both $\dot{x}_2$ and $\dot{x}_3$ are positive. The relations $\dot{x}_1 + \dot{x}_2 = 0$ and $\dot{x}_3 = 2k_4$ are satisfied, which implies that $x_1 + x_2 = c$, where $c \in \mathbb{R}$, and $x_3(t) = 2k_4t$. Since the plane is not invariant, this information indicates that the trajectories move with a positive slope. However, on each x_1 and x_2-axis, $\dot{x}_1 = \dot{x}_2 = 0$ and $\dot{x}_3 > 0$. This indicates that near the axes, the trajectories move upward toward the x_3-axis. This information helps us predict the direction of the trajectories.

By integrating the information obtained from Figs. 2-a, 2-b and the x_1x_2-plane, along with the dynamics at infinity, the complete information in Fig. 3 is derived. This information is useful for understanding the trajectory directions around the positive critical point E, which can be stable, unstable or a center in different cases.

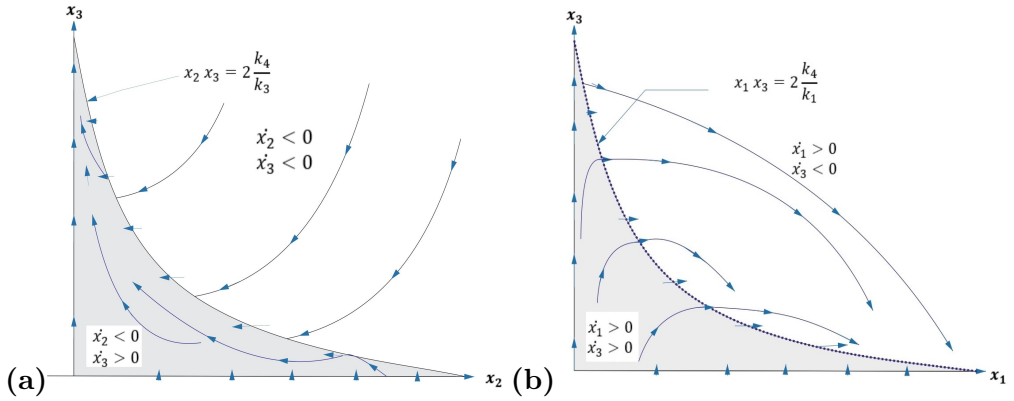

Figure 2: The trajectory directions of system (1) on the planes are shown. **(a)** trajectory direction on x_2x_3-plane. **(b)** trajectory direction on x_1x_3-plane. The dotted lines indicate the isoclines.

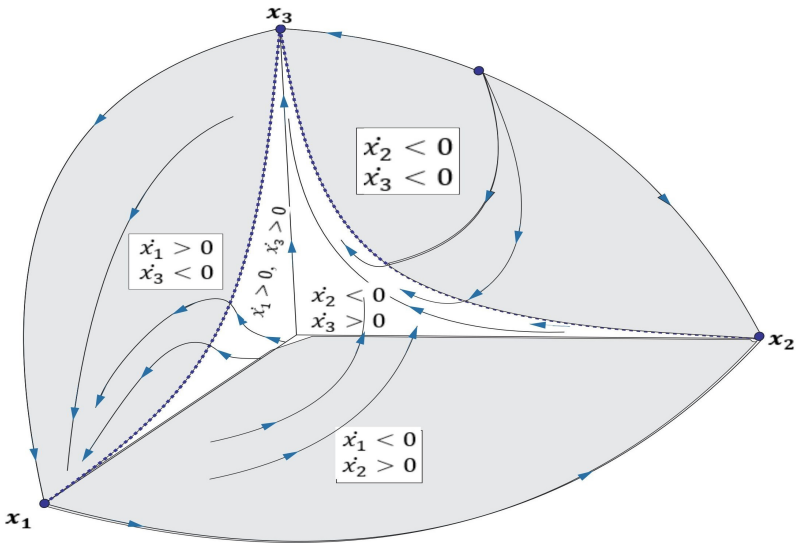

Figure 3: Directions of the trajectory of system (1) in the three planes.

4. Bifurcation Analysis

Bifurcations describe significant changes in the behavior of solution curves within a dynamical system as certain parameter values, called bifurcation values, are varied. This section examines both Hopf and center bifurcations in system (1), emphasizing the conditions under which they occur.

4.1. Hopf Bifurcation

Consider the following dynamical system in three dimensions:

$$\dot{X} = f(X, \mu), \tag{4}$$

where X is an element of $\mathbb{R}^3$, f is a real analytic function and μ belongs to $\mathbb{R}^k$, serving as the bifurcation parameter. The essential conditions for the occurrence of a Hopf bifurcation are now presented. It is assumed that the system possesses an equilibrium point (E_0, μ_0) at which the following criteria are satisfied:

i. The Jacobian matrix $J = Df(E_0, \mu_0)$ possesses a unique pair of purely imaginary eigenvalues $\lambda(\mu_0)$ and $\bar{\lambda}(\mu_0)$, while the remaining eigenvalues are non-zero.

ii. $\frac{dRe(\lambda(\mu_0))}{d\mu} \neq 0$.

Subsequently, the system defined by (4) experiences a Hopf bifurcation at the equilibrium point (E_0, μ_0) [14]. System (4), satisfying the conditions above, can be transformed into the following canonical form:

$$\begin{aligned} \dot{x}_1 &= -\omega x_2 + f_1(x_1, x_2, x_3; \mu), \\ \dot{x}_2 &= \omega x_1 + f_2(x_1, x_2, x_3; \mu), \\ \dot{x}_3 &= \lambda x_3 + f_3(x_1, x_2, x_3; \mu), \end{aligned} \tag{5}$$

where $\omega > 0$, $\lambda \neq 0$ and $f_i(x_1, x_2, x_3; \mu) = \sum_{k=2}^{\infty} f_i^k(x_1, x_2, x_3; \mu)$ for $i = 1, 2, 3$ and $f_i^k(x_1, x_2, x_3; \mu)$ are homogeneous polynomials of degree k.

Proposition 2. *For system (1), the Hopf bifurcation occurs at the equilibrium point E when the parameter k_1 passes through k_1^* where $k_1^* = k_2 + k_3$.*

Proof. By applying the linear transformation $x_1 \to x_1 + \sqrt{\frac{k_3 k_4}{k_1 k_2}}, x_2 \to x_2 + \sqrt{\frac{k_1 k_4}{k_2 k_3}}$ and $x_3 \to x_3 + \sqrt{\frac{k_2 k_4}{k_1 k_3}}$, the equilibrium point E is relocated to the origin, resulting in the transformation of system (1) into:

$$\begin{aligned} \dot{x}_1 &= \left(\sqrt{\frac{k_3 k_4}{k_1 k_2}} + x_1 \right) (-k_2 x_2 + k_1 x_3), \\ \dot{x}_2 &= \left(\sqrt{\frac{k_1 k_4}{k_2 k_3}} + x_2 \right) (k_2 x_1 - k_3 x_3), \\ \dot{x}_3 &= -\sqrt{\frac{k_1 k_2 k_4}{k_3}}\, x_1 - \sqrt{\frac{k_2 k_3 k_4}{k_1}}\, x_2 - 2\sqrt{\frac{k_1 k_3 k_4}{k_2}}\, x_3 - k_1 x_1 x_3 - k_3 x_2 x_3. \end{aligned} \tag{6}$$

The characteristic equation corresponding to the Jacobian matrix of system (6) evaluated at the origin is

$$\lambda^3 + 2\sqrt{\frac{k_1 k_3 k_4}{k_2}}\lambda^2 - k_4 (k_3 - k_1 - k_2)\lambda + 4k_4\sqrt{k_1 k_2 k_3 k_4} = 0, \tag{7}$$

Letting $k_1 = k_1^*$, then Eq. (7) can be rewritten as

$$\left(\lambda + \frac{2}{\omega}\sqrt{k_3k_4\left(\omega^2 + 2k_4k_3\right)}\right)\left(\lambda^2 + \omega^2\right) = 0,$$

where $\omega = \sqrt{2k_2k_4}$. Clearly, Eq. (7) has two complex conjugate roots $\lambda_{1,2} = \pm i\omega$ and one real root $\lambda_3 = -\frac{2}{\omega}\sqrt{k_3k_4\left(\omega^2 + 2k_4k_3\right)}$. Thus, the initial requirement for the Hopf bifurcation theorem, which is the first condition, is fulfilled. It is important to note that, in general, $\lambda = \lambda(k_1)$. From Eq. (7), we can then express the relation as follows:

$$f(\lambda(k_1), k_1) = \left(\lambda(k_1) + \frac{2}{\omega}\sqrt{k_3k_4\left(\omega^2 + 2k_4k_3\right)}\right)\left(\lambda^2(k_1) + \omega^2\right).$$

Then, the root $\lambda = \lambda(k_1)$ of Eq. (7) satisfies the following

$$f(\lambda(k_1), k_1) = 0. \tag{8}$$

Differentiating Eq. (8) with respect to k_1 yields

$$\frac{\partial f}{\partial \lambda(k_1)}\ \frac{d\lambda(k_1)}{dk_1} + \frac{\partial f}{\partial k_1} = 0,$$

this implies that

$$\frac{d\lambda(k_1)}{dk_1} = -\frac{\partial f}{\partial k_1}\ \left(\frac{\partial f}{\partial \lambda(k_1)}\right)^{-1} = -\frac{k_2k_4\left(\lambda^2 + \sqrt{\frac{k_1k_2k_4}{k_3}}\,\lambda + 2k_2k_4\right)}{\sqrt{\frac{k_1k_2k_4}{k_3}}\,\left(3k_2\lambda^2 + 4\sqrt{k_1k_2k_3k_4}\,\lambda + k_2k_4\left(k_1 + k_2 - k_3\right)\right)}. \tag{9}$$

By taking the root $\lambda(k_1^*) = \lambda_{1,2}(k_1^*)$, we find that $\lambda_{1,2}(k_1^*) = \pm i\omega$. Substituting the value of λ_1 into Eq. (9), we obtain:

$$\frac{d}{dk_1}Re(\lambda_{1,2}(k_1))|_{k_1=k_1^*} = -\frac{k_4\omega\sqrt{k_3k_4\left(\omega^2 + 2k_3k_4\right)}}{\omega^4 + 4k_3k_4\left(\omega^2 + 2k_3k_4\right)} \neq 0.$$

Thus, the second condition for a Hopf bifurcation is met. Consequently, at E, system (1) undergoes a Hopf bifurcation when $k_1 = k_1^*$.

It is straightforward to determine the Lyapunov coefficients corresponding to system (6) at $k_1 = k_1^*$. Since the equilibrium point is a center, the $k-$th Lyapunov coefficients vanish for all k at k_1^* [15]. Therefore, by the Lyapunov theorem, system (1) exhibits a vertical Andronov-Hopf bifurcation as k_1 passes through k_1^*.

4.2. Center Bifurcation

Research in bifurcation theory currently focuses on the bifurcation of limit cycles from critical points. A limit cycle can be achieved by perturbing a focus or center. A widely used method is center bifurcation, which helps estimate cyclicity and examine the bifurcation of limit cycles from the center (see [16] and [17]). Here, we consider system (5). The set of all parameters in $f_i(x_1, x_2, x_3)$ for $i = 1, 2, 3$ is denoted by Λ and $\mathbf{K}$ is the corresponding parameter space.

4.2.1. A Technique to Examine the Cyclicity

This subsection describes a technique used for analyzing cyclicity. As previously noted, Christopher [18] explored a method for analyzing cyclicity bifurcating from a center in two-dimensional systems by linearizing the Lyapunov quantities. Salih [11] extended this approach to three-dimensional systems to estimate the cyclicity of the center, applying it for the first time to three-dimensional Lotka-Volterra systems. The technique used to estimate cyclicity in three-dimensional differential systems can be summarized in the following steps:

(i) Select a point on a center variety.

(ii) Linearize the Lyapunov quantities around this point.

(iii) Determine the codimension of the point. If the codimension of the selected point on the center variety is r and the first r linear terms of the Lyapunov quantities are linearly independent, then the cyclicity is $r-1$. This means that $r-1$ limit cycles can bifurcate from a small perturbation.

Defining the Lyapunov function and computing its focal values is a traditional approach to assess the number of limit cycles and their stability. This method involves looking for a function of the following form:

$$F(x_1, x_2, x_3) = x_1^2 + x_2^2 + \sum_{k=3}^{\infty} F_k(x_1, x_2, x_3), \tag{10}$$

where $F_k = \sum_{i=0}^{k} \sum_{j=0}^{i} C_{k-i,i-j,j} x_1^{k-i} x_2^{i-j} x_3^j$ for system (5) and the coefficients of F_k satisfy

$$\mathcal{X}(F) = L_1(x_1^2 + x_2^2) + L_2(x_1^2 + x_2^2)^2 + L_3(x_1^2 + x_2^2)^3 + ..., \tag{11}$$

where $L_i, i = 1, 2, ..$ are polynomials in the parameters of the system and the L_i is called the $i-$th Lyapunov constant (focal value). To explain the technique in greater detail, it is assumed that the center critical point of (5) corresponds to $0 \in \mathbf{K}$, using a perturbation method in the parameters. This can be written:

$$\begin{aligned} \mathcal{X} &= \mathcal{X}_0 + \mathcal{X}_1 + \mathcal{X}_2 + ..., \\ F &= F_0 + F_1 + F_2 + ..., \\ L_i &= L_{i0} + L_{i1} + L_{i2} + ..., \qquad i = 1, 2, ..., \end{aligned} \tag{12}$$

where $\mathcal{X}_0, F_0$ and L_{i0} are calculated at the unperturbed parameters, $\mathcal{X}_1, F_1$ and L_{1i} are obtained at a perturbed parameters of first order (they contain the terms of degree one in Λ), $\mathcal{X}_2, F_2$ and L_{2i} are obtained at a perturbed parameters of second order (they contain the terms of degree two in Λ) and so forth. The Lyapunov function F_i and the Lyapunov

quantity L_i are both of degree i in terms of parameters. By substituting Eq. (12) into Eq.(11), we obtain:

$$\begin{gathered}\mathcal{X}_0F_0=0,\quad \mathcal{X}_0F_1+\mathcal{X}_1F_0=L_{11}(x_1^2+x_2^2)+L_{21}(x_1^2+x_2^2)^2+\dots\,,\\ \mathcal{X}_0F_2+\mathcal{X}_1F_1+\mathcal{X}_2F_0=L_{12}(x_1^2+x_2^2)+L_{22}(x_1^2+x_2^2)^2+\dots\end{gathered}\tag{13}$$

and more general,

$$\mathcal{X}_0F_i+\dots+\mathcal{X}_iF_0=L_{1i}(x_1^2+x_2^2)+L_{2i}(x_1^2+x_2^2)^2+\dots\qquad,i=1,2,3,\dots\tag{14}$$

The linear terms of the Lyapunov quantities L_k (modulo the $L_i, i<k$) can be obtained by simultaneously solving the two equations in (13) using linear algebra. Eq. (14) is then used to derive the higher-order terms of the Lyapunov quantities.

4.2.2. Cyclicities Bifurcated from the Center Equilibrium Point

To apply the above technique, we choose point $(k_1,k_2,k_3,k_4)=(\frac{3}{2},\frac{1}{2},1,1)$ on center variety and let

$$\begin{aligned}k_1&=\frac{3}{2}+a_1+a_2,\\ k_2&=\frac{1}{2}+b_1+b_2,\\ k_3&=1+c_1+c_2\qquad\text{and}\\ k_4&=1+d_1+d_2\end{aligned}\tag{15}$$

are defined where a_1,b_1,c_1,d_1 and a_2,b_2,c_2,d_2 are parameters introduced by perturbation in the system of first and second order, respectively. Therefore, the unperturbed vector field $\mathcal{X}_0$, the first-order perturbed vector field $\mathcal{X}_1$ and the second-order perturbed vector field $\mathcal{X}_2$ are defined as follows:

$$\begin{aligned}\mathcal{X}_0&=\frac{1}{6}\left(2\sqrt{3}+3x_1\right)(3x_3-x_2)\frac{\partial}{\partial x_1}+\frac{1}{2}(x_1-2x_3)\left(x_2+\sqrt{3}\right)\frac{\partial}{\partial x_2}\\ &\quad-\frac{1}{6}\left(3\sqrt{3}\,x_1+2\sqrt{3}x_2+12\sqrt{3}x_3+9x_1x_3+6x_2x_3\right)\frac{\partial}{\partial x_3},\\ \mathcal{X}_1&=(e_2x_2+e_3x_3-b_1x_1x_2+a_1x_1x_3)\frac{\partial}{\partial x_1}+(e_1x_1-e_3x_3+b_1x_1x_2-c_1x_2x_3)\frac{\partial}{\partial x_2}\\ &\quad+(e_2x_2-2e_3x_3-a_1x_1x_3-c_1x_2x_3)\frac{\partial}{\partial x_3},\\ \mathcal{X}_2&=(f_2x_2+f_3x_3+a_2x_1x_3-b_2x_1x_2)\frac{\partial}{\partial x_1}+(f_1x_1-f_3x_3+b_2x_1x_2-c_2x_2x_3)\frac{\partial}{\partial x_2}\\ &\quad+(f_2x_2-2f_3x_3-a_2x_1x_3-c_2x_2x_3)\frac{\partial}{\partial x_3},\end{aligned}\tag{16}$$

where

$$e_1=\frac{\sqrt{3}}{12}(2a_1+6b_1-3c_1+3d_1)\,,\ e_2=\frac{\sqrt{3}}{18}(2a_1-6b_1-3c_1-3d_1)\,,\ e_3=\frac{\sqrt{3}}{6}(2a_1-6b_1+3c_1+3d_1)\,,$$

$$f_1 = \frac{\sqrt{3}}{144}(-4a_1^2 + 24b_1a_1 - 12a_1c_1 + 12a_1d_1 - 36b_1^2 - 36b_1c_1 + 36b_1d_1 + 27c_1^2 - 18c_1d_1 - 9d_1^2 + 24a_2 + 72b_2 - 36c_2 + 36d_2),\ f_2 = \frac{\sqrt{3}}{72}(-4a_1^2 + 8b_1a_1 + 4a_1c_1 + 4a_1d_1 + 12b_1^2 - 12b_1c_1 - 12b_1d_1 + 3c_1^2 - 6c_1d_1 + 3d_1^2 + 8a_2 - 24b_2 - 12c_2 - 12d_2) \quad \text{and}$$

$$f_3 = \frac{\sqrt{3}}{72}(-4a_1^2 - 24b_1a_1 + 12a_1c_1 + 12a_1d_1 + 108b_1^2c - 36b_1c_1 - 36b_1d_1 - 9c_1^2 + 18c_1d_1 - 9d_1^2 + 24a_2 - 72b_2 + 36c_2 + 36d_2).$$

The main result regarding the bifurcated limit cycle from the center equilibrium point, using the technique described above, is the following theorem.

Theorem 1. *For system (1), when $k_1 = k_2 + k_3$, using first-order perturbation, only a single limit cycle can bifurcate from the equilibrium point at E.*

Proof. Instead of analysing system (1) at E, system (6) is examined at the origin. Using the linear transformation

$$X = PY,\ P = \begin{bmatrix} -2\sqrt{3} & -2 & -1/6 \\ 2\sqrt{3} & -3 & 1/4 \\ 0 & 1 & 5/12 \end{bmatrix}, \tag{17}$$

where $X = (x_1, x_2, x_3),\ Y = (x, y, z)$, the linear part of system (6) at the origin can be written in the real canonical form as

$$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -2\sqrt{3} \end{bmatrix},$$

and the new system is given by

$$\begin{aligned} \dot{x} &= -y - \sqrt{3}x^2 + xy + \frac{7\sqrt{3}}{13}y^2 + \frac{5\sqrt{3}}{156}yz + \frac{\sqrt{3}}{312}z^2, \\ \dot{y} &= x + \sqrt{3}\,xy + \frac{5\sqrt{3}}{12}xz + \frac{3}{13}y^2 + \frac{5}{26}yz + \frac{25}{624}z^2, \\ \dot{z} &= -2\sqrt{3}z + \frac{180}{13}y^2 + \frac{72}{13}yz - \frac{5}{52}z^2. \end{aligned} \tag{18}$$

The transformation described in Eq. (17) is applied to the first order perturbed vector field component of system (6), leading to the following results:

$$\dot{x} = -\frac{1}{13}(4e_1 + 15e_2)\,x - \frac{\sqrt{3}}{78}(8e_1 - 45e_2 + e_3)y - \frac{\sqrt{3}}{936}(8e_1 + 45e_2 + 5e_3)z + \frac{1}{13}(3a_1 + 13b_1 + 2c_1)xy + \frac{1}{156}(15a_1 - 65b_1 + 10c_1)xz + \frac{\sqrt{3}}{78}(3a_1 - 2c_1)yz - 2\sqrt{3}b_1x^2 + \frac{\sqrt{3}}{13}(a_1 + 13b_1 - c_1)y^2$$

$$
\begin{aligned}
&+\frac{\sqrt{3}}{1872}(5a_1-13b_1+5c_1)z^2,\\
\dot{y}=&\frac{\sqrt{3}}{13}(5e_1-4e_2)x+\frac{1}{13}(5e_1+6e_2-e_3)y+\frac{1}{156}(5e_1-6e_2-5e_3)z+\frac{2\sqrt{3}}{13}(3a_1+2c_1)xy\\
&+\frac{5\sqrt{3}}{78}(3a_1+2c_1)xz+\frac{1}{13}(3a_1-2c_1)yz+\frac{6}{13}(a_1-c_1)y^2+\frac{5}{312}(a_1+c_1)z^2,\\
\dot{z}=&-\frac{12\sqrt{3}}{13}(e_1-6e_2)x-\frac{1}{13}(12e_1+108e_2+60e_3)y-\frac{1}{13}(e_1-9e_2+25e_3)z+\frac{24\sqrt{3}}{13}(2a_1-3c_1)xy\\
&+\frac{10\sqrt{3}}{13}(2a_1-3c_1)xz+\frac{12}{13}(2a_1+3c_1)yz+\frac{12}{13}(4a_1+9c_1)y^2+\frac{5}{156}(4a_1-9c_1)z^2.
\end{aligned}
\tag{19}
$$

Now, the unperturbed Lyapunov function, F_0, and the first-order perturbed Lyapunov function, F_1, are defined by:

$$
\begin{aligned}
F_0&=x^2+y^2+\sum_{k=3}^{N}\sum_{i=0}^{k}\sum_{j=0}^{i}C_{k-i,i-j,j}x^{k-i}y^{i-j}z^j,\\
F_1&=\sum_{k=3}^{N}\sum_{i=0}^{k}\sum_{j=0}^{i}D_{k-i,i-j,j}x^{k-i}y^{i-j}z^j,
\end{aligned}
\tag{20}
$$

where $N\geq 3$. It is easy to show that the Lyapunov function, F_0, of Eq. (18) is satisfied by $\mathcal{X}_0F_0=0$. Using the computer algebra package MAPLE, the following linearly independent terms of Lyapunov quantities are given by Eq. (13):

(i) $L_{11}=-\frac{\sqrt{3}}{156}(14a_1-54b_1-9c_1-15d_1)$.

(ii) $L_{21}=\frac{3\sqrt{3}}{21632}(2254a_1-4534b_1-1969c_1-855d_1)$.

The origin of system (6) is weak focus of order one if and only if

$$
a_1=\frac{1}{14}(54b_1+9c_1+15d_1). \tag{21}
$$

Since the Jacobian of L_{11} and L_{21} with respect to a_1 and b_1 is non-zero, it indicates that, by suitable perturbation of the coefficients of the Lyapunov quantities, only one limit cycle can be bifurcated from the equilibrium point E of system (1) in the neighborhood of that point.

If we take $b_1=c_1=d_1=0.1$ as a numerical example, then from equation (21), we obtain $a_1=\frac{39}{70}$ and a limit cycle is observed from the first-order perturbation. From Fig. 4, we note that the blue trajectory moves inward toward the equilibrium point, while the red trajectory moves outward. This predicts that there may be a limit cycle located in a region between the two initial points, although determining the existence of the limit cycle is not an easy task.

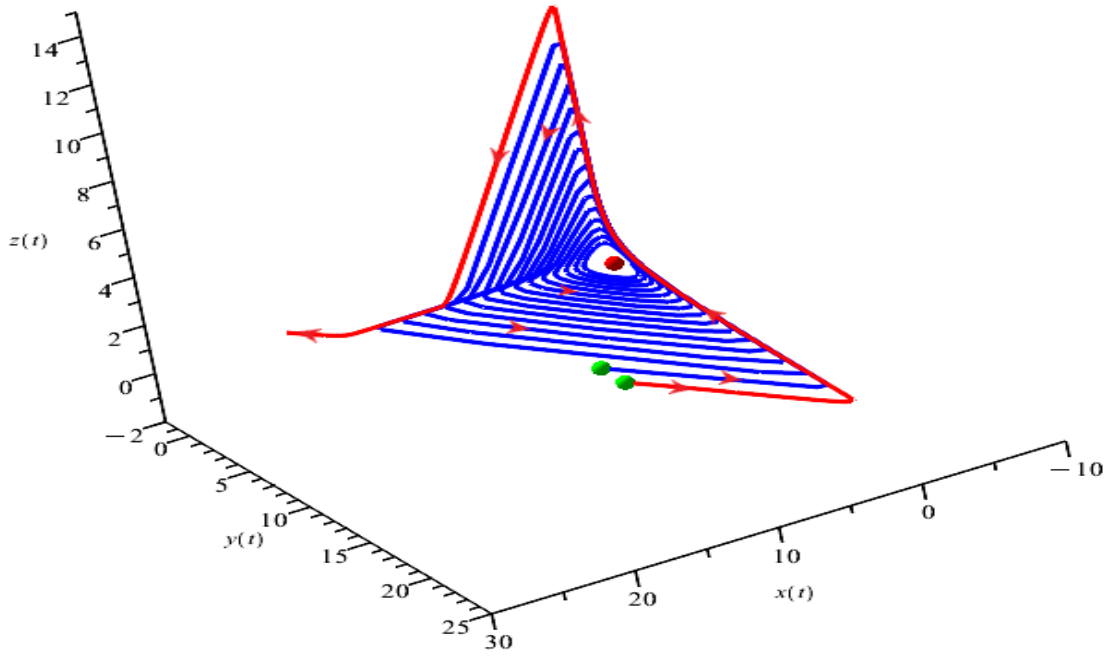

Figure 4: The phase portrait of system (1) around the positive equilibrium point is shown. The red and green balls indicate the equilibrium point and the initial points, respectively.

It is also observed that applying the second-order perturbation in Eq. (14) does not change the outcome regarding the number of perturbed limit cycles, which remains one.

Understanding the uniqueness of the limit cycle in bimolecular mass-action systems has important implications for chemical reaction dynamics and computational chemistry. This framework enhances our comprehension of chemical behavior under varying conditions, aiding in the prediction of real-world reaction outcomes. Additionally, these findings can improve computational models, enhancing the accuracy of simulations for complex chemical networks. By connecting theory with practical applications, this research fosters a deeper understanding of chemical systems and supports future advancements in the field.

5. Conclusions

In this paper, the smallest bimolecular mass-action system exhibiting a center equilibrium point is studied. It has previously been shown that when a key reaction rate parameter k_1 satisfies $k_1 = k_2 + k_3$, the positive equilibrium point was classified as a center and a vertical Andronov-Hopf bifurcation was observed. The novelty of this research lies in determining how many limit cycles can bifurcate from the center equilibrium point. Using a perturbation technique, the number of limit cycles bifurcating from the center equilibrium point is estimated and it is concluded that only one limit cycle can emerge. These findings enhance the understanding of the dynamics of bimolecular reaction networks and provide a foundation for further research on the bifurcation behavior of

complex chemical systems. The presence of the limit cycle is important because it offers valuable insights into the stability and behavior of chemical reaction networks, forming a foundation for comprehending more complex systems. Future studies could focus on higher-dimensional mass-action systems, which might display more complex bifurcation patterns. Furthermore, examining the implications of these results in practical chemical processes and integrating them into computational models could deepen our understanding and application of dynamical systems in chemistry.

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