QUALITATIVE STUDY OF A GENERALISED BRUSSELATOR TYPE EQUATION

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Abstract. In this paper we discuss a system of equations which is a generalisation of the Brusselator equations [13]. Such equations usually deal with some autocatalytic reactions. Some equations related to non-allosteric enzyme reactions which are similar to the Michaelis-Menten equations with regard to functional response term are also analysed.
Keywords: Autocatalytic reactions, Poincare compactification, enzyme reactions.

1. Introduction and Motivation

The classic tri-molecular Brusselator reaction model is known to display complex behaviour [4],[3],[6],[7]. In this paper we consider a multimolecular Brusselator type of reaction with a special emphasis on the trimolecular reaction. The generalised Brusselator type equations based on a multimolecular reaction could have a possible form

$$\frac{dx}{dt} = 1 - ax - x^p y^q, \qquad \frac{dy}{dt} = b(x^p y^q - y), \tag{1}$$

where $x, y \geq 0$, integers $p, q \geq 0$ and parameters $a \geq 0, b \geq 0$ [10]. Several authors have investigated the cases where $a = 0$ (see for example [11]).

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Usually such reactions from which the differential equation (1) is derived are enzyme reactions. As with all such reactions this reaction follows the law of mass action which states that the rate of a reaction is proportional to the product of the concentrations of the reactants. This is a nonlinear phenomenon and several people have explained the mechanism [12]. This is not surprising since enzymes are biological catalysts. The Brusselator equation as is well-known represents an autocatalytic reaction (for example Belousov-Zhabotinsky reaction, see [13]). Enzymes alter the rates of reactions in cells without being changed themselves during the course of a reaction. Our interest in this paper is with (apart from other enzyme reactions) non-allosteric enzymes [1]. Non-allosteric enzymes are a part of enzymes that are involved in the control and regulation of biological processes.

The Michaelis Menten [12] enzyme reaction has been studied by several authors. We are interested in this model as well and we propose a new model were in we introduce a functional response term of the Michaelis Menten type output into the generalised Brusselator equations. This is in Section 4.

We study the following equations in this paper

$$\frac{dx}{d\tau} = a - bx - x^p y^q, \qquad \frac{dy}{d\tau} = x^p y^q - \frac{cy}{y+1}. \tag{2}$$

In this paper we discuss, amongst several cases the case where in equations (2), $q = 1, b = 0$. Equations (2) would then become

$$\frac{dx}{d\tau} = a - x^n y, \qquad \frac{dy}{d\tau} = x^n y - \frac{cy}{y+1}. \tag{3}$$

2. The reaction diffusion system of the generalised Brusslator reaction

If the entities x and y represent chemicals then the equations (1) to (3) would be the rate of reactions corresponding to some reaction kinetics. Taking a hint from [13], the reaction diffusion equations can be written. Such equations would study the instability induced in a reaction (chemical) by diffusion [16]. Thus the corresponding equations with the inclusion of the diffusion term would be

$$\frac{\partial \tilde{x}}{\partial t} = D_1 \nabla^2 \tilde{x} + a - b\tilde{x} + \tilde{x}^p \tilde{y}^q, \quad \frac{\partial \tilde{y}}{\partial t} = D_2 \nabla^2 \tilde{y} + b(\tilde{x}^p \tilde{y}^q - \tilde{y}),$$

where $\nabla^2 \tilde{x}$ and $\nabla^2 \tilde{y}$ are the diffusion terms with D_1 and D_2 the diffusion coefficients, $a - b\tilde{x} + \tilde{x}^p \tilde{y}^q$ and $b(\tilde{x}^p \tilde{y}^q - \tilde{y})$ would be the reaction terms. We study the reaction diffusion reaction related to a Brusselator model as the Brusselator *is a perfectly acceptable model for the study of cooperative processes in chemical kinetics* (to quote Prigogine [13]). According to Prigogine the Brusselator model plays a somewhat similar role as the harmonic oscillator or the Heisenberg model in ferromanetism which are studied to illustrate the basic laws of classical

and quantum mechanics. Prigogine stresses on the importance of trimolecular steps (shown by the x^2y and y^2x terms in the equations) because such cubic nonlinearities give rise to 'cooperative' behaviour.

3. Analysis of the generalised Brusselator reaction

Let us consider the system of equations (2).

Choose $b = 0$ and use cy in place of $\dfrac{cy}{y+1}$ (for the sake of some insight into a simpler system).

$$\frac{dx}{dt} = a - x^p y^q, \qquad \frac{dy}{dt} = x^p y^q - cy. \tag{4}$$

This is a planar polynomial system. Solving these two equations for the equilibrium points, (by equating the derivatives on the left hand sides to zero), one of the equilibrium points is $x = a^{1/p}(\frac{c}{a})^{q/p},\ y = \frac{a}{c}$.

Linearising the system about this equilibrium point would give the Jacobian matrix J as

$$J = \begin{bmatrix} \dfrac{1-q}{p}\, a^{\frac{1-q}{p}} c^{\frac{q}{p}} (\frac{a}{c})^{-1+p} (\frac{a}{c})^q & -qa^{1-q}c^q(\frac{a}{c})^{-1+q} \\ p(a^{\frac{1-q}{p}} c^{\frac{q}{p}})^{-1+p}(\frac{a}{c})^q & -c + qa^{1-q}c^q(\frac{a}{c})^{-1+q} \end{bmatrix}.$$

Its eigenvalues are

$$\lambda_{41} = \frac{1}{2}[-c - a^{\frac{-1+q}{p}}(\frac{a}{c})^q c^{\frac{-q}{p}} a^{1-q}c^q p + (\frac{a}{c})^{-1+q} a^{1-q}c^q q] - \frac{1}{2}a^{\frac{-1-p}{p}} c^{\frac{-q}{p}} \times$$
$$\sqrt{-4a^{\frac{1+2p+q}{p}}(\frac{a}{c})^q c^{\frac{p+q}{p}} a^{1-q}c^q p + [a^{1+\frac{1}{p}} c^{\frac{p+q}{p}} + a^{\frac{p+q}{p}}(\frac{a}{c})^q a^{1-q}c^q p - a^{\frac{1}{p}}(\frac{a}{c})^q c^{\frac{p+q}{p}} a^{1-q}c^q q]^2}$$

and

$$\lambda_{42} = \frac{1}{2}[-c - a^{\frac{-1+q}{p}}(\frac{a}{c})^q c^{\frac{-q}{p}} a^{1-q}c^q p + (\frac{a}{c})^{-1+q} a^{1-q}c^q q] + \frac{1}{2}a^{\frac{-1-p}{p}} c^{\frac{-q}{p}} \times$$
$$\sqrt{-4a^{\frac{1+2p+q}{p}}(\frac{a}{c})^q c^{\frac{p+q}{p}} a^{1-q}c^q p + [a^{1+\frac{1}{p}} c^{\frac{p+q}{p}} + a^{\frac{p+q}{p}}(\frac{a}{c})^q a^{1-q}c^q p - a^{\frac{1}{p}}(\frac{a}{c})^q c^{\frac{p+q}{p}} a^{1-q}c^q q]^2}.$$

To study the special trimolecular case referred to earlier, let us choose $p+q = 3$ with $p = 2$ and $q = 1$. The system is

$$\frac{dx}{dt} = a - x^2 y, \qquad \frac{dy}{dt} = x^2 y - cy. \tag{5}$$

Its equilibrium points are $(-\sqrt{c}, \frac{a}{c})$ and $(\sqrt{c}, \frac{a}{c})$.

The eigenvalues at $(-\sqrt{c}, \frac{a}{c})$ are

$$\lambda_{51} = \frac{a}{\sqrt{c}} - \frac{\sqrt{a^2 + 2ac^{3/2}}}{\sqrt{c}}, \qquad \lambda_{52} = \frac{a}{\sqrt{c}} + \frac{\sqrt{a^2 + 2ac^{3/2}}}{\sqrt{c}}.$$

The eigenvalues at $(\sqrt{c}, \frac{a}{c})$ are

$$\lambda_{53} = \frac{-a}{\sqrt{c}} - \frac{\sqrt{a^2 - 2ac^{3/2}}}{\sqrt{c}}, \qquad \lambda_{54} = \frac{-a}{\sqrt{c}} + \frac{\sqrt{a^2 - 2ac^{3/2}}}{\sqrt{c}}.$$

- Observing λ_{51} and λ_{52} it is apparent that they will not take on complex values for $c > 0$, $a > 0$ and hence the equilibrium point $(-\sqrt{c}, \frac{a}{c})$ is either a node or a saddle point (depending on the sign of the eigenvalues).

- λ_{53} and λ_{54} can take on complex values for $a^2 - 2ac^{3/2} < 0$ or $a < 2c^{3/2}$. In this case, since the real part of λ_{53} and λ_{54} is negative one would expect a spiral sink for the equilibrium point $(\sqrt{c}, \frac{a}{c})$.

This case is illustrated in Figure 1.

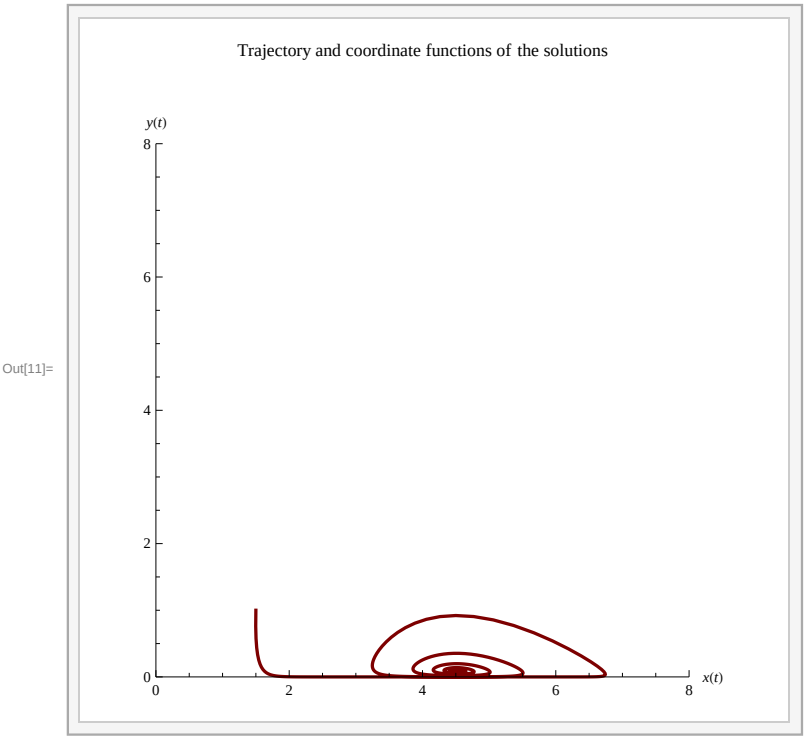

Figure 1: A spiral sink for the system (5) for some particular values $a = 1.8$, $c = 20.345$, $p = 2$, $q = 1$

In Figure 1 a spiral sink for the system (5) is shown for some particular values of a, b, c.

A simulation of equation (2)

We now consider a simulation of equation (2) by replacing the term cy by $\dfrac{cy}{y+1}$. It can be seen that a limit cycle appears for some values of parameters.

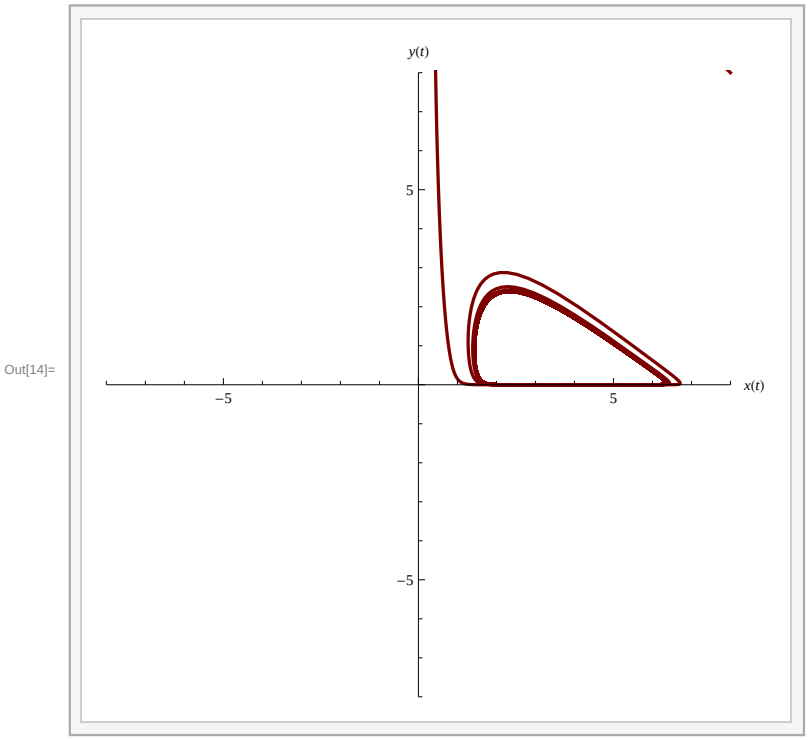

Figure 2: A Limit Cycle for the system (2) for some particular values $a = 1.8$, $b = 0$, $c = 4.8$, $p = 2$, $q = 1$

4. A generalised Brusselator type equation with a Michaelis-Menten functional response term

C.S.Holling studied the factors involved in the utilization of resources by predators. He described the changes in the feeding rate of organisms as "the functional response term". He showed that there were three categories of functional response [15].

- Type 1. Refers to animals which consume food proportional to the rate of their encounter with food items.
- Type 2. Where the organisms take some time to eat and to capture their prey.

- Type 3. In this category the organism will not consume the prey if it is below a certain threshold density.

There is a remarkable parallel between enzyme reactions and the predator-prey Holling functional response [2]. The Michaelis-Menten enzyme reaction follows a type 2 functional response. Keeping this type of functional response in mind we propose the following model and analyse it.

$$\frac{dx}{dt} = a - bx - x^p y^q, \qquad \frac{dy}{dt} = x^p y^q - \frac{cxy}{y+1}. \tag{6}$$

For the purpose of understanding and analysis, we take $b = 0$, $p = 2$, $q = 1$. Equations (6) reduce to

$$\frac{dx}{dt} = a - x^2 y, \qquad \frac{dy}{dt} = x^2 y - \frac{cxy}{y+1}. \tag{7}$$

The equilibrium points of equation (7) are

$$(\frac{1}{2}[c - \sqrt{-4a + c^2}], \frac{-2a + c^2 + c\sqrt{-4a + c^2}}{2a})$$

and

$$(\frac{1}{2}[c + \sqrt{-4a + c^2}], \frac{-2a + c^2 - c\sqrt{-4a + c^2}}{2a}).$$

Let (x_0, y_0) be an equilibrium point chosen from amongst the two equilibrium points of equation (7) so that $x_0 > 0$, $y_0 > 0$. This is possible if $c^2 > 4a$. Linearising the system (7) about its equilibrium point, the Jacobean matrix is

$$M = \begin{bmatrix} -2x_0y_0 & -x_0^2 \\ 2x_0y_0 - \dfrac{cy_0}{1+y_0} & x_0^2 + \dfrac{cx_0y_0}{(1+y_0)^2} - \dfrac{cx_0}{1+y_0} \end{bmatrix},$$

where the elements in the linearised matrix are to be treated as the functions of the parameter c. The characteristic equation of this matrix has the form $\lambda^2 - s\lambda + D = 0$ where

$$s(c) = \text{the trace of } M = -2x_0y_0 + x_0^2 + \frac{cx_0y_0}{(1+y_0)^2} - \frac{cx_0}{1+y_0}$$

and $D = \text{determinant of } M = -\frac{2cx_0^2y_0^2}{(1+y_0)^2} + \frac{cx_0^2y_0}{1+y_0}$. Let the two eigenvalues of this matrix be λ_1 and λ_2. These can be represented as a function of c.

$$\lambda_1, \lambda_2 = \frac{1}{2}[s(c) \pm \sqrt{s^2(c) - 4D(c)}].$$

We will now show that a Hopf bifurcation can occur in this equation for some values of the parameter c. A Hopf bifurcation condition would require that ([9], see page 91) the real part (Re) of the eigenvalues is equal to zero and

the imaginary part (Im) is nonzero $\Re\mathrm{e} = \theta(c) = \frac{1}{2}s(c)$ and $\Im\mathrm{m} = \nu(c) = \frac{1}{2}\sqrt{s^2(c) - 4D(c)}$ (see [8]). Solving for the parameter c after setting the trace to zero

$$(1) \qquad x_0^2 - 2x_0y_0 + \frac{cx_0y_0}{(1+y_0)^2} - \frac{cx_0}{1+y_0} = 0 \Rightarrow c = (x_0 - 2y_0)(1+y_0)^2$$

$$(2) \qquad \frac{d}{dc}(\text{Trace}) = \frac{x_0y_0}{(1+y_0)^2} - \frac{x_0}{1+y_0} \neq 0.$$

(1) is the non-hyperbolicity condition and (2) is the transversality condition. Thus showing the existence of a Hopf bifurcation for the parameter c. A simulation of the limit cycle is shown in Figure 3.

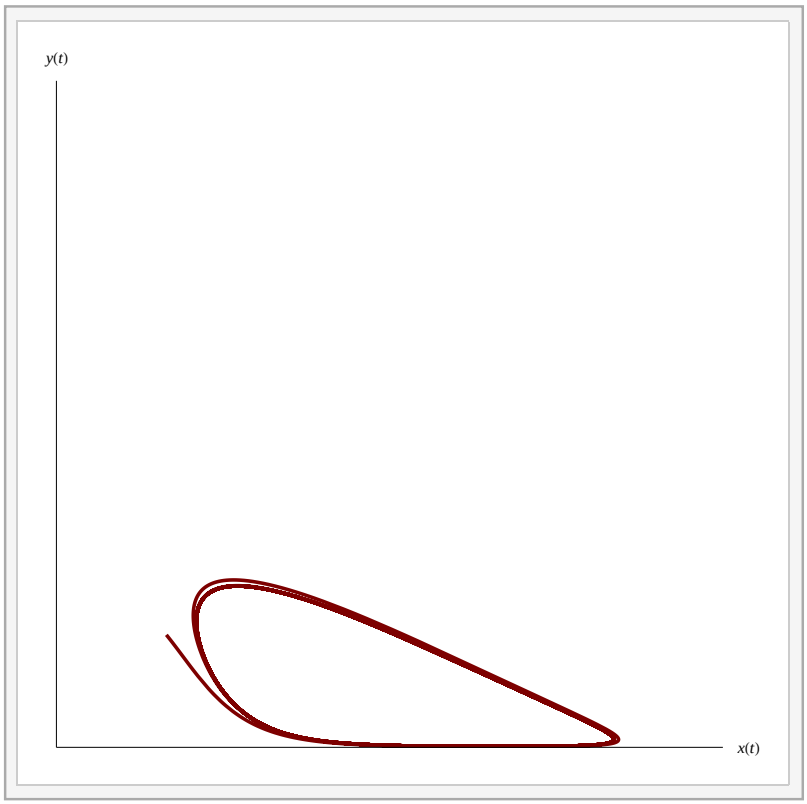

Figure 3: A limit cycle for the values of the parameter $a = 1.8$, $c = 1$, $p = 2$, $q = 1$

The generalised Brusselator equation (1) is a planar polynomial system. Usually in such systems one needs to study not just its finite equilibria but also the equilibria at infinity. When related to a chemical reaction this would mean that one studies the tendency of the concentrations of the chemicals over a large range. So for this it is appropriate to use a Poincaré Compactification.

5. A Brief Outline of Poincaré Compactification

In order to study the behaviour of the trajectories of a planar differential system near infinity we use a compactification. A good approach for studying the behaviour of trajectories near infinity is to use the Poincaré sphere, introduced by Poincaré [14]. It has the advantage that the singular points at infinity are spread out along the equator of the sphere. In order to draw the phase portrait of a vector field, we would have to work over the complete real plane $\mathbb{R}^2$, which is not very practical. If the functions defining the vector field are polynomials, we can apply Poincaré compactification, which will tell us how to draw it in a finite region. It controls the orbits which tend to or come from infinity. Here we use (x_1, x_2) as coordinates instead of (x, y) (in order to differentiate).

Let $X = P\partial/\partial x_1 + Q\partial/\partial x_2$ be a polynomial vector field (the functions P and Q are polynomials of arbitrary degree in the variables x_1 and x_2), or in other words:

$$\begin{aligned} \dot{x_1} &= P(x_1, x_2) \\ \dot{x_2} &= Q(x_1, x_2). \end{aligned}$$

The degree of X is represented as d where d is the maximum of the degrees of P and Q. Poincaré compactification works as follows: First we consider $\mathbb{R}^2$ as the plane in $\mathbb{R}^3$ defined by $(y_1, y_2, y_3) = (x_1, x_2, 1)$. We consider the sphere $\mathbb{S}^2 = \{y \in \mathbb{R}^3 : y_1^2 + y_2^2 + y_3^2 = 1\}$ which we will call here Poincaré sphere; it is tangent to $\mathbb{R}^2$ at the point $(0, 0, 1)$. We may divide this sphere into $H_+ = \{y \in \mathbb{S}^2 : y_3 > 0\}$ (the northern hemisphere), $H_- = \{y \in \mathbb{S}^2 : y_3 < 0\}$ (the southern hemisphere) and $\mathbb{S}^1 = \{y \in \mathbb{S}^2 : y_3 = 0\}$ (the equator). Now we consider the projection of the vector field X from $\mathbb{R}^2$ to $\mathbb{S}^2$ given by the central projections $f^+ : \mathbb{R}^2 \to \mathbb{S}^2$ and $f^- : \mathbb{R}^2 \to \mathbb{S}^2$. More precisely, $f^+(x)$ (respectively $f^-(x)$) is the intersection of the straight line passing through the point y and the origin with the northern (respectively, southern) hemisphere of $\mathbb{S}^2$.

$$f^+(x) = \left(\frac{x_1}{\triangle(x)}, \frac{x_2}{\triangle(x)}, \frac{1}{\triangle(x)}\right),$$

$$f^-(x) = \left(\frac{-x_1}{\triangle(x)}, \frac{-x_2}{\triangle(x)}, \frac{-1}{\triangle(x)}\right),$$

where

$$\triangle(x) = \sqrt{(x_1)^2 + (x_2)^2 + 1}.$$

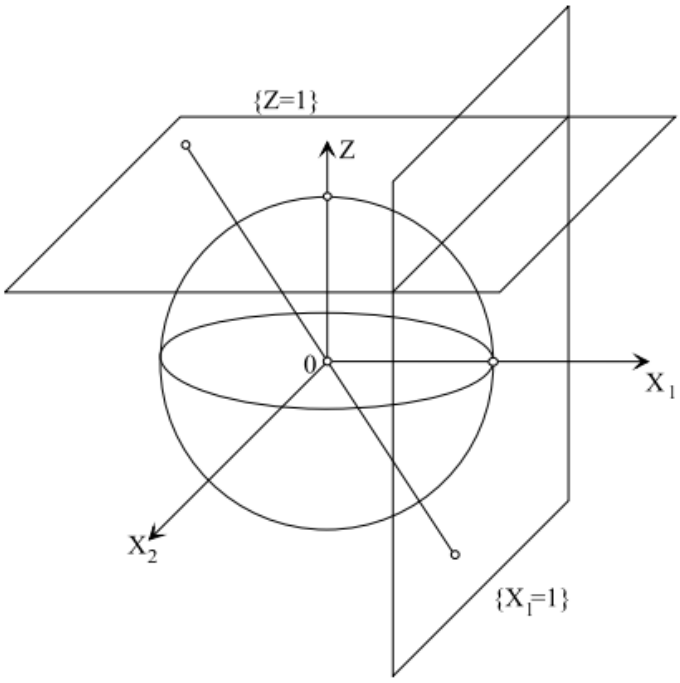

Figure 4: Poincaré Sphere

In this way we obtain induced vector fields in each hemisphere. (For more details see page 150 of [5]).

We now consider a Poincaré compactification of equation (2).
Let

$$\hat{P}(x,y) = a - bx - x^p y^q,$$
$$\hat{Q}(x,y) = x^p y^q - \frac{cy}{y+1}.$$

For the local chart U_1 (see [5]), x is transformed to $\frac{1}{v}$ and y is transformed to $\frac{u}{v}$.

$$\hat{P}(\frac{1}{v},\frac{u}{v}) = a - \frac{b}{v} - \frac{u^q}{v^{p+q}},$$
$$\hat{Q}(\frac{1}{v},\frac{u}{v}) = \frac{u^q}{v^{p+q}} - \frac{cu}{u+v}.$$

The extended vector on $\mathbb{S}^2$ which is called the Poincaré compactification of the vector field X on $\mathbb{R}^2$ is denoted by $p(X)$. The expression for $p(X)$ in the local chart (U_1, ϕ_1) is given by

$$\begin{aligned} \dot{u} &= v^d[-u\hat{P}(\frac{1}{v},\frac{u}{v}) + \hat{Q}(\frac{1}{v},\frac{u}{v})], \\ \dot{v} &= -v^{d+1}\hat{P}(\frac{1}{v},\frac{u}{v}). \end{aligned}$$

where d=(maximum of the degrees of $\hat{P}$ and $\hat{Q}$)=$p+q$. Therefore,

$$\begin{aligned}\dot{u} &= v^{p+q}[-au + \frac{bu}{v} + \frac{u^{q+1}+u^q}{v^{p+q}} - \frac{cu}{u+v}]\\ \dot{v} &= -v^{p+q+1}[a - \frac{b}{v} - \frac{u^q}{v^{p+q}}].\end{aligned}$$

For the local chart U_2, x is transformed to $\frac{u}{v}$ and y is transformed to $\frac{1}{v}$. The expression for chart (U_2, ϕ_2) is given by

$$\begin{aligned}\dot{u} &= v^d[\hat{P}(\frac{u}{v}, \frac{1}{v}) - u\hat{Q}(\frac{u}{v}, \frac{1}{v})],\\ \dot{v} &= -v^{d+1}\hat{Q}(\frac{u}{v}, \frac{1}{v}).\end{aligned}$$

Therefore

$$\begin{aligned}\dot{u} &= v^{p+q}[a - \frac{bu}{v} - \frac{u^{p+1}+u^p}{v^{p+q}} - \frac{c}{v+1}],\\ \dot{v} &= -v^{p+q+1}[\frac{u^p}{v^{p+q}} - \frac{c}{v+1}].\end{aligned}$$

In order to illustrate this compactification process, using these equations we evaluate the local charts U_1 and U_2. We choose some specific values for the various parameters in equation (2) as $a = 1, b = 0, c = 1, p = 2, q = 1$. The system is

$$\begin{aligned}\frac{dx}{dt} &= (1 - x^2y)(y+1),\\ \frac{dy}{dt} &= x^2y(y+1) - y.\end{aligned}$$

The expression for the local chart U_1 is

$$\begin{aligned}\dot{u} &= u(u+v)(1+u-v^3) - uv^3,\\ \dot{v} &= v(u+v)(u-v^3).\end{aligned}$$

For the local chart U_2

$$\begin{aligned}\dot{u} &= (1+v)(v^3 - u^2 - u^3) + uv^3,\\ \dot{v} &= v^4 - vu^2(1+v).\end{aligned}$$

In figure 5 there are many equilibrium points visible on the Poincaré sphere. One of them is an unstable node as can be seen from the trajectories moving away from the equilibrium point and a stable node where the trajectories move towards the equilibrium point. For the system

$$\begin{aligned}\frac{dx}{dt} &= (0.35 - x^2y)(y+1),\\ \frac{dy}{dt} &= x^2y(y+1) - 5y.\end{aligned}$$

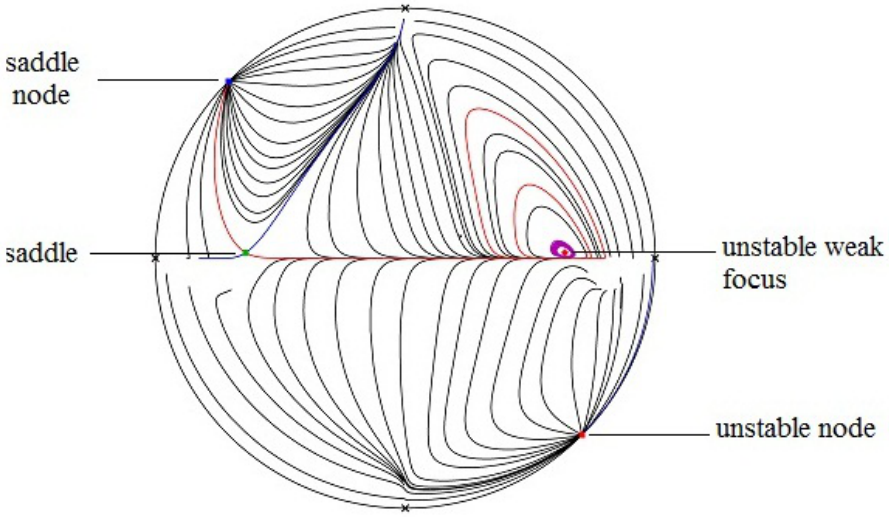

Figure 5: Phase portrait on the Poincaré sphere

The expression for the local chart U_1 is $\dot{u} = u(u+v)(1+u-0.35v^3) - 5uv^3$, $\dot{v} = v(u+v)(u-0.35v^3)$.

For the local chart U_2, is $\dot{u} = (1+v)(0.35v^3 - u^2 - u^3) + 5uv^3$, $\dot{v} = 5v^4 - vu^2(1+v)$.

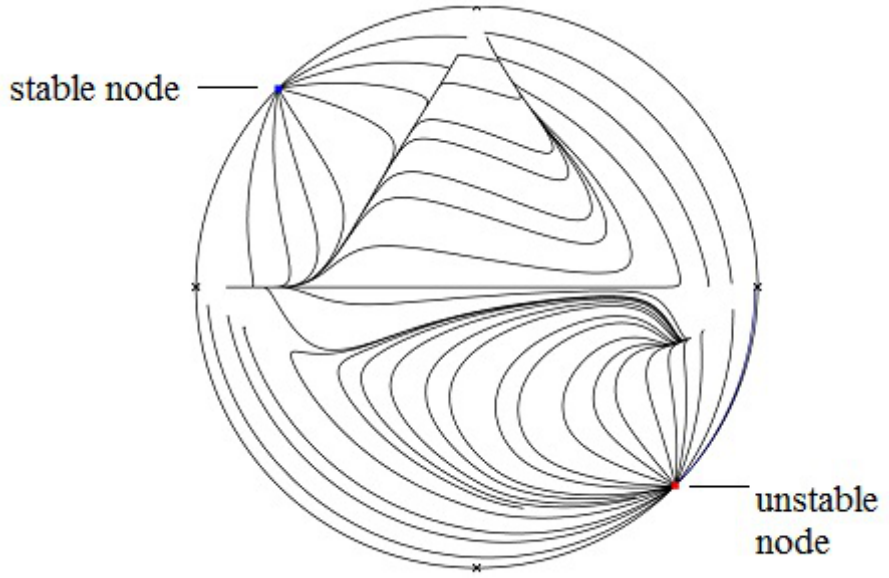

Figure 6: Phase portrait on the Poincaré sphere

With the change of the values of the parameters, the phase portrait on the Poincaré sphere has in addition to the stable and unstable nodes, a saddle point and a focus as can be seen from the figure 6.

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