

Networks Induced in Nonlinear Chemical Reaction System by Symmetries of Transformation Groups

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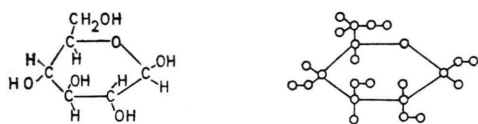
Z. Naturforsch. **34a**, 380–386 (1979); received December 12, 1978

Physical systems possess a structure and display dynamics. The article describes how a structure of one class of systems, which are encountered in chemical kinetics, can be revealed. The structure may be represented by a graph that has some similarities with the graph used to display the structure of chemical molecules. The graphs are induced by one-parameter transformation groups in nonlinear systems. The model system of Dreitlein and Smoes is treated as an example.

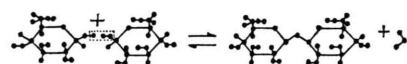
Introduction

Systems consist of components, which mutually interact. The interactions of the components comprise the dynamic aspect of the system. However, a system also possesses a structure, i.e. a characteristic mode of assembly of the components, which defines the network of interactions between the components. The network is usually represented by a graph.

Consider, e.g., the chemical formula of glucose:



If every atom of glucose is replaced by a full circle, the above graph on the right-hand is obtained. The graph represents the static structure of connections in the molecule. However, if a glucose molecule is considered a component of a solution of interacting molecules, then e.g. two glucoses may form a trehalose molecule:



The dynamics are introduced by assuming an interaction between two structured components, here the glucose molecules, which ultimately may lead to new components, here trehalose and water. The dynamics of such processes are described by the theory of chemical reaction kinetics.

In this paper, we shall derive a similar graph in which the atoms (nodes) of a molecule represent

kinetic states of a reacting chemical system (e.g. a stationary state or a limit cycle state). As interaction (reaction) between the molecules the diffusion of chemical components is introduced to give an equivalent to the chemical reaction equation. We shall mathematically treat a reaction-diffusion system proposed by Dreitlein and Smoes [1] as model of such a process.

The Chemical Reaction Model and Its Graph

The kinetics of a system of chemical reactions has been studied mathematically by Dreitlein and Smoes [1]. This model has been selected because the corresponding nonlinear differential Eqs. (1) can be solved analytically:

$$\begin{aligned}\frac{\partial}{\partial t} a_1 &= (E - a_1^2 - a_2^2) a_1 + S_1 a_2 - 2 R a_1, \\ \frac{\partial}{\partial t} a_2 &= (E - a_1^2 - a_2^2) a_2 - S_2 a_1 + 2 R a_2\end{aligned}\quad (1)$$

where a_1, a_2 are time dependent species quantities (e.g. concentrations of chemicals) and E, S_1, S_2, R parameters. Unfortunately, no chemical system has so far been discovered, which obeys such kinetics. The Eqs. (1) are given in a dimensionless form [2]. The choice of $R=0$ converts the elliptic limit cycle of the system to a circle of radius E [1]. This modification facilitates the calculations very much without effecting its structural components of that state. Figure 1B shows a concentration diagram of the limit cycle state, which may be so projected on a sphere that the south pole represents the origin, the north pole the infinity of the phase plane (see Fig. 2) and the equator the limit cycle. This allows us to assign a generator to each of the elements of the sphere, e.g. the Northern half sphere, the

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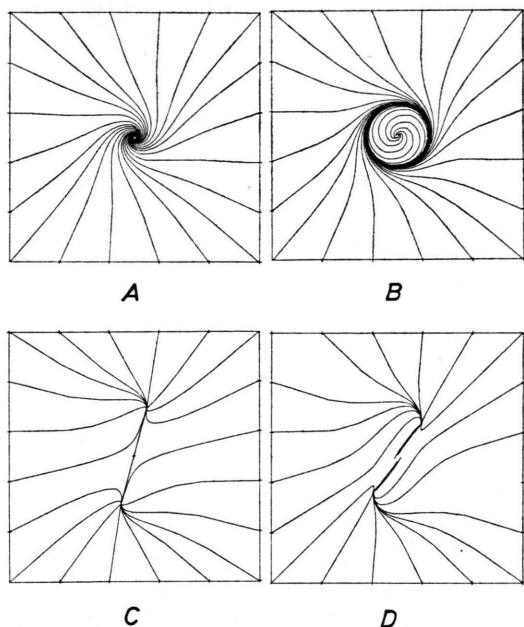


Fig. 1. Families of trajectories for the different domains of the differential equation system (1). Each family A–D in the state space (a_1, a_2) —(a_2 abscissa) corresponds to a graph (see Fig. 3). The transition from one type of family to another is accompanied by a change in the structure of the graph. The transition occurs at the boundaries of the parameter space. The parameters of Eqs. (1) are: $S_1=S_2=2$ and for A) $E=-1$, $R=0$; B) $E=1$, $R=0$; C) $E=-1$, $R=1$; D) $E=1$, $R=1.04$.

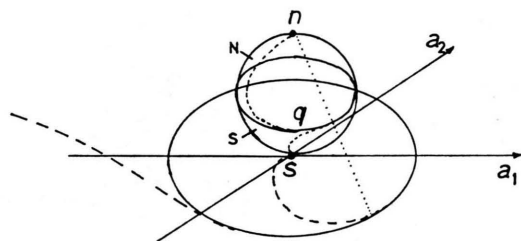


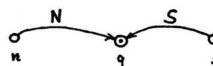
Fig. 2. Geometric projection of the a_1, a_2 plane onto a sphere. Points in the plane are mapped onto the sphere by connecting the north pole of the sphere with the point in the plane by a straight line. The intersection of the line with the sphere is the image of the point. The particular plane diagram of Fig. 1B is shown here. The mapping is so performed that the limit cycle is mapped onto the equator of the sphere.

Southern half sphere, the equator, the North pole and the South pole may be assigned to the generators N, S, q, n, s respectively. Introduction of a boundary operator ∂ gives the relation between topographic localities on the sphere [3]:

$$\partial N = q - n, \quad \partial S = q - s,$$

i.e. on the Northern hemisphere, a curve of Eqs. (1) will leave North pole (negative orientation at n) and enter (positive orientation) its other boundary, the equator. The same is true for the Southern part. Thus, the boundary of S is $q - s$.

The system can only stay indefinitely in the elements q, n, s , whereas N, S are areas of transitions between the states q, n, s . A graph displaying the connectivity has the nodes (points, states) q, n, s and the branches N, S :



The graph is independent of the initial conditions of the equation system (1), but it is dependent on the system parameters. When E is approaching zero, the limit cycle will move toward the singular point at the origin (Figure 1B). For $E=0$, the limit cycle vanishes in the singular point. Hence, for negative values of E , there are only two singular points, n and s , left. The corresponding graph is:



The structure of the system may suddenly change (from Fig. 1B to 1A), as demonstrated above, by altering the system parameters. Hence, one may establish diagrams of parameters of the system, displaying the different structures of the system (like phase diagrams of crystals of solids). Dreitlein and Smoes [1] have drawn such a diagram for the Equations (1). A transition to a different graph resembles in many respect a phase transition. Now, we have derived a graph, which corresponds to the one of glucose in the introduction, but the graphs and their concentration diagrams are very simple and do not reflect all aspects involved. More details are revealed if $R \neq 0$ in Equations (1).

Since Eqs. (1) still are analytically soluble for $R \neq 0$, this model is treated in the following.

The substitution

$$a_1 = z \cos \varphi \quad \text{and} \quad a_2 = z \cos(\varphi + \alpha)$$

in Eqs. (1) results in the equation system:

$$\begin{aligned} \frac{d\varphi}{dt} = & S_1 \sin \alpha + (2R - S_1 \cos \alpha) \sin(2\varphi) \\ & + \frac{1}{\sin \alpha} [S_2 - S_1 \\ & + 2 \cos \alpha \cdot (S_1 \cos \alpha - 2R)] \cos^2 \varphi, \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{dz}{dt} = & [E - z^2(\cos^2(\varphi + \alpha) + \cos^2 \varphi)] \\ & \cdot z + z(S_1 \cos \alpha - 2R) \\ & \cdot (\cos^2 \varphi - \sin^2 \varphi) + \frac{z}{2 \sin \alpha} \\ & \cdot [S_2 - S_1 + 2 \cos \alpha (S_1 \cos \alpha - 2R)] \\ & \cdot \sin 2\varphi \end{aligned}$$

where α is a time independent parameter.

The value of α may be determined from

$$S_2 - S_1 = 2 \cos \alpha (2R - S_1 \cos \alpha),$$

so that Eqs. (2) simplifies to:

$$\frac{d\varphi}{dt} = S_1 \sin \alpha + Q \sin 2\varphi, \quad (3a)$$

$$\begin{aligned} \frac{dz^2}{dt} = & 2[E - z^2(\cos^2(\varphi + \alpha) + \cos^2 \varphi)] \\ & \cdot z^2 + z^2 Q \cdot 2 \cos 2\varphi \end{aligned} \quad (3b)$$

where $Q = 2R - S_1 \cos \alpha = (S_2 - S_1)/2 \cos \alpha$ since the last term in Eq. (2) vanishes.

Equation (3b) divided by Eq. (3a) is a differential equation of the Riccati type:

$$dz^2/d\varphi = Vz^2 + Wz^4 \quad (4)$$

where

$$\begin{aligned} W = & -2 \frac{\cos^2(\varphi + \alpha) + \cos^2 \varphi}{S_1 \sin \alpha + Q \sin 2\varphi}; \\ V = & 2 \frac{E + Q \cos 2\varphi}{S_1 \sin \alpha + Q \sin 2\varphi}. \end{aligned}$$

By substituting $z^2 = -\frac{1}{W} \frac{p}{\int p d\varphi}$, Eq. (4) gives

$$\frac{dp}{d\varphi} = \left(\frac{1}{W} \frac{dW}{d\varphi} + V \right) p$$

which has the solution:

$$p = W \text{Ei } V d\varphi \quad \text{where} \quad \text{Ei} \exp \int.$$

Hence, the solution of Eqs. (3) in a form which emphasises the integration constants C and t_0 is:

$$\begin{aligned} \text{Ei } V d\varphi \left(\frac{1}{z^2} + \text{Ei} - V d\varphi \cdot \int W \text{Ei } V d\varphi d\varphi \right) = C, \\ \int (S_1 \sin \alpha + Q \sin 2\varphi)^{-1} d\varphi = t - t_0. \end{aligned} \quad (5)$$

If $S_1 = S_2 = S$, Eqs. (5) simplify to:

$$\begin{aligned} \exp \{V_0 \varphi\} \cdot \left(\frac{1}{z^2} - \frac{1}{E} - \frac{1}{E} \right. \\ \left. \cdot \cos \alpha \sin \beta \sin(2\varphi + \alpha + \beta) \right) = C, \end{aligned}$$

$$\varphi = (S \sin \alpha)(t - t_0) \quad (6)$$

where $V_0 = 2E/S \sin \alpha$, $\cos \beta = 1/\sqrt{1 + (V_0/2)^2}$ and $\cos \alpha = 2R/S$.

Let $\Omega = S \sin \alpha$; $a = \cos \alpha \sin \beta$ and $\gamma = \alpha + \beta$. Then Eqs. (6) take the compact form:

$$\begin{aligned} \exp \{2E\varphi/\Omega\} \cdot \left(\frac{E}{z^2} - 1 - a \sin(2\varphi + \gamma) \right) \\ = C' = CE, \end{aligned} \quad (7a)$$

$$\varphi = \Omega(t - t_0). \quad (7b)$$

When the term within the outer paranthesis in Eq. (7a) set to zero the equation for the limit cycle, an ellipse expressed in polar coordinates, appears:

$$\begin{aligned} z^2 = & \frac{E}{1 + a \sin(2\varphi + \gamma)} \\ = & \frac{E/(1 - a)}{1 + 2a/(1 - a) \cos^2(\varphi + \delta)} \end{aligned} \quad (8)$$

where $\delta = (\gamma - \pi/2)/2$.

Note, that z and φ only are polar coordinates in the plane a_1, a_2 if $\alpha = \pi/2$.

Equation (7a) permits a second transformation:

$$\begin{aligned} \frac{1}{r_*^2} = & \frac{1}{z^2} - \frac{a}{E} \sin(2\varphi + \gamma), \\ \varphi_* = & \varphi \end{aligned} \quad (9)$$

which gives Eq. (7) the form:

$$\begin{aligned} \exp \left\{ \frac{2E\varphi}{\Omega} \right\} \left(\frac{E}{r_*^2} - 1 \right) = C', \\ \varphi_* = \Omega(t - t_0). \end{aligned} \quad (10)$$

This system has been extensively discussed in a previous paper [4]. Here, we derive the infinitesimal generator of the group U which leaves the solutions of Eqs. (1) for $S_1 = S_2 = S$ invariant. From Eq. (24) of that paper:

$$U = \left(\frac{\partial}{\partial \varphi_*} z \right) \frac{\partial}{\partial z} + \left(\frac{\partial}{\partial \varphi_*} \varphi \right) \frac{\partial}{\partial \varphi}$$

we calculate:

$$U = \frac{a}{E} z^3 \cos(2\varphi + \gamma) \frac{\partial}{\partial z} + \frac{\partial}{\partial \varphi}. \quad (11)$$

The associated differential equation system admits the solution:

$$z^2 = \frac{1}{K - (a/E) \sin(2\varphi + \gamma)} \quad (12)$$

where K is the integration constant of the family of curves. Again, Eq. (12) has the form of Eq. (8) i.e. of a conical section. Hence, the curves may be elliptic or hyperbolic.

Finally, from Eq. (7a) a differential form may be obtained by:

$$dC' = \frac{\partial C'}{\partial z} dz + \frac{\partial C'}{\partial \varphi} d\varphi = 0 \quad (13)$$

from which the system of differential equations:

$$\begin{aligned} \mu dz/dt &= \partial C'/\partial z, \\ \mu d\varphi/dt &= -\partial C'/\partial \varphi \end{aligned} \quad (14)$$

may be derived. μ is the integrating factor of the differential form (13). Integrating factors are closely related to the differential systems and the groups which they admit [5]. Equations (14) are the Eqs. (2) multiplied by the factor μ . Hence, introduction of a time interval $d\tau = dt/d\mu$ would result in a system of differential equations like the ones known from Hamiltonian systems. If the singularities of the Eq. (14) are evaluated by setting the time derivatives equal to zero, another interesting fact is revealed:

$$\begin{aligned} C' &= C'(Z, \varphi, E, R, S_1, S_2), \\ \partial C'/\partial z &= 0, \quad \partial C'/\partial \varphi = 0, \end{aligned} \quad (15)$$

where C' is Equation (7a).

Equations (15) are suitable for a discussion of the problem of singularities in the catastrophe theory [6]. We shall use Eqs. (1) to discuss the singularities, but the Eqs. (15) could be used equally well.

Singular Points

The singular points are essential constituents of the graph. Therefore, they must be considered. They are obtained from Eqs. (1) by setting the time derivatives equal to zero. One singular point is the origin ($a_1 = a_2 = 0$). The other points may be obtained by considering Eqs. (1) as a linear equation system in a_1 and a_2 . For $a_1, a_2 \neq 0$, the determinant has to be zero, i.e.

$$\begin{vmatrix} E - 2R - \varrho & S_1 \\ -S_2 & E + 2R - \varrho \end{vmatrix} = 0 \quad (16)$$

where $\varrho = a_1^2 + a_2^2$.

Hence,

$$\begin{aligned} \varrho &= E \pm \sqrt{4R^2 - S_1 S_2}, \\ \frac{a_2}{a_1} &= \frac{2R \mp \sqrt{4R^2 - S_1 S_2}}{S_1} = \text{ctg } \varphi. \end{aligned}$$

The parameters ϱ and φ may be interpreted as polar coordinates. The critical transition occurs if the term under the square root turns negative or if the radius ϱ becomes negative.

Therefore, the critical curves are:

$$4R^2 = S_1 S_2 \quad \text{and} \quad E^2 = 4R^2 - S_1 S_2. \quad (17)$$

The same result can be obtained more systematically by regarding ϱ in Eq. (16) as a complex quantity:

$$\begin{vmatrix} E - 2R - u - iv & S_1 \\ -S_2 & E + 2R - u - iv \end{vmatrix} = 0. \quad (18)$$

The real and imaginary terms of the determinant give the equations:

$$\begin{aligned} (E - 2R)(E + 2R) + S_1 S_2 - Eu \\ + u^2 - v^2 &= 0, \\ -Ev + 2uv &= 0. \end{aligned}$$

The Eqs. (17) may also be obtained from the conditions $u=0$ or $v=0$, where ϱ turns from a real positive to a negative or a complex value.

The three dimensional parameter space generated by E , R and $\bar{S} = \sqrt{S_1 S_2}$ is sectioned by the Eqs. (17) into domains. A specific graph belongs to each domain (see Fig. 1 and 3).

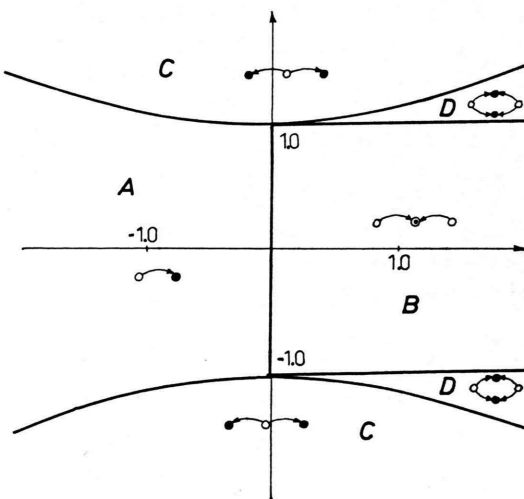
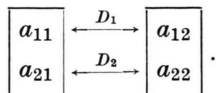


Fig. 3. Domains in the parameter space (R , E) with $S_1 = S_2 = 2$ of the differential equation system (1). Each domain belongs to a different type of solution, to which a graph may be assigned. The nodes in the graph represent: ● stable point, ○ unstable point and ⊙ limit cycle. The identifiers A–D of the domains correspond to the diagrams in Fig. 1.

Coupling of Model Systems by Diffusion

Let a_{11} , a_{21} and a_{12} , a_{22} be the variables of two systems (distinguished by the latter subscript 1, 2 resp.) of the type given by the Equations (1). The systems may be illustrated by two boxes:



The substance a_1 may be exchanged by a law of the diffusion type, characterized by the diffusion constant D_1 . The same is true for a_2 . The corresponding equation set is obtained by addition of diffusion terms to the Equations (1):

$$\begin{aligned}\frac{\partial}{\partial t} a_{11} &= q_1 a_{11} + S_{11} a_{21} - 2 R_1 a_{11} \\ &\quad + D_1 (a_{12} - a_{11}), \\ \frac{\partial}{\partial t} a_{12} &= q_2 a_{12} + S_{12} a_{22} - 2 R_2 a_{12} \\ &\quad + D_2 (a_{22} - a_{12}), \\ \frac{\partial}{\partial t} a_{21} &= q_1 a_{21} - S_{21} a_{12} + 2 R_1 a_{21} \\ &\quad + D_1 (a_{11} - a_{12}), \\ \frac{\partial}{\partial t} a_{22} &= q_2 a_{22} - S_{22} a_{12} + 2 R_2 a_{22} \\ &\quad + D_2 (a_{21} - a_{22})\end{aligned}\quad (19)$$

where $q_1 = E_1 - a_{11}^2 - a_{21}^2$ and $q_2 = E_2 - a_{12}^2 - a_{22}^2$.

The coupling between the upper two and the lower two equations is furnished by the added terms. Introduction of polar coordinates will not considerably simplify Eqs. (19) and the condition $D_1 = D_2 = D$ and $R = 0$ will result in an equation system which can be solved analytically. However, the solution contains no essentially new features.

As in Eq. (18), one may find the curves sectioning the parameter space by solving the determinant:

$$\begin{vmatrix} E_{11} - \varrho_1 & S_{11} & D_1 & 0 \\ -S_{12} & E_{12} - \varrho_1 & 0 & D_2 \\ D_1 & 0 & E_{21} - \varrho_2 & S_{21} \\ 0 & D_2 & -S_{22} & E_{22} - \varrho_2 \end{vmatrix} = 0 \quad (20)$$

where $\varrho_i = a_{i1}^2 + a_{i2}^2$, ($i = 1, 2$)

$$E_{11} = E_1 - 2 R_1 - D_1 \quad \text{and}$$

$$E_{12} = E_1 + 2 R_1 - D_2$$

for the complex quantities

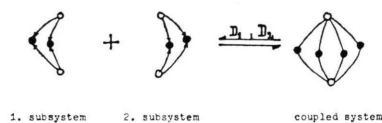
$$\varrho_1 = u_1 + i v_1 \quad \text{and} \quad \varrho_2 = u_2 + i v_2.$$

The equation sets $u_1, u_2, v_1, v_2 = 0$ resp. separate domains of different topological properties in the space of solutions.

Since the calculations are extensive and the result will only deal with the separation of the phase space by the singular points and not with other phenomena like e.g. limit cycles, this approach is abandoned here. Nevertheless, Eqs. (20) demonstrate some peculiar properties. If initially $a_{12} = a_{11}$, $a_{21} = a_{22}$ and both subsystems are equal e.g. $E = E_1 = E_2$, $R = R_1 = R_2$, $S = S_{11} = S_{21}$, then the diffusion terms have no influence on the solution, i.e. the system behaves as if it were uncoupled.

Thus, we shall find the solutions of the uncoupled system among the solutions of the coupled system. The singular points and the limit cycle of the uncoupled systems are also among the singularities of the coupled system. Another special situation is encountered if diffusion terms dominate, e.g. by strong coupling (where D_1 and D_2 have very large values). Then, $a_{11} = -a_{12}$ and $a_{22} = -a_{21}$ approximate singular conditions. Moreover, far from the origin, e.g. at infinity, the contribution of the diffusion term becomes negligible. Therefore, curves at infinity take a course as if the subsystems were uncoupled. These facts roughly describe the state space of the system.

A picture of the structural relationship is obtained, if the parameters in the subsystem are so selected that two stable and three unstable points occur (see Figure 1D). The coupling of two equal subsystems may then be graphically represented by the structural equation:



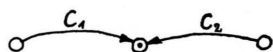
where the left side of the equation represents the uncoupled system and the right side the structure of the coupled system. The constants D_1 and D_2 involved in the interaction are fixed to the arrows, which symbolize the transition. The structure of the coupled system may either be obtained by numerical calculation or from the above reflections. Firstly, there have to be curves which in both subsystems approach the same singular point, since the system behaves as if it were uncoupled when both subsystems have equal initial conditions. Secondly, one subsystem must approach the opposite

singular point in the other subsystem. The resulting singular points no longer have the same coordinates as those in the uncoupled system, but are strongly influenced by the coupling. Curves entering the singular points come either from infinity or from the unstable origin. Hence, here the coupling of the two systems is mainly attained by the coalescence of the unstable nodes.

Discussion

The chemical model system, treated by Dreitlein and Smoes, can be solved analytically to study the phenomena inherent in some non-linear differential-equation systems. Particularly the structural aspect, which manifests itself in the networks, is considered here. These networks are closely related to the symmetries which are induced by one-parameter transformation groups. Each branch of the network graph corresponds to a solution (or path in the state space) of the system. All the solutions, which can be transformed into one another by the transformation group are represented by one branch in the graph. Since the state space is continuously covered by paths, all transformations of a path by the group form a domain in the state space. The paths join at the boundary of the domain. The ends of the path (or its boundary) form a subspace in the state space, which is represented by a node in the graph of the network. Frequently, paths of different domains meet in the same subspace, thus generating the network. The physical meaning of the subspace, is, that all points within the domain are uniquely determined by the transformation group. At the boundary, the uniqueness is destroyed, e.g. at a limit cycle the same point may be encountered at different times.

Moreover, one may specify a path in a domain by a constant, which may be the parameter of the transformation group or the integration constant belonging to that curve (see Equation (7a)). Thus, one may weight the graph (G):



The nodes may be singular points, but not all singular points are nodes. Some of the singular points of the Eqs. (1) are part of the contours which separate different domains (separatrix). Whereas the paths (branches) can be transformed into each

other, the nodes have an individual character. They may be limit cycles, stable or unstable points (similar to the different atoms in the introduction). It seems that their number, at least for a two dimensional state space, is limited. Since the evaluation of the singularities has a bearing on the catastrophe theory, the classification of this theory may be helpful in classifying the nodes.

The graph is independent of the initial conditions of the differential Eqs. (1), but it changes its structure when the parameters of Eqs. (1) cross certain boundaries in the parameter (phase) space. In this respect, it has much in common with phase transitions. The introduction of new parameters into the Eqs. (1) by introducing diffusion as a new interaction, as it was done to establish the Eqs. (19), causes the appearance of new networks. If the interaction between subsystems is introduced, then in many cases the transition to the new network may be represented by formulas similar to the ones used in chemistry. Note, that in chemical reaction formulas the number of atoms on both sides remains constant. This does not seem to apply to these graphs since they do not require that atoms are defined as conservative quantities.

The new network created by coupling of subsystems by interactions of the diffusion type is one method of generating new structures. In the case treated, the network structure does not change drastically. However, under strong coupling it may in other systems happen, that above a certain threshold the system assumes a different structure. Such cases seem to be more relevant to life processes, since the latter permit two individual systems to coexist and yield an entity which has properties that cannot be attributed to individuals alone.

Furthermore, it should be noted, that the trajectories in Eqs. (1) are curves with a boundary. There are several other types of curves, e.g. path curves in chaotic regimes [7] or the closed path curves which belong to the one parameter transformation group [see Eq. (18)]. They are either ellipses or path curves which originate in infinity and disappear in infinity (close through infinity). The duality between closed and open curves seem to be related to physical phenomena [8].

The graphs of the network induce a boundary operator ∂ , which may be represented by a matrix [9]. This matrix represents a map of a free abelian

group folded into itself (endomorphism). It has the property $\partial^2 = 0$. Such operators are known to produce homologies [3], and to have particular properties. The free abelian group can be coded by a set of generators and a set of relations [10] between the generators. The relations contain the information of the network in an especially coded form. In chemical kinetics, these relations are coded in the stoichiometric matrix. In biology, the network structure is somehow coded in the DNA of the cells. This code seems to correspond to non-abelian free groups. If this is so, the coding capacity would

allow the construction of still more complex structures.

Finally, it has to be mentioned that there is an essential aspect which has not been considered in this paper. In real systems, some quantities, e.g. concentrations, are limited: They can only be positive and the sum of the concentrations of some constituents cannot in a closed system at any time exceed their total at initial time. The limits of the quantities may establish another boundary in the physical state space. The constraints which generate boundaries are important parts of the real system.

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