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HOPF AND TURING BIFURCATIONS IN FLUCTUATIONAL MODELS OF SELF-ORGANIZATION

A.V.Chalyi[(1)], D.A.Khiznyak[(2)], Ya.V.Tsehmister[(1)]

[(1)] *Chair of Biophysics*
Ukrainian State Medical University
13 Shevchenko Blvd., UA–252004 Kiev, Ukraine

[(2)] *Institute of Physics*
Ukrainian National Academy of Sciences
46 Nauki Av., UA–252650 Kiev, Ukraine

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The fluctuation models of self-organization are proposed with fluctuation Hamiltonians taken into account. Conditions of the Hopf and Turing bifurcations are examined, special attention is paid for the analysis of limit-cycle and focus solutions. The principal possibility of the formation of ordered structures in the fluctuation models of self-organization are discussed for open systems in a stationary states.

1. Introduction

The problem of self-organization and related problem of the formation of spatial and temporal structures, i.e. the Turing and Hopf bifurcations, seems to be important up to now (see [1-3]). The development of the general theory of self-organization has been stimulated by the latest advance connecting with the universal behavior of the systems having different physical natures near the continuous phase transition point and critical (bifurcation) points. The modern theory of self-organization (synergetics) is based on such powerful and well-developed methods as those of nonlinear mechanics, kinetic models and physics of phase transition. It is obvious that the phase-transition methods using fundamental ideas of scaling invariance [4], renormalization group [5], collective variables [6] are preferable because various systems (not only physical but chemical, biological, sociological, etc.) exhibit an anomalous high susceptibility to external influences.

The main idea of our approach to study the development of the space, time and spatio-temporal structures in open systems is based on the assumption that many processes in chemically (biochemically) reacting systems can be treated as those isomorphous to the second-order phase transitions. It means that fluctuational effects must be taken into consideration near the critical (bifurcation) points. Thus, the corresponding fluctuation models of the processes of self-organization have to be proposed on the background of the phase transition theory.

2. Effective fluctuation Hamiltonian for chemically reacting systems

For a system with chemical reactions the main governing mode (in terms of synergetics [2]) or the order parameter (in terms of physics of phase transitions [4-7]) is the degree of completeness (coordinate) ξ_α defined by the formula

$$d\xi_\alpha = d_\alpha n_i / \nu_{i\alpha}, \tag{1}$$

where $d_\alpha n_i$ is the variation of the number of moles, $\nu_{i\alpha}$ are the stoichiometric coefficients. The quantity conjugate to of ξ_α (in the thermodynamic sense) is the reaction affinity

$$A_\alpha = \left(\frac{\partial G}{\partial \xi_\alpha}\right)_{T,P,\xi_{\gamma\neq\alpha}} = \sum_i \nu_{i\alpha}\left(\frac{\partial G}{\partial n_i}\right)_{T,P,n_{j\neq i}} = \sum_i \nu_{i\alpha}\mu_i \tag{2}$$

represented by a linear combination of the chemical potentials μ_i.

Near the boundary of stability the chemical reaction susceptibility

$$\chi = -\left(\frac{\partial \xi}{\partial A}\right)_{T,P,\{\xi\}}, \qquad \chi^{-1} = \sum_{i,j} \nu_i \nu_j (\partial \mu_i / \partial n_i)_{P,T,n_k \neq n_j} \tag{3}$$

goes to infinity. This principal circumstance allows to use the basic assumptions of the phase transition theory, namely to expand the fluctuation part of the Gibbs potential into a functional Taylor series

$$G[\xi] = \sum_{n\geq 0} = \frac{1}{n!}\int \cdots \int \frac{\delta^n G[\xi]}{\delta\xi(\vec{r_1})\cdots\delta\xi(\vec{r_n})}|_{\xi(\vec{r_i})=0} \cdot \prod_{j=1}^{n} \xi(\vec{r_i}) d\vec{r_i}. \tag{4}$$

It is natural to choose this fluctuational part in the generalized well-known Landau-Ginzburg form. For the case of two chemical reactions with order parameters

$$x = \xi_1 - \langle \xi_1 \rangle, \qquad y = \xi_2 - \langle \xi_2 \rangle \tag{5}$$

the effective fluctuational Hamiltonian has the following form

$$\begin{aligned}
\mathcal{H} &= \Delta G_{fl}[x,y] = \int g(\vec{r})\mathrm{d}\vec{r}, \\
g(\vec{r}) &= A_x x + A_y y + C^{(0)}_{xx} x^2 + 2C^{(0)}_{xy} xy + C^{(0)}_{yy} y^2 \\
&+ C^{(0)}_{xxx} x^3 + C^{(0)}_{yyy} y^3 + 3C^{(0)}_{xxy} x^2 y + 3C^{(0)}_{xyy} x y^2 \\
&+ C^{(0)}_{xxxx} x^4 + C^{(0)}_{yyyy} y^4 + 4C^{(0)}_{xxxy} x^3 y + 4C^{(0)}_{xyyy} x y^3 \\
&+ 6C^{(0)}_{xxyy} x^2 y^2 + C^{(2)}_{xx} (\vec{\nabla} x)^2 + C^{(2)}_{yy} (\vec{\nabla} y)^2 + 2C^{(2)}_{xy} (\vec{\nabla} x \vec{\nabla} y) + \cdots,
\end{aligned} \tag{6}$$

Here $C^{(0)}_{\alpha\beta}$ and $C^{(2)}_{\alpha\beta}$ are the zeroth and second spatial moments of the direct correlation function

$$\begin{aligned}
C^{(0)}_{\alpha,\beta} &= \int_V C_{\alpha\beta}(\vec{r_1},\vec{r_2})\mathrm{d}\vec{r_1}\mathrm{d}\vec{r_2} = \left(\frac{\partial^2 G}{\partial\xi_\alpha \partial\xi_\beta}\right)_{P,T} = \left(\frac{\partial A_\alpha}{\partial \xi_\beta}\right)_{P,T,\xi_\alpha}, \\
C^{(2)}_{\alpha,\beta} &= \frac{1}{2}\int_V C_{\alpha\beta}(\vec{r_1},\vec{r_2})(\vec{r_2}-\vec{r_1})^2 \mathrm{d}\vec{r_1}\mathrm{d}\vec{r_2}.
\end{aligned} \tag{7}$$

Thus, the value of χ^{-1}_α, i.e. the zeroth moments $C^{(0)}_{\alpha\alpha}$, specifies the coefficients in front of the squares of order parameters in the expansion (6) for the fluctuation part of the Gibbs potential.

3. Kinetic equations and theorems on bifurcation

According to (6), the equations of motion have the form of the known kinetic equations of the Landau-Ginzburg time-dependent theory

$$\begin{aligned} \dot{x}(\vec{r},t) &= -\text{ч}_x \frac{\delta \Delta G_{fl}}{\delta x(\vec{r},t)}, \\ \dot{y}(\vec{r},t) &= -\text{ч}_y \frac{\delta \Delta G_{fl}}{\delta y(\vec{r},t)}, \end{aligned} \tag{8}$$

or

$$\begin{aligned} \dot{x} &= \psi(x,y) + D_1 \nabla^2 x, \\ \dot{y} &= \theta(x,y) + D_2 \nabla^2 y, \end{aligned} \tag{9}$$

where ч_i are the Onsager coefficients, D_i are the diffusion coefficients, and ψ and θ are nonlinear functions of the order parameters. One can easily see that these kinetic equations coincide in their form with the kinetic equations of the reaction-diffusion models widely used in synergetics [2].

Next step is the analyzing of the type of singular points according to the Poincare classification and of the stability of stationary solutions with respect to small perturbations

$$\begin{aligned} \delta x &= x(\vec{r},t) - \tilde{x}(\vec{r},t), \\ \delta y &= y(\vec{r},t) - \tilde{y}(\vec{r},t), \\ \delta x_i(\vec{r},t) &= \int \sum_{\vec{k}} \delta x_i(\lambda,\vec{k}) e^{\lambda t + i\vec{k}\vec{r}} \mathrm{d}\lambda, (x,y \to x_i). \end{aligned} \tag{10}$$

The corresponding characteristic equation has the form

$$\det[\hat{U}_0 - \hat{D}k^2 - \hat{J}\lambda] = 0 \tag{11}$$

and gives the dispersion law and relates the damping coefficient λ to the wave vector k. Here

$$\hat{U}_0 = \begin{pmatrix} \frac{\partial\psi}{\partial x} & \frac{\partial\psi}{\partial y} \\ \frac{\partial\theta}{\partial x} & \frac{\partial\theta}{\partial y} \end{pmatrix}, \qquad D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}, \tag{12}$$

and J is the unit matrix. Another form of the equation (11) is

$$(2\lambda + E_1 + E_2)^2 = (E_1 - E_2)^2 + 4E_3, \tag{13}$$

where

$$\begin{aligned} E_1 &= D_1 k^2 - \frac{\partial\psi}{\partial x}, \\ E_2 &= D_2 k^2 - \frac{\partial\theta}{\partial y}, \\ E_3 &= \frac{\partial\psi}{\partial y} \cdot \frac{\partial\theta}{\partial x}. \end{aligned} \tag{14}$$

In [3] a series of statements (theorems) determining the conditions of the Hopf and Turing bifurcations were formulated and proved for the fluctuation models (9):

1. Oscillatory solutions appear if

$$\begin{vmatrix} E_1 - E_2 & 4E \\ -1 & E_1 - E_2 \end{vmatrix} < 0, \tag{15}$$

under the additional conditions $E_1 + E_2 >< 0$ the stable and unstable focus is realized, respectively.

2. For periodic solutions in the form of limit cycle, it is necessary and sufficiently if the following conditions are realized, respectively:

2.1

$$E_1 + E_2 = 0, \quad E_1 \neq E_2 \neq 0, \quad E_3 - E_1 E_2 < 0;$$

2.2

$$E_1 + E_2 = 0, \quad E_1 \neq E_2 \neq 0, \quad D_1 + D_2 = 0, \quad D_1 \neq D_2 \neq 0,$$
$$-|\hat{U}_{0j}| - [|\hat{U}_{0j}| + |\hat{U}_0|]^{1/2} < D_i k^2 < -|\hat{U}_{0j}| + [|\hat{U}_{0j}| + |\hat{U}_0|]^{1/2},$$
$$\hat{U_{01}} = \begin{pmatrix} \frac{\partial\psi}{\partial x} & \frac{\partial\psi}{\partial y} \\ 0 & 1 \end{pmatrix}, \quad \hat{U_{02}} = \begin{pmatrix} 1 & 0 \\ \frac{\partial\theta}{\partial x} & \frac{\partial\theta}{\partial y} \end{pmatrix}; \tag{16}$$

2.3

$$E_1 + E_2 = 0, \quad E_1 \neq E_2 \neq 0, \quad |\hat{U}_{01}| = |\hat{U}_{02}|,$$
$$|\hat{U}_{0j}| - [-E_3]^{1/2} < D_i k^2 < |\hat{U}_{0j}| + [-E_3]^{1/2}, \quad E_3 < 0;$$

2.4

$$E_1 + E_2 = 0, \quad E_1 \neq E_2 \neq 0, \quad D_1 = D_2, \quad [D_i k^2]^2 - |\hat{U}_0| < 0;$$

2.5

$$E_1 + E_2 = 0, \quad E_1 \neq E_2 \neq 0, \quad D_1 = 0, \quad D_2 \neq 0, \quad D_2 k^2 |\hat{U}_{01}| - |\hat{U}_0| < 0;$$

2.6

$$E_1 = E_2 = 0, \quad E_3 < 0.$$

Omitting some details, it is worthy to stress the main result which follows from (16): the ordered structures appear inside the boundary of stability under the spinodal curve. It means that a system which is thermodynamically unstable in this region becomes stable due to the formation of the spatial, temporal or spatio-temporal structures.

4. Singular points in fluctuation models of self-organization

We shall now investigate the concrete fluctuation models with two order parameters.

The first model is the fluctuation model similar to well-known kinetic "brusselator" model [1,2]:

$$\begin{aligned} \dot{x} &= A - Cx + By - xy^2 + D_x \frac{\partial^2 x}{\partial \rho^2}, \\ \dot{y} &= Bx - x^2 y + D_y \frac{\partial^2 y}{\partial \rho^2}. \end{aligned} \tag{17}$$

The difference between the "brusselator" model and model (17) is in the form of the nonlinear cubic term: the "brusselator" model produces the term x^2y on the motion equation for x i.e. the same term as in the motion equation for y.

One can obtain the following stationary states for the fluctuation model (17)

$$\tilde{x}_1 = \frac{A}{C}, \quad \tilde{y}_1 = \frac{BC}{A}; \quad \tilde{x}_2 = 0, \quad \tilde{y}_2 = -\frac{A}{B} \tag{18}$$

and investigate its stability considering the corresponding system of differential equations

$$\delta\dot{\vec{r}} = \hat{M}\delta\vec{r} + \hat{D}\nabla^2\delta\vec{r}, \tag{19}$$

where

$$\delta\dot{\vec{r}} = \begin{pmatrix} \delta x \\ \delta y \end{pmatrix}, \quad \hat{M} = \begin{pmatrix} -C - \tilde{y} & B - 2\tilde{x}\tilde{y} \\ B - 2\tilde{x}\tilde{y} & -\tilde{x}^2 \end{pmatrix}, \quad \hat{D} = \begin{pmatrix} D_x & 0 \\ 0 & D_y \end{pmatrix}. \tag{20}$$

Then by taking into account the characteristic equation

$$\begin{aligned} &\det(\hat{M} - \hat{D}k^2 - \lambda\hat{I}] = 0, \quad \lambda^2 - (\mathrm{Sp}\ \hat{M})\lambda + \Delta = 0, \\ &\mathrm{Sp}\ \hat{M} = T_1 + T_2, \quad \Delta = T_1T_2 - B^2, \\ &T_1 = -\left(1 + \frac{CB^2}{A^2}\right)C + D_xk^2, \quad T_2 = -\left(\frac{A}{C}\right)^2 + D_yk^2 \end{aligned} \tag{21}$$

one can obtain the necessary conditions of the Turing bifurcation

$$D_xD_yk^2 - [D_x\tilde{x}^2 + D_y(\tilde{y}^2 + C)]k^2 + \tilde{x}^2(\tilde{y}^2 + C) - (2\tilde{x}\tilde{y} - B)^2 = 0. \tag{22}$$

The second fluctuation model is the model similar to the Landau-Ginzburg model with two order parameters and the forth-order interaction

$$\mathcal{H}_{int}[x, y] = a_4 \int x^2y^2\mathrm{d}\vec{r}. \tag{23}$$

Corresponding kinetic equations

$$\begin{aligned} \dot{x} &= Ax + C_1x^3 + Q_1xy^2 + D_x\frac{\partial^2 x}{\partial\rho^2}, \\ \dot{y} &= By + C_2y^3 + Q_2x^2y + D_y\frac{\partial^2 y}{\partial\rho^2}, \end{aligned} \tag{24}$$

have a number of stationary states

$$\begin{aligned} \tilde{x}_1 &= \tilde{y}_1 = 0; \quad \tilde{x}_2 = (-A/C_1)^{1/2}; \quad \tilde{y}_2 = 0; \\ \tilde{x}_3 &= 0, \quad \tilde{y}_3 = (-B/C_2)^{1/2}; \\ \tilde{x}_4 &= [(A/C_1) - Q_1(AQ_2 - BC_1)/C_2(C_1C_2 - Q_1Q_2)]^{1/2}, \\ \tilde{y}_4 &= [(AQ_2 - BC_1)/(C_1C_2 - Q_1Q_2)]^{1/2}. \end{aligned} \tag{25}$$

It follows from a characteristic equation

$$\begin{aligned}
&\lambda^2 - (\mathrm{Sp}\ \hat{M})\lambda + \Delta = 0,\\
&\mathrm{Sp}\ \hat{M} = \kappa_1 + \kappa_2, \quad \Delta = |\hat{M}| = \kappa_1\kappa_2 - \kappa_3,\\
&\kappa_1 = A - 3C_1\tilde{x}^2 + Q_1\tilde{y}^2 + D_x k^2,\\
&\kappa_2 = B + C_2\tilde{y}^2 + Q_2\tilde{x}^2 + D_y k^2,\\
&\kappa_3 = 4Q_1Q_2\tilde{x}^2\tilde{y}^2
\end{aligned} \tag{26}$$

that conditions of the Hopf bifurcation

$$Q_1Q_2 < 0, \quad \text{ч}_1\text{ч}_2 < 0 \tag{27}$$

realize only on the non-thermodynamic branch of states.

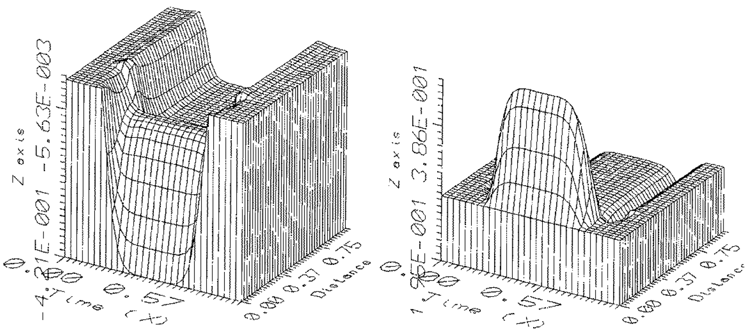

Figure 1.

These results are confirmed by the numerical calculations performed in [8]. Namely, singular points exist under the following conditions $\text{ч}_1\text{ч}_2 < 0$, i.e. on the non-thermodynamic branch of states in which the change of the coefficients A_i and (or) D_i takes place. Computer simulations of the ordered structure formation give three different types of structures: (a) so called "contrast" structures with many sharp peaks (figure 1), (b) quasi-periodic structures slowly decaying in space and time (figure 2), and (c) soliton-like structures exhibiting a self-organization process within the range of parameters predicted theoretically (figure 3).

5. Fluctuation effects in stationary states of open systems

According to the Prigogine's definition of the stationary states of open systems the total entropy remains constant due to the complete compensation of the entropy increase ΔS_i connecting with the dissipative processes inside a system and the entropy flow ΔS_e from this system outside:

$$\Delta S = \Delta S_i + \Delta S_e = 0. \tag{28}$$

Here

$$\Delta S_i = \int_V \sigma dV \mathrm{d}T > 0, \tag{29}$$

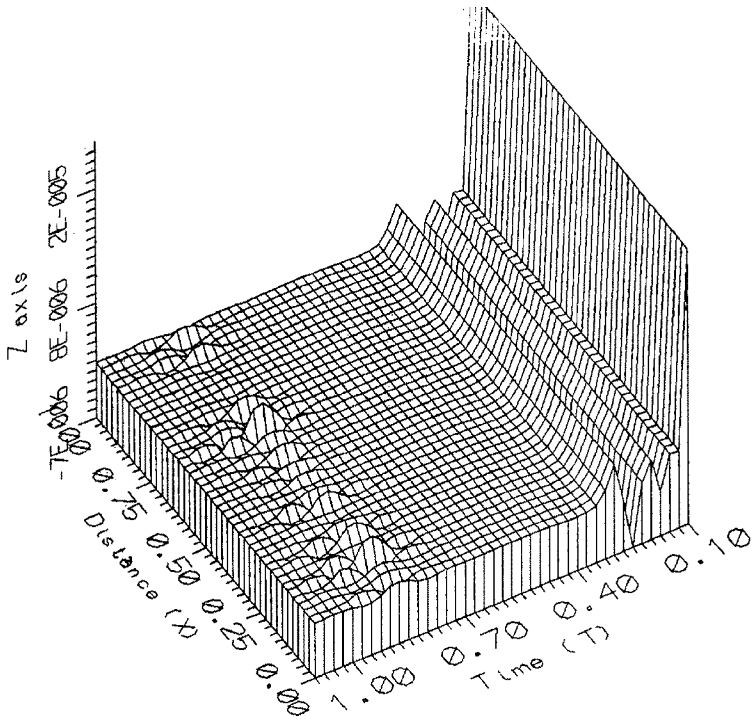

Figure 2.

$$\Delta S_e = -\int_\Omega J_s d\Omega \mathrm{d}t < 0. \tag{30}$$

Let us generalize a definition of stationary states given by Prigogine on the cases of arbitrary open systems with ordered structures. The entropy change consists of two contributions it the processes of the ordered structures formation are taking into account:

1) positive entropy changes $\Delta S_i^{(d)}$ caused by of dissipative processes inside a system, 2) negative entropy changes $\Delta S_i^{(j)}$ connecting with the ordered structures formation, i.e.

$$\Delta S_i = \Delta S_i^{(d)} + \Delta S_i^{(s)}. \tag{31}$$

In these cases stationary states can be guaranteed as follows: a) if $\Delta S_i^{(d)} > \Delta S_i^{(s)}$, then $\delta S_i > 0$ and in order to fulfil the condition of the entropy conservation $\Delta S = 0$ the following inequality similar to the Prigogine condition of stationarity has to take place:

$$\Delta S_e = -|\Delta S_i^{(d)} - \Delta S_i^{(s)}| < 0; \tag{32}$$

2) if $\Delta S_i^{(d)} < |\Delta S_i^{(s)}|$, then $\Delta S_i < 0$ and in this case an entropy flow from outside $\Delta S_e > 0$ becomes necessary, i.e.

$$\Delta S_e = |\Delta S_i^{(s)} - \Delta S_i^{(d)}| > 0; \tag{33}$$

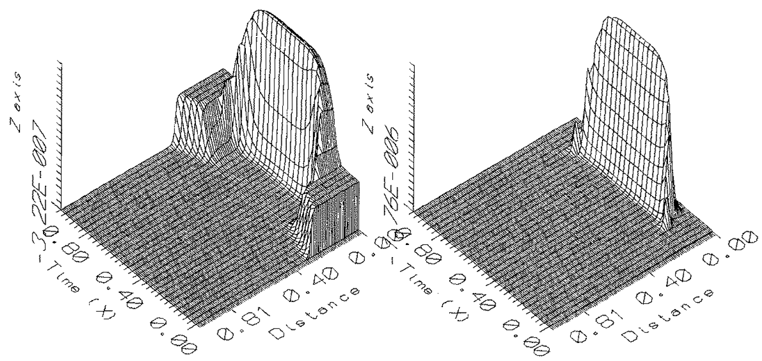

Figure 3.

The last inequality gives a generalization of the Prigogine's definition of the stationary states of open systems.

It is important to stress that fluctuation effects must be taken into account in treating the formation of the spatial, temporal, and spatio-temporal structures near the bifurcation points. Therefore, the formula for the full entropy change reads as follows

$$\Delta S = \Delta S_i^{(d)} + \Delta S_i^{(s)} + \Delta S_e + \Delta S_{fl}. \tag{34}$$

It is seen from (34) that under the conditions of stationarity (32) or (33) the last term describing fluctuation effects gives the only contribution to ΔS_{fl} . For the fluctuational part of the free energy one has respectively:

$$\Delta F_{fl} = -T\Delta S_{fl}. \tag{35}$$

It gives a necessary grounding to use the fluctuation Hamiltonians of the Landau-Ginzburg form for investigation of the ordered structures formation in stationary states of open systems.

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References

[1] Nikolis G., Prigogine I. Self-organization in non-equilibrium systems. Moscow, Mir, 1979 (in Russian).

[2] Haken H. Synergetics. Moscow, Mir, 1980 (in Russian).

[3] Chalyi A.V., Tsehmister Ya.V. Fluctuation models of the self-organization processes. Kiev, Ukrainian Medical University, comment, 1994 (in Russian).

[4] Patashinskii A.Z., Pokrovskii V.L. Fluctuation theory of phase transitions. Moscow, Nauka, 1982 (in Russian).

[5] Wilson K.G., Kogut J. The renormalization group and ϵ-expansion. Moscow, Mir, 1975 (in Russian).

[6] Yukhnovskii I.R. Phase transitions of the second order. Collective variables method. Kiev, Naukova Dumka, 1985 (in Russian).
[7] Chalyi A.V. Non-homogeneous liquids near the critical point and the boundary of stability. // Sov. Sci. Rev. A. Phys., 1992, vol. 16, p. 1-103.
[8] Chalyi A.V., Khiznyak D.A., Tsehmister Ya.V. Ordered structures in model with forth-order interaction. // Ukr. Fiz. Zhurn. (in press).

БІФУККАЦІЇ ХОПФА ТА ТЮРІНГА В ФЛУКТУАЦІЙНІЙ МОДЕЛІ САМООРГАНІЗАЦІЇ

А.В.Чалий, Д.А.Хижняк, Я.В.Цехмістер

Пропонується флуктуаційна модель самоорганізації з врахуванням флуктуаційного гамільтоніана. Досліджуються умови Хопфової та Тюрінгової біфуркацій, особлива увага звертається на граничний цикл та фокусні розв'язки. Обговорюється принципова можливість утворення впорядкованих структур у флуктуаційній моделі самоорганізації у стаціонарних станах.