A note on the existence of heteroclinic connecting orbits in the Belousov–Zhabotinskii system

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We prove for a concrete system the occurence of heteroclinic orbits via the Conley index. Because this system is bistable, we have two different connecting orbits. If we include the parameter dependence of the reaction term, there exists two families of connecting orbits. At the ends of the parameter interval, where bistability occurs, we have bifurcation points.

1. Introduction

In this note we describe the occurrence of heteroclinic orbits in a bistable system. A heteroclinic orbit is a solution ψ of the system

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(u), \quad u \in \mathbf{R}^m, \quad t \in \mathbf{R},$$
(1)

which connects two different steady states:

$$\lim_{t \to -\infty} \psi(t) = u^{(1)},$$
$$\lim_{t \to \infty} \psi(t) = u^{(2)},$$

where $f(u^{(1)}) = f(u^{(2)}) = 0$, $u^{(1)} \neq u^{(2)}$. Such heteroclinic orbits may be the reason for the existence of waves in the corresponding reaction-diffusion system. Using topological methods, especially the Conley index, for some types of reaction systems it was proved that there exist travelling waves if one has connecting orbits for the reaction system. This was done for gradient systems by Mischaikow [10] and

¹ Present address: Fachhochschule Lippe, Fachbereich Elektrotechnik, Liebigstraße 87, D-32657 Lemgo, Germany. Reineck [11], and for Lotka–Volterra-Systems by Gardner [3]. The system we consider has this property, too. This will be outlined in another paper [5]. Our system describes a real chemical reaction, the so-called Belousov–Zhabotinskii reaction (BZR). For the investigation of spatial structures and travelling waves the preferred reaction mixture contains malonic acid, bromate, and ferroin in diluted sulfuric acid. In this system a sharp color change from red (Fe(phen)₃²⁺) to blue (Fe(phen)₃³⁺) occurs. Therefore, it is easy to detect the chemical structure visually. Kuhnert et al. found waves in this system, and determined their velocities in dependence of some parameters, see [6,8].

We shall include a parameter, too. This parameter φ controls the autocatalytic oxidation of the catalyst Fe(phen)₃²⁺ when the BZ system is photosensitive [7]. If not, φ corresponds to the inhibitor release by oxygen diffusing from the air into the liquid layer, see [9]. The parameter dependence yields the existence of a family of connecting orbits. Because we have two stable restpoints and one unstable restpoint if $\varphi \in (\varphi_{\min}, \varphi_{\max})$, there are exactly two families. For $\varphi = \varphi_{\min}$ or $\varphi = \varphi_{\max}$, we have bifurcation points. We shall mainly use topological methods. For basic knowledge we refer the reader to the books of Conley [2] and Smoller [12].

We shall prove the existence of heteroclinic orbits for a concrete system. Nevertheless this result may be applied for some other similar systems, which have both an unstable restpoint $u^{(1)}$ and a stable restpoint $u^{(2)}$, but no periodic orbit.

2. Results

Let us consider here the following model of the BZR [4,6,7]:

$$\frac{\partial u_1}{\partial t} = d_1 \frac{\partial^2 u_1}{\partial x^2} + u_1 (1 - u_1 - u_2) + q u_2, \qquad (2)$$

$$\frac{\partial u_2}{\partial t} = d_2 \frac{\partial^2 u_2}{\partial x^2} - b u_1 u_2 - m u_2 + \varphi \,. \tag{3}$$

This model involves bistability for some parameter values q, b, m, φ . In what follows we assume that $b, m, \varphi > 0$, and

$$0 < q < 1. \tag{4}$$

Let us briefly summarize the results of [4] concerning the reaction scheme

$$\frac{\mathrm{d}u_1}{\mathrm{d}t} = u_1(1 - u_1 - u_2) + qu_2, \qquad (5)$$

$$\frac{\mathrm{d}u_2}{\mathrm{d}t} = -bu_1u_2 - mu_2 + \varphi \,. \tag{6}$$

Stationary solutions of (5) and (6) are completely described by

$$bu_1^3 + (m-b)u_1^2 + (\varphi - m)u_1 - q\varphi = 0$$
,

$$u_2=\frac{\varphi}{bu_1+m}.$$

Figure 1 shows the stability diagram. Zero eigenvalues occur at the turning points only.

We are interested in positive solutions u_1, u_2 only, hence they represent concentrations of the chemical substances. Let us denote the stable branches by $u^{(1)}, u^{(3)}$, and the unstable ones by $u^{(2)}$. Let $u_1^{(3)} > u_1^{(2)} > u_1^{(1)}$. Define

$$\mathcal{D} := \{(u_1, u_2) \in \mathbf{R}^2 : q < u_1 < 1, 0 < u_2 < \varphi m^{-1}\}.$$

Then the following two theorems hold:

THEOREM 1. [4]

Assume (4) and $u_0 \in \mathcal{D}$. Then the solution u(t) of (5) and (6) with $u(0) = u_0$ exists for all t > 0 and is bounded $(\forall t \ge 0)$, and $u(t) \in \mathcal{D} \ \forall t \ge 0$.

Moreover, by means of the Dulac criterion it was shown that there do not exist any periodic solutions u(t).

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THEOREM 2. [4]
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Closed trajectories do not exist in \mathcal{D} .

Our main result will be the following.



Fig. 1. Bistability diagram for u_1 in dependence on φ for fixed values m = 0.008, b = 8.0, q = 0.001. The upper branch (full line) corresponds to $u_1^{(1)}$, the middle branch (broken line) to $u_1^{(2)}$, and the lower branch (full line) to $u_1^{(3)}$.

THEOREM 3

For each $\varphi \in (\varphi_{\min}, \varphi_{\max})$ there exist exactly two heteroclinic orbits $\psi^{(1)}$ and $\psi^{(2)}$ of (5) and (6) included in \mathcal{D} . Moreover, we have

$$\begin{split} \psi^{(1)}(t) &\to u^{(1)}, \quad t \to +\infty, \\ \psi^{(2)}(t) &\to u^{(3)}, \quad t \to +\infty, \\ \psi^{(i)}(t) &\to u^{(2)}, \quad t \to -\infty, \quad i = 1, 2, \end{split}$$

Now, we shall consider the parameter values $\varphi = \varphi_{\min}$ and $\varphi = \varphi_{\max}$. At these points exist heteroclinic orbits, too.

THEOREM 4

For $\varphi = \varphi_{\min}$ or $\varphi = \varphi_{\max}$ there exists a heteroclinic orbit $\psi^{(1)}$ or $\psi^{(2)}$, respectively, of (5) and (6) included in \mathcal{D} . Moreover, we have

$$\begin{split} \psi^{(1)}(t) &\to u^{(1)}, \quad t \to +\infty, \quad \varphi = \varphi_{\min}, \\ \psi^{(2)}(t) &\to u^{(3)}, \quad t \to +\infty, \quad \varphi = \varphi_{\max}, \\ \psi^{(i)}(t) &\to u^{(2)}, \quad t \to -\infty, \quad i = 1, 2, \quad \varphi = \varphi_{\min}, \varphi_{\max}. \end{split}$$

Before we state our last theorem about bifurcation let us define a bifurcation point of heteroclinic orbits. Let $f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ be a continuous map. Consider a parametrized family of differential equations

$$\dot{\boldsymbol{u}} = f(\boldsymbol{u}, \boldsymbol{\varphi}) \tag{7}$$

and choose a point $(u_0, \varphi_0) \in \mathbb{R}^n \times \mathbb{R}$ such that $f(u_0, \varphi_0) = 0$. This point (u_0, φ_0) is said to be a bifurcation point of heteroclinic orbits of (7) if for any open neighborhood \mathcal{U} of $(u_0, \varphi_0) \in \mathbb{R}^n \times \mathbb{R}$ there exists a heteroclinic orbit of (7) included in \mathcal{U} .

THEOREM 5

The points $(u^{(1)}, (\varphi_{\min}), \varphi_{\min})$ and $(u^{(3)}(\varphi_{\max}), \varphi_{\max})$ are bifurcation points of (5) and (6).

Compare fig. 2.

3. Proofs

First, we given the proof of theorem 3.

Proof of theorem 3

Fix $\varphi \in (\varphi_{\min}, \varphi_{\max})$. Theorems 1 and 2 imply that \mathcal{D} is an isolating block of

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Fig. 2. The flow in the phase space for $\varphi \in (\varphi_{\min}, \varphi_{\max}), \varphi = \varphi_{\min}, \varphi < \varphi_{\min}$, respectively.

some invariant set $K \subset \text{ int } \mathcal{D}$ in the sense of Conley. The Conley index of K is given by $I_{\mathbb{C}}(K) = [S^0, *]$.

Since there are no homoclinic or periodic orbits in \mathcal{D} , each stationary solution of (5), (6) is an isolated invariant set. Moreover, each stationary stable solution of (5), (6) is the limit set of the flow of the system (5), (6) considered in some of its neighborhoods, and thus it is there an attractor. Consequently, $I_C(u^{(1)}) = I_C(u^{(3)})$ $= [S^0, *]$. On the other hand, there is no trajectory leaving \mathcal{D} . Thus, the Browder topological degree of F on \mathcal{D} is equal to 1. Topological degrees of F computed on sufficiently small neighborhoods of stable stationary solutions are also equal to 1. Thus, for a sufficiently small neighborhood of the unstable stationary solution this degree must be equal to -1. Since the linearization of the vector field F at $u^{(2)}$ is an isomorphism, it has to have two real eigenvalues of opposite signs. By the Conley theory, $I_C(u^{(2)}) = [S^1, *]$.

Now, let us consider two rectangles $G' = [0, u_1^{(3)}] \times [0, \varphi/m] \subset \mathbb{R}^2_+$ and $G'' = [u_1^{(1)}, 1] \times [0, \varphi/m] \subset \mathbb{R}^2_+$. It is easy to check that both rectangles are isolating blocks of some invariant sets K', K'' including $\{u^{(1)}, u^{(2)}\}$ and $\{u^{(2)}, u^{(3)}\}$, respectively. Computing the Conley indices of K' and K'' we obtain $I_{\mathbb{C}}(K') = I_{\mathbb{C}}(K'')$

= [*,*]. From the "sum property" of the Conley index we get the following equations:

$$I_{\mathcal{C}}(\{u^{(1)}\} \cup \{u^{(2)}\}) = I_{\mathcal{C}}(\{u^{(1)}\}) + I_{\mathcal{C}}(\{u^{(2)}\}) = [S^0, *] + [S^1, *] = [S^0 \vee S^1, *],$$

and similarly

$$I_{\mathbf{C}}(\{u^{(2)}\} \cup \{u^{(3)}\}) = [S^0 \vee S^1, *].$$

Since $I_{\mathbb{C}}(K') = [*, *] \neq [S^0 \vee S^1, *] = I_{\mathbb{C}}(\{u^{(1)}\} \cup \{u^{(2)}\})$ we obtain by the "sum theorem" the existence of a nonstationary bounded solution of (5), (6), denoted by $\psi^{(1)}$ and lying in the interior of G'.

Analogously for G'' we conclude that there exists at least on nonstationary bounded solution of (5), (6), say $\psi^{(2)}$, included in the interior of G''.

Obviously, the limit set of $\psi^{(1)}$ (resp. $\psi^{(2)}$) consists of exactly two points $\{u^{(1)}\}, \{u^{(2)}\}$ (resp. $\{u^{(2)}\}, \{u^{(3)}\}$), and $\lim \psi^{(1)}(t) = u^{(1)}, \lim \psi^{(2)}(t) = u^{(3)}$ as $t \to \infty$. Now, let us consider the linearization of F at $u^{(2)}$, which has exactly two trajectories running away from $u^{(2)}$, when t goes to infinity. Since the flows of the vector field F and its linearization at $u^{(2)}$ are locally homeomorphic we obtain the uniqueness of $\psi^{(1)}$ and $\psi^{(2)}$.

Now, we shall give the proofs of the theorems 4 and 5.

Proof of theorem 4

If $\varphi = \varphi_{\min}$ there are exactly two stationary solutions $u^{(1)} \equiv u^{(2)}$ and $u^{(3)}$, of (5), (6) in \mathcal{D} . Since there are no closed trajectories in \mathcal{D} each stationary solution is an isolated set.

It is well known (see [2]) that every stationary solution in the plane, which attracts locally all other solutions, has the Conley index equal to $[S^0, *]$. The continuation of the stationary solution $u^{(1)}$ for $\varphi < \varphi_{\min}$ does not exist, and therefore $I_{\rm C}(u^{(1)}) = [*, *]$. Consequently, $u^{(1)}$ does not attract locally all other solutions, which implies the existence of at least one trajectory running away from $u^{(1)} \equiv u^{(2)}$ and tending to $u^{(3)}$.

The proof for $\varphi = \varphi_{\max}$ is the same.

Proof of theorem 5

Let us consider the point $(u^{(1)}(\varphi_{\min}, \varphi_{\min}))$. By the same arguments as above, $\{u^{(1)}\}$ is an isolated invariant set in the sense of Conley. In fact, every sufficiently small disc centered at $u^{(1)}$ is an isolating neighborhood for $u^{(1)}$. The fundamental result in the Conley theory states that for every isolating neighborhood \mathcal{U} of an invariant set \mathcal{S} there exists an isolating block \mathcal{B} such that $\mathcal{S} \subseteq \mathcal{B} \subseteq \mathcal{U}$, compare [1]. Let (\mathcal{D}_k) be a descending sequence of discs in \mathbb{R}^2 centered at $u^{(1)}$ such that $\bigcap \mathcal{D}_k = \{u^{(1)}\}$. Now, for each $k \in \mathbb{N}$ there exists an isolating block $\mathcal{B}_k \subseteq \mathcal{D}_k$ for $u^{(1)}$. By the continuation property of the Conley index we have $I_{\mathbb{C}}(u^{(1)}) = [*,*]$.

In order to prove the assertion, it is enough to show that for every open neighborhood \mathcal{U} of $(u^{(1)}, \varphi_{\min}) \in \mathbb{R}^3$ there exists a heteroclinic orbit of (5), (6) in \mathcal{D} .

Fix an open neighborhood \mathcal{U} of $(u^{(1)}, \varphi_{\min}) \in \mathbb{R}^3$. Then $\mathcal{B}_k \subset \mathcal{U}$ if $k \in \mathbb{N}$ is sufficiently large. Since \mathcal{B}_k is compact, we obtain $\mathcal{B}_k \times (\varphi_{\min} - \epsilon, \varphi_{\min} + \epsilon) \subset \mathcal{U}$ if $\epsilon > 0$ is small enough. Let $\varphi \in (\varphi_{\min}, \varphi_{\min} + \epsilon)$. Then $\mathcal{B}_k \times \{\varphi\}$ is an isolating block for some invariant set containing $u^{(1)}$ and $u^{(2)}$. Since

$$egin{aligned} &I_{\mathrm{C}}(\mathcal{B}_k imes \{arphi\}) = [*,*]\,, \ &I_{\mathrm{C}}igg(u^{(1)} imes \{arphi\}igg) = [S^0,*]\,, \ &I_{\mathrm{C}}igg(u^{(2)} imes \{arphi\}igg) = [S^1,*]\,, \end{aligned}$$

we obtain from the "sum theorem" the existence of a heteroclinic orbit in $\mathcal{B}_k \times \{\varphi\} \subset \mathcal{U}$.

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