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ORGANIZING CENTERS FOR DISCRETE REACTION DIFFUSION MODELS

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1. INRRODUCTION

This paper supplements the two papers [1,2] in this book. Our references are included in the list of references of [1,2]. We will refer to the j-th reference in [1], [2] by $[j]_1$, $[j]_2$, respectively.

Let us consider an assemblage of finitely many chemical cells as described in the introduction of [2]. More generally, we allow for more than just two cells to be connected to the outside reservoir via membranes. If h_j is the width of the j-th cell, if E_j is the diffusion constant between the j-th cell and the outside reservoir and if D_j is the diffusion coefficient between the (j-1)-th cell and the j-th cell, then the corresponding system reads

(1a) $$(E_1+D_2)x_1-D_2x_2 = h_1f(x_1,\lambda),$$

(1b) $$-D_jx_{j-1}+(E_j+D_j+D_{j+1})x_j-D_{j+1}x_{j+1} = h_jf(x_j,\lambda), \quad (j=2,\dots,N-1)$$

(1c) $$-D_Nx_{N-1}+(E_N+D_N)x_N = h_Nf(x_N,\lambda).$$

The case $E_j=0$ describes a cell which is not connected to the outside reservoir. The generation term f is qualitatively given by Fig.3 of [2]. There we have given examples in $(4)_2$ (we refer to the formula (j) in [2] as $(j)_2$). λ is again a control parameter. We consider our assemblage to be made up of end units (see Fig.1a, 1c) and middle units (see Fig.1b). For any unit, the number of cells which are not connected to the outside reservoir is arbitrary but at least one for end units and at least two for middle units. Hence the smallest assemblage constructed in this way consists of seven cells and is given in Fig.1.

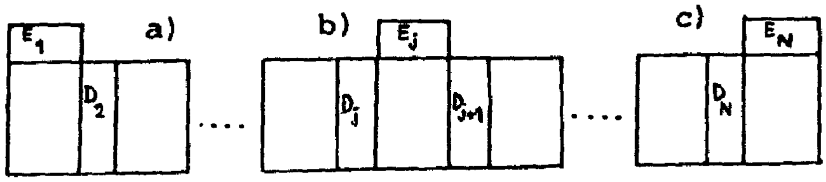


Fig.1

To understand the solution set of (1) we visualize all the parameters E_j, D_j, h_j, λ $(j=1,\dots,N)$

as control parameters and combine them in the control parameter vector $v \in \mathbb{R}^p$ where p is a sufficiently large natural number. Then an abbreviation for the system (1) is

(2) $$F(x,v) = \Theta, \quad x \in \mathbb{R}^N, \quad v \in \mathbb{R}^p.$$

Here for any $v \in \mathbb{R}^p$ the function F maps $\mathbb{R}^N$ into itself. We are trying to construct an organizing center (see $[7]_1$ for this notion) in the solution set of (1) or (2) which determines the structure of this set in the neighborhood of the center. An organizing center is a singularity. Its universal unfolding structurally gives the complete picture of our solution set in the neighborhood of the center. In section 2 we first obtain the type of the singularity in a heuristic way. In section 3 we test our intuition numerically: Structures in the solution diagram of the universal unfolding of the singularity must have their counterpart in the solution set of (1) and vice versa. Hence we take some characteristic structures in one of the two diagrams and try to find a diffeomorphic picture in the other diagram by perturbation of suitable parameters. The results show remarkable agreement of the predictions and the answers. For all structures we have picked in one diagram we could find a counterpart in the other. We note that we only publish some of our tests in this paper. In fact, we tried many more situations and always found the expected answer.

2. A SINGULARITY

In the spirit of [2] we take our assemblage of cells apart into finitely many pieces of the form given in Fig.1. These are two end units and finitely many middle units as described in the introduction.

Let us first take a closer look at an end unit. In the case considered in section 2 of [2] the solution set of an end unit is given by Fig.5 in [2]. Let us concentrate on one of the hysteresis loops (see Fig.5 in [2]) which disappears during the transition described in [2]. We have seen in [2] that this dynamics can be understood by a perturbation of the solution set of the following simple algebraic equation

(3) $$z^3 - \lambda = 0$$

(see $(15)_2$). Numerical studies on the system (1) for the middle unit show that also a middle unit produces hysteresis phenomena which behave like perturbations of the polynomial equation (3).

We now turn to the general case of our assemblage of cells. We assume that we can fix all control parameters except for λ such that the solution curve of any unit with respect to the parameter λ shows a hysteresis loop in the neighborhood of a common value λ_o of the control parameter. All these loops are supposed to behave like a perturbation of (3) if some of the other control parameters in (1) undergo suitable perturbations. Then it is tempting to conjecture that the whole system (1) describing the complete assemblage of cells works locally like a perturbation of equations of the form (3) yielding the system

$$z_j^3 - \lambda = 0, \quad j = 1,\dots,K, \tag{4}$$

where K is the number of units which make up our complete assemblage. For each unit we simply put down an equation of the form (3). Eliminating λ from the system (4) we are left with the system

$$z_j^3 - z_{j+1}^3 = 0 , \quad j = 1,\dots,K-1. \tag{5}$$

This describes a singularity at the point $(0,\dots,0) \in \mathbb{R}^{K-1}$ which defines our organizing center mentioned in the introduction. We proceed now as described at the end of the introduction: The unfolding of (5) at the origin gives the solution pictures which we have to spot in the solution set of (1).

It is very difficult to obtain a universal unfolding for (5) in general. So we retreat in this paper to the two cases K=2 and K=3. Here we can give the universal unfolding of (5). We then know the perturbation pictures predicted by the singularity (5) and can try to adjust the parameters D_j, E_j, h_j $(j=1,\dots,N)$ in (1) to find qualitatively the same pictures in the solution set of (1).

The case K=2 has already been considered in [2], $[3b,4d]_2$. Here our assemblage consists of two end units or an end unit and a middle unit or two middle units. In particular, the case of two end units has been studied [2], $[3b,4d]_2$ with the result that we could observe all predictions of the singularity

$$z_1^3 - z_2^3 = 0 \tag{6}$$

(note K=2 in (5)) for the corresponding system which is in this case the system $(1)_2$. In particular the three pictures of Fig.6 in [2] are part of the universal unfolding of (6) which reads

(7) $$z_1^3 - z_2^3 + \alpha_1 + \alpha_2 z_1 + \alpha_3 z_2 + \alpha_4 z_1 z_2 = 0.$$

This unfolding is discussed in detail in $[1]_1$.

3. THE CASE K=3

In this section we are concerned with the case K=3. We join the three parts of Fig.1 via membranes and arrive at a total of seven cells, three of which are connected to the outside reservoir and separated from each other by two cells with no connection to this reservoir. We assume the generation term f to be of the form $(4a)_2$ with

(8) $$\lambda_1 = 10^{1.4}, \quad \lambda_2 = 4, \quad \lambda_3 = \lambda = \text{control parameter}.$$

The corresponding system (1) takes the form

(9a)
$$\begin{aligned} (E_1+D_2)x_1 - D_2x_2 &= h_1 f(x_1,\lambda) \\ -D_2x_1 + (D_2+D_3)x_2 - D_3x_3 &= h_2 f(x_2,\lambda) \end{aligned}$$

(9b)
$$\begin{aligned} -D_3x_2 + (D_3+D_4)x_3 - D_4x_4 &= h_3 f(x_3,\lambda) \\ -D_4x_3 + (E_4+D_4+D_5)x_4 - D_5x_5 &= h_4 f(x_4,\lambda) \\ -D_5x_4 + (D_5+D_6)x_5 - D_6x_6 &= h_5 f(x_5,\lambda) \end{aligned}$$

(9c)
$$\begin{aligned} -D_6x_5 + (D_6+D_7)x_6 - D_7x_7 &= h_6 f(x_6,\lambda) \\ -D_7x_6 + (D_7+E_7)x_7 &= h_7 f(x_7,\lambda) \end{aligned}$$

Here (9a) and (9c) govern the two end units and the three equations (9b) the middle unit. We now have to find diffusion constants E_j, D_j and cell lenghts h_j such that all three parts (9a), (9b) and (9c) show hysteresis behaviour with respect to the control parameter λ.

This situation occurs if we put

(10) $$E_j = 1 \ (j=1,4,7), \quad D_i = .3, \quad h_i = 1 \ (i=1,\dots,7).$$

Then we can combine for the control parameter $\lambda=9$ out of three solutions for any of the subsystems (9a), (9b), (9c) a total of 27 solutions for the full system (9). We start a continuation procedure at each of these points and find a net of branches as shown in Fig.2a. In the net four bifurcation points occur which we have marked by P1 to P4. The remaining intersections in Fig.2a do not correspond to bifurcation points of the system (9), they are caused by the choice of functionals which we made to draw the bifurcation diagram. In fact, the picture is simplified considerably if we plot the same branches in a (x_1, x_4, x_7) coordinate system as it is done in Fig.2b. This change of view may be compared with the elimination of the parameter λ from the singular system (4) (the vertical axis in Fig.2a is $(x_1+2x_4+3x_7)/6$).

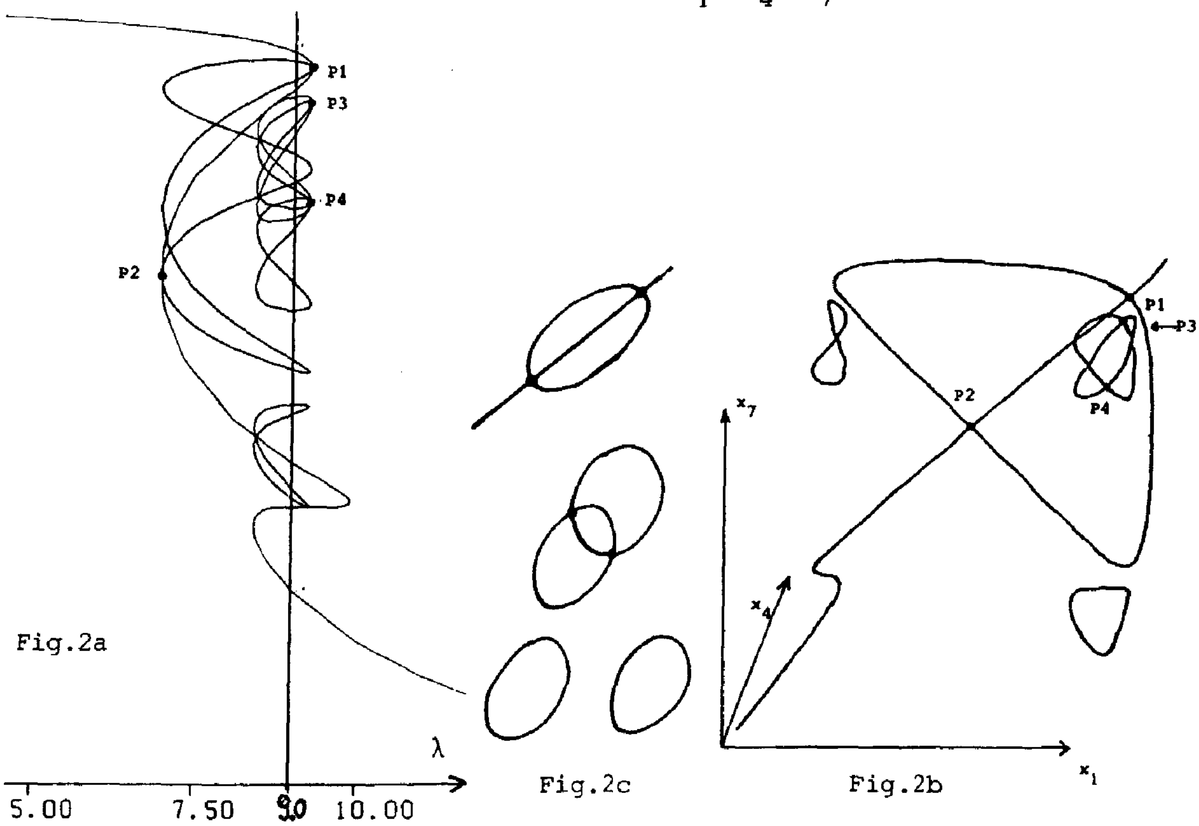


Fig.2a

Fig.2c

Fig.2b

A further simplification occurs if we draw a picture showing the topological type of the net without any reference to the values of the variables $x_1, \dots, x_7, \lambda$. The resulting diagram is given in Fig.2c. It consists of one open curve and five closed curves, one of which is connected to the open curve at two bifurcation points and two of which are tied together at two bifurcation points. The remaining two curves form isolas which are disconnected from each other and from the other branches.

Let us first try to retrieve this configuration from the universal unfolding of the singularity (5) with K=3. In this case we may rewrite (5) as

(11) $\quad x^3-y^3 = 0, \quad z^3-y^3 = 0.$

From the theory in $[6]_2$ we find that a universal unfolding of (11) needs 28 parameters and a particular one is given by

$$
\begin{aligned}
U_1(x,y,z,\alpha) &= x^3-y^3+\alpha_1+\alpha_2x+\alpha_3y+\alpha_4z+\alpha_5xy+\alpha_6y^2+\alpha_7yz+\alpha_8z^2 \\
&\quad +\alpha_9xz+\alpha_{10}xy^2+\alpha_{11}xz^2+\alpha_{12}xyz+\alpha_{13}y^2z+\alpha_{14}yz^2+\alpha_{15}xy^2z+\alpha_{16}xyz^2 \\
U_2(x,y,z,\alpha) &= z^3-y^3+\alpha_{17}+\alpha_{18}x+\alpha_{19}y+\alpha_{20}z+\alpha_{21}x^2+\alpha_{22}xy+\alpha_{23}yz \\
&\quad +\alpha_{24}xz+\alpha_{25}zx^2+\alpha_{26}xyz+\alpha_{27}yx^2+\alpha_{28}x^2yz\ .
\end{aligned} \tag{12}
$$

Of course it is impossible to grasp all types of solution branches of the system $U_1=0$, $U_2=0$ when α varies in $\mathbb{R}^{28}$. Therefore we are compelled to drop many of the parameters from the unfolding (12). Here we are guided by special properties of the system (9) with the values of (10) which should be reflected by the unfolding. In particular, we keep in mind that the variables x,y,z correspond to the concentrations x_1,x_4,x_7 in those cells which are connected to the reservoir.

I. Symmetry

The complete system (9) at the values of (10) is invariant under the transformation $x_i \longrightarrow x_{8-i}$ $(i=1,\ldots,7)$. Hence we require $U_1(x,y,z,\alpha)=U_2(z,y,x,\alpha)$ which leaves us with a total of 12 parameters instead of 28 in (12).

II. Decoupling

$U_1=0$ models the coupling of the left end unit and the middle unit whereas $U_2=0$ does the same for the middle unit and the right end unit. It seems therefore reasonable to let U_1 be independent of z and U_2 be independent of x. This condition reduces the number of parameters in (12) to 10.

If we impose both conditions I and II on the universal unfolding (12) then we end up with the following 4-parameter unfolding

(13a) $\quad F_1(x,y,\beta) = x^3-y^3+\beta_1+\beta_2x+\beta_3y+\beta_4xy = 0$

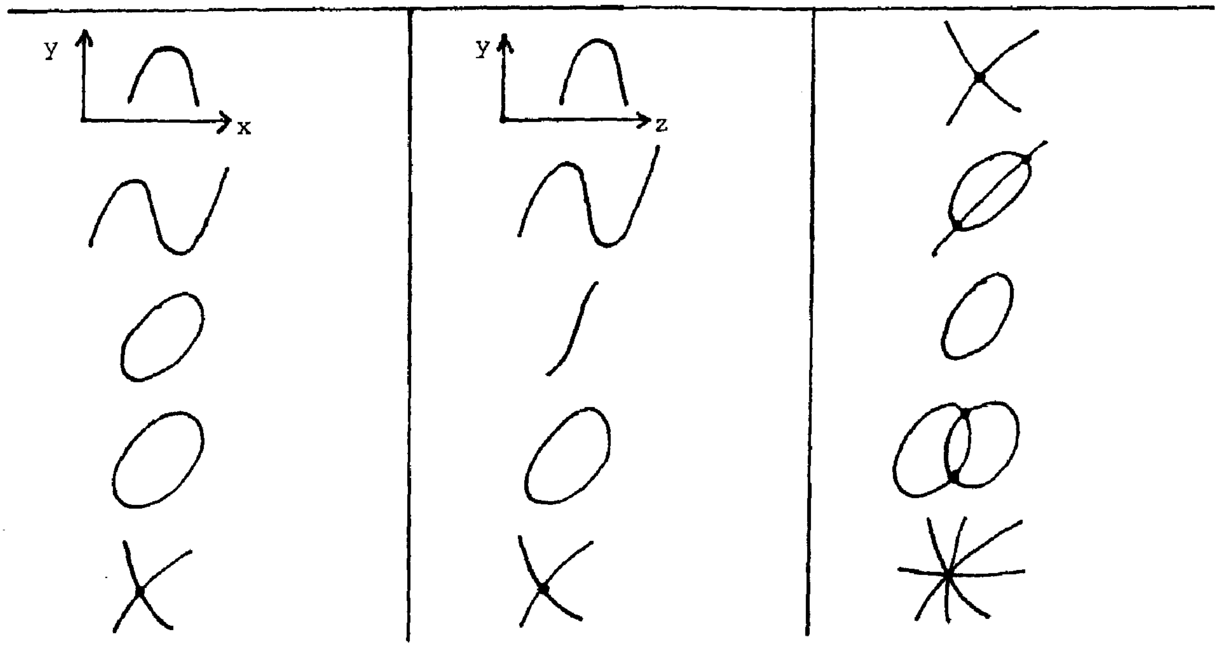
(13b) $\quad F_2(x,y,\beta) = z^3-y^3+\beta_1+\beta_2z+\beta_3y+\beta_4zy = 0\ .$

We recognize that this system contains the unfolding (7) two times with a coupling through the variable y. Projecting the solution sets of (13) onto the (x,y)-plane and the (y,z)-plane will therefore yield the known solution curves of (7) (cf.[1]). On the other hand we can combine the solution set of (13) from the single curves (13a) and (13b). This combination follows some simple rules which we have illustrated in an obvious way in Tab.1. These rules apply to any system of the type

(14) $F(x,y) = 0, \quad F(z,y) = 0$

and could in fact be put into rigorous theorems.

(x,y)-branch of $F(x,y) = 0$	and	(z,y)-branch of $F(z,y) = 0$	combines to	(x,y,z)-branch of (14)



Tab.1

For example, if we consider the parameter set $\beta_1=\varepsilon$, $\beta_2=-1$, $\beta_3=1$, $\beta_4=0$ ($\varepsilon > 0$ small), then the cubic curves (13a), (13b) are of the following form

Fig.3

Combining the two pictures according to the rules of Tab.1 we get a structure which is diffeomorphic to the one given in Fig.2c. Hence we have found the counterpart of the structure of Fig.2a in an unfolding of the organizing center (11).

An even more interesting solution net of the system (9) occurs for the following set of parameters

(15) $E_1=E_7=1,\quad E_4=2,\quad D_i=.3\quad (i=1,\dots,7),\quad h_i=1\quad (i=1,\dots,7,i\neq4),\ h_4=2$.

This situation differs from (10) only in E_4 and h_4. In the (x_1,x_4,x_7)-space we obtain a solution picture for (9) as shown in Fig.4.

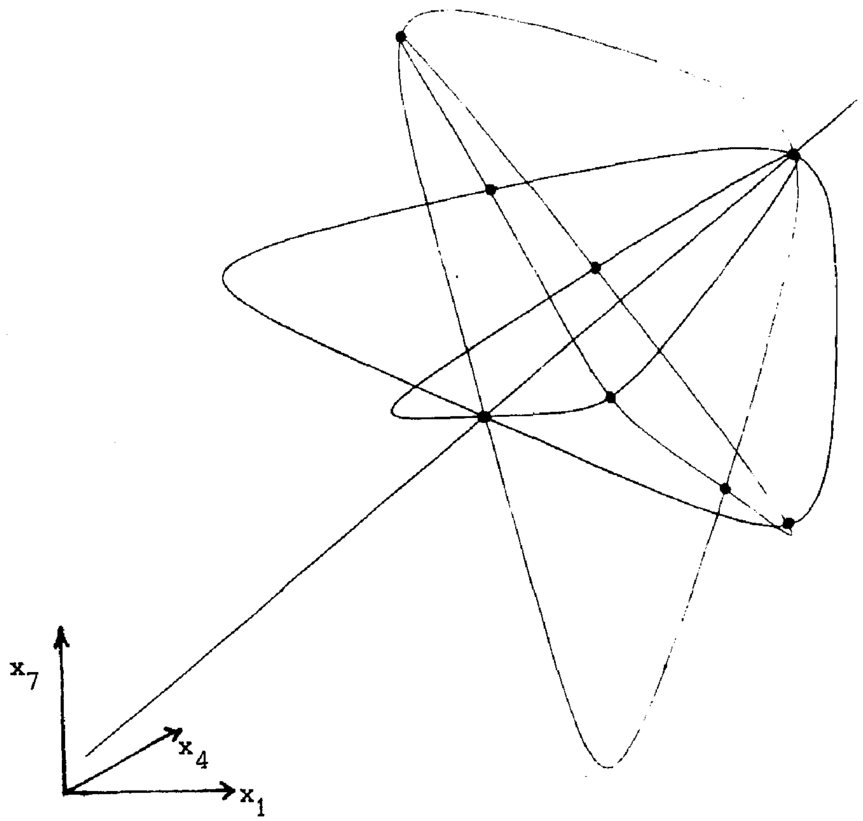


Fig.4

Let us postpone for the moment the explanation of this picture from the universal unfolding (12).

Instead we look at some typical solution curves of (13a) which occur for parameter sets $(\beta_1,\beta_2,\beta_3,\beta_4)$ close to (0,-1,1,0). Combining these curves by the rules of Tab.1 yields the solution nets in the small pictures below. We compare these pictures with three perturbations of the situation (15) which are obtained by varying E_4 and h_4.

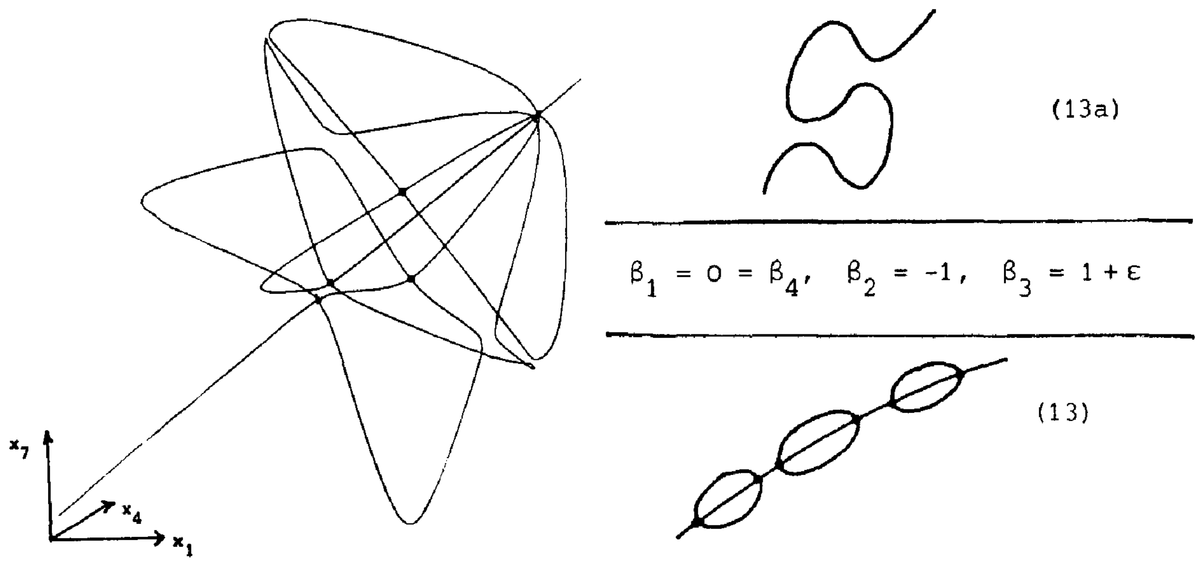


Fig.5 (h_4=2.055, E_4=2.051)

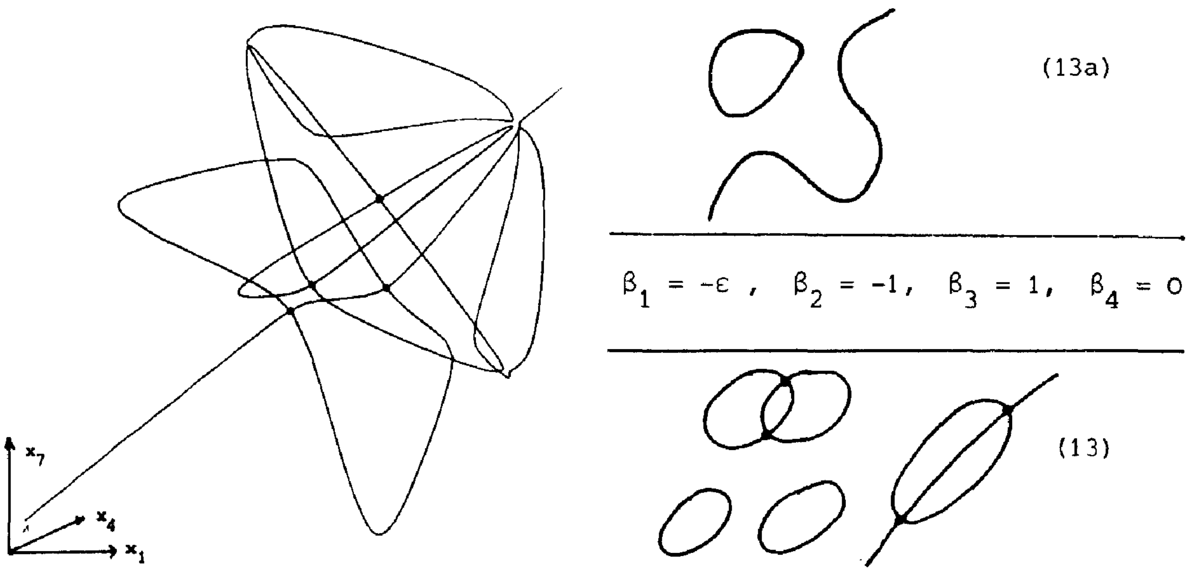


Fig.6 (h_4=2, E_4=2.02)

The case of Fig.6 is of course topologically equivalent to that of Fig.2. As a result, the small pictures in the figures 5, 6, 7 are the forecasts of the singularity (11) to the corresponding figures given by our system (9).

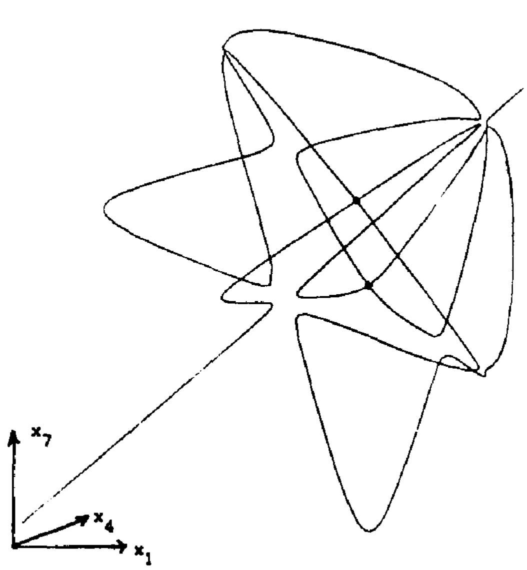
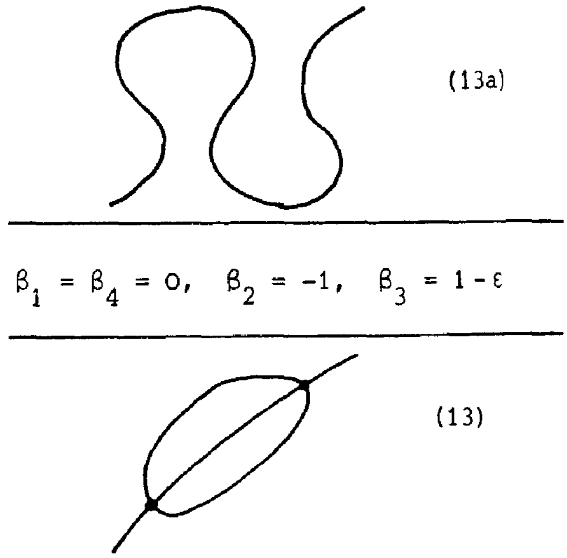


Fig.7 (h_4=1.948, E_4=1.952)



Let us return to the case (15). The special feature of it is that the system (9) has in addition to our symmetry I the following subsymmetry:

III. Subsymmetry.

In the subspace of symmetric vectors x (i.e. $x_i=x_{8-i}$, i=1,...,7) the system (9) is invariant under the transformation $x_i \longrightarrow x_{5-i}$ (i=1,...,4). Therefore we require $U_1(x,y,x,\alpha) = -U_1(y,x,y,\alpha)$ in (12).

Imposing this condition on (13) yields the one parameter unfolding

$$(16) \qquad \begin{aligned} x^3-y^3-\gamma(x-y) &= 0 \\ z^3-y^3-\gamma(z-y) &= 0. \end{aligned}$$

The solution net of this system for $\gamma > 0$ consists of one straight line, three ellipses and one circle. These are coupled by 6 simple and 2 multiple bifurcation points as indicated in Fig. 8a.

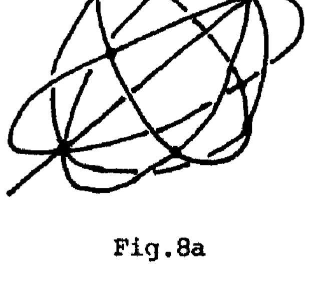


Fig.8a

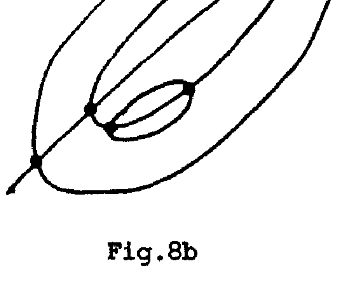


Fig.8b

This seems to explain Fig.4. However, a close inspection of the branching structure of the system (9) with values (15) showed that in fact the topological type of Fig.8b obtains numerically. The deviations cannot be visualized in the scale of Fig.4, but we have indicated them in Fig.4 of [1].

The problem now is that Fig.8b is not possible in the partial unfolding (13). Hence we are forced to skip at least one of the simplifying assumptions I, II or III. The obvious candidate is the decoupling condition II which was only expected to hold approximately. If we impose the two symmetry conditions in the universal unfolding (12) we find the five parameter unfolding

$$x^3-y^3+\delta_1(x-y)+\delta_2(z-y)+(\delta_3y+\delta_4z+\delta_5yz)(x-z) = 0$$
$$z^3-y^3+\delta_1(z-y)+\delta_2(x-y)+(\delta_3y+\delta_4x+\delta_5yx)(z-x) = 0.$$

After some calculations it turns out that this system exhibits the net structure of Fig.8b for the parameter set

$$\delta_1=-\gamma+\varepsilon,\ \delta_2=-\varepsilon \quad (0<\varepsilon\ll\gamma),\quad \delta_3=\delta_4=\delta_5=0.$$

Moreover, this situation is a perturbation of the system (16).

This ends the explanation of the situation (15) via the unfolding of the organizing center (11).

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