METHODOLOGICAL NOTES

PACS numbers: 05.45. - a, 47.54. - r, 82.40.Bj, 82.40.Ck

Turing patterns and Newell-Whitehead-Segel amplitude equation

E P Zemskov

DOI: 10.3367/UFNe.0184.201410j.1149

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Abstract. Two-dimensional (2D) reaction—diffusion type systems with linear and nonlinear diffusion terms are examined for their behavior when a Turing instability emerges and stationary spatial patterns form. It is shown that a 2D nonlinear analysis for striped patterns leads to the Newell—Whitehead—Segel amplitude equation in which the contribution from spatial derivatives depends only on the linearized diffusion term of the original model. In the absence of this contribution, i.e., for the normal forms, standard methods are used to calculate the coefficients of the equation.

1. Introduction

Pattern formation in nonlinear reaction—diffusion systems is encountered in many branches of physics, chemistry, biology, and other sciences [1–6]. The classical approach to identifying the mechanism of pattern formation was proposed by Turing [7] in 1952. Turing's idea was that pattern formation hinges on coupling between the diffusion and reaction kinetics. In the framework of this approach, the analysis of system stability allows one to find the values of model parameters whereat a pattern-forming instability develops. The analysis of system stability also includes a weakly nonlinear treatment, whereby the original mathematical problem is reduced to the so-called amplitude equations which, in their form, represent the real parts of the Ginzburg—Landau equations.

The subject of this work is a reaction—diffusion system. The result of its weakly nonlinear analysis is the amplitude equation on the complex-valued amplitude W, with coefficients dependent on the parameters of the original reaction—diffusion model. Earlier [8–10], we derived amplitude equations for systems with a crossing [8] and nonlinear [9, 10] diffusion, being limited to one-dimensional models alone. The goal of this study is to demonstrate how the weakly

E P Zemskov Department of Continuous Mechanics, Dorodnitsyn Computing Centre, Russian Academy of Sciences, ul. Vavilova 40, 119333 Moscow, Russian Federation E-mail: zemskov@ccas.ru

Received 25 December 2013, revised 11 February 2014 *Uspekhi Fizicheskikh Nauk* **184** (10) 1149–1151 (2014) DOI: 10.3367/UFNr.0184.201410j.1149 Translated by S D Danilov; edited by A Radzig

nonlinear approach can be applied in a *two-dimensional* case to the derivation of the Newell–Whitehead–Segel amplitude equation which was obtained in monograph [3] from symmetry considerations.

2. Stripe patterns and the Newell-Whitehead-Segel equation

In this section, we consider a reaction—diffusion system at the onset of the Turing instability that leads to the build up of the stationary spatial stripe pattern in those cases when the diffusion coefficient is constant (classical linear diffusion) or depends on the system components (nonlinear diffusion).

2.1 Linear diffusion

The basic system is described by the following vector equation:

$$\frac{\partial \mathbf{Z}}{\partial t} = \mathbf{F}(\mathbf{Z}) + \nabla(\mathbf{D}\nabla\mathbf{Z}), \qquad \nabla = \left(\frac{\partial}{\partial r_x}, \frac{\partial}{\partial r_y}\right), \tag{2.1}$$

where F(Z) is the vector reaction function, Z is the n-dimensional vector with the components u, v, \ldots , and D denotes the diagonal matrix of diffusion coefficients, which are assumed to be constant.

A perturbation written down as the deviation $\mathbf{X} = \mathbf{Z} - \mathbf{Z}_0$ from the equilibrium position \mathbf{Z}_0 satisfying the equation $\mathbf{F}(\mathbf{Z}_0) = 0$ defines the expansion of Eqn (2.1) in a series in \mathbf{X} as follows:

$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{L}\mathbf{X} + \mathbf{M}\mathbf{X}\mathbf{X} + \mathbf{N}\mathbf{X}\mathbf{X}\mathbf{X} + \dots, \tag{2.2}$$

with the linear operator $\mathbf{L} = \mathbf{J} + \mathbf{D}\Delta$, where \mathbf{J} is the Jacobian, $\Delta = \partial^2/\partial r_x^2 + \partial^2/\partial r_y^2$ is the two-dimensional Laplace operator, and the quadratic (Hessian) **MXX** and cubic **NXXX** forms are written in the standard way [11].

By introducing new variables for time (T) and space (R_x, R_y) , the respective derivatives are modified as [12]

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial T}, \qquad (2.3)$$

$$\frac{\partial}{\partial r_x} \to \frac{\partial}{\partial r} + \mu^{1/2} \frac{\partial}{\partial R_x} , \qquad \frac{\partial}{\partial r_y} \to \mu^{1/4} \frac{\partial}{\partial R_y} . \tag{2.4}$$

In deriving formula (2.4) we kept in mind that $\partial \mathbf{X}/\partial r_y = 0$ [12]. We also introduced the notation $r_x \equiv r$ and the measure $\mu = (\phi - \phi_{\rm crit})/\phi_{\rm crit}$ which characterizes the deviation of a governing parameter ϕ from its critical value $\phi_{\rm crit}$ whereat the system loses its stability. We also assume that the following standard expansions [11] hold for the operators $\mathbf{H} = \{\mathbf{J}, \mathbf{M}, \mathbf{N}\}$: $\mathbf{X} = \mu^{1/2}\mathbf{X}_1 + \mu\mathbf{X}_2 + \mu^{3/2}\mathbf{X}_3 + \dots$ and $\mathbf{H} = \mathbf{H}_0 + \mu\mathbf{H}_1 + \mu^2\mathbf{H}_2 + \dots$

Inserting these expansions into the series (2.2) results in a system of equations which correspond to combinations of terms with equal powers of μ . For $\mu^{1/2}$, μ , and $\mu^{3/2}$, we get equations $(\partial_t - \mathbf{L}_0)\mathbf{X}_l = \mathbf{B}_l$ with l = 1, 2, 3, where $\mathbf{L}_0 = \mathbf{L}(\mathbf{J} \to \mathbf{J}_0)$, \mathbf{J}_0 is the zeroth-order Jacobian, $\mathbf{J}_0 = \mathbf{J}|_{\mu=0}$, and $\partial_t \equiv \partial/\partial t$. The right-hand sides of these equations are written as $\mathbf{B}_1 = 0$, namely

$$\mathbf{B}_{2} = 2\mathbf{D} \frac{\partial^{2} \mathbf{X}_{1}}{\partial r \partial R_{x}} + \mathbf{D} \frac{\partial^{2} \mathbf{X}_{1}}{\partial R_{x}^{2}} + \mathbf{M}_{0} \mathbf{X}_{1} \mathbf{X}_{1}, \qquad (2.5)$$

$$\mathbf{B}_{3} = -\frac{\partial \mathbf{X}_{1}}{\partial T} + \mathbf{J}_{1}\mathbf{X}_{1} + \mathbf{D} \frac{\partial^{2}\mathbf{X}_{1}}{\partial R_{x}^{2}} + 2\mathbf{D} \frac{\partial^{2}\mathbf{X}_{2}}{\partial r \partial R_{x}} + \mathbf{D} \frac{\partial^{2}\mathbf{X}_{2}}{\partial R_{y}^{2}} + 2\mathbf{M}_{0}\mathbf{X}_{1}\mathbf{X}_{2} + \mathbf{N}_{0}\mathbf{X}_{1}\mathbf{X}_{1}\mathbf{X}_{1}.$$
(2.6)

Here, the notation $J_1 = (dJ/d\mu)_{\mu=0}$ was introduced. In a two-component system, one has

$$\frac{\partial u}{\partial t} = F_1(u, v) + D_{11} \Delta u, \qquad (2.7)$$

$$\frac{\partial v}{\partial t} = F_2(u, v) + D_{22} \Delta v. \tag{2.8}$$

The right U (column) and left U^* (row) eigenvectors of the matrix L_0 take the form

$$\mathbf{U} = \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \exp(ik_{c}r), \quad \mathbf{U}^{*} = \frac{1}{1 + \alpha\beta} (1, \beta) \exp(ik_{c}r), \quad (2.9)$$

where k_c is the critical value of the wave vector at the onset of the Turing instability, and

$$\alpha = -\frac{L_{11}^0}{L_{12}^0} = -\frac{L_{21}^0}{L_{22}^0}, \quad \beta = -\frac{L_{11}^0}{L_{21}^0} = -\frac{L_{12}^0}{L_{22}^0}.$$
 (2.10)

Here, $L_{mn}^0 = J_{mn}^0 - k_c^2 D_{nm} \delta_{mn}$, m, n = 1, 2, and J_{mn}^0 are the elements of Jacobian \mathbf{J}_0 , $\delta_{mn} = 1$ at m = n and $\delta_{mn} = 0$ for $m \neq n$.

For stripe patterns, the perturbations of the first and second orders, X_1 and X_2 , are written down as [1, 13]

$$\mathbf{X}_{1} = \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \left[W \exp\left(\mathrm{i}k_{\mathrm{c}}r\right) + \bar{W} \exp\left(-\mathrm{i}k_{\mathrm{c}}r\right) \right], \tag{2.11}$$

$$\mathbf{X}_{2} = \begin{pmatrix} a_{0} \\ b_{0} \end{pmatrix} + \begin{pmatrix} a_{1} \\ b_{1} \end{pmatrix} \exp\left(\mathrm{i}k_{\mathrm{c}}r\right) + \begin{pmatrix} a_{2} \\ b_{2} \end{pmatrix} \exp\left(2\mathrm{i}k_{\mathrm{c}}r\right) + \mathrm{c.c.}, \tag{2.12}$$

where a_s , b_s , s = 0, 1, 2 are the coefficients depending on the model parameters and the amplitude W, and c.c. implies complex conjugation. The expressions for perturbations (2.11) and (2.12) are substituted into the two-component version of equations $(\partial_t - \mathbf{L}_0)\mathbf{X}_l = \mathbf{B}_l$. In this case, from the second-order (l = 2) equation it follows that the coefficients a_1 and b_1 are coupled by the relationship

$$\alpha a_1 - b_1 = \frac{D_{11}}{J_{12}^0} \left(2ik_c \frac{\partial}{\partial R_x} + \frac{\partial^2}{\partial R_y^2} \right) W, \tag{2.13}$$

which leads to the cubic amplitude equation: 1

$$(1+\alpha\beta)\frac{\partial W}{\partial T} = \eta W + g|W|^2 W + \frac{D_{11}^2}{\alpha J_{12}^0} \left(2ik_c \frac{\partial}{\partial R_x} + \frac{\partial^2}{\partial R_y^2}\right)^2 W,$$
(2.14)

called the Newell-Whitehead-Segel equation [14, 15]. The difference in terms with spatial x- and y-derivatives in this equation is the consequence of the chosen reference frame in which the patterns (stripes) are oriented perpendicular to the abscissa [3]. Equation (2.14) is of a general form for system (2.7), (2.8); the behavior details stemming from the reaction functions $F_{1,2}$ depend on the g and η coefficients, which can be computed in the standard way [1, 13]. The expressions for the coefficients g and η contain the critical values of the wave vector k_c and governing parameter ϕ_{crit} (in the Jacobian \mathbf{J}_0); the sign of g defines the type of instability: a supercritical bifurcation occurs for a negative one, and a subcritical bifurcation for a positive one. The critical values of parameters can be found from a linear stability analysis, which also allows one to identify the domain in the parameter space where patterns may form (as, for example, was done in Ref. [10]).

2.2 Nonlinear diffusion

In some cases [2, 4, 16], the diffusion coefficient is not constant but depends on concentrations of reacting substances [4, 17]. Since the Turing instability is diffusion-based, such systems call for a separate treatment.

In the simplest case of nonlinear diffusion [17], when the matrix of diffusion coefficients can be written down as $\mathbf{D} + \mathbf{Q}\mathbf{Z}$ [9], with diagonal \mathbf{D} and \mathbf{Q} matrices being independent of \mathbf{Z} , i.e., constant, the system is described by the following equation

$$\frac{\partial \mathbf{Z}}{\partial t} = \mathbf{F}(\mathbf{Z}) + \nabla [(\mathbf{D} + \mathbf{Q}\mathbf{Z})\nabla \mathbf{Z}], \qquad (2.15)$$

and expansion (2.2) takes the form

$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{L}\mathbf{X} + \mathbf{M}\mathbf{X}\mathbf{X} + \mathbf{N}\mathbf{X}\mathbf{X}\mathbf{X} + \mathbf{Q}\nabla(\mathbf{X}\nabla\mathbf{X}) + \dots, \quad (2.16)$$

where $\mathbf{L} = \mathbf{J} + \hat{\mathbf{D}}\Delta$ and $\hat{\mathbf{D}} = \mathbf{D} + \mathbf{Q}\mathbf{Z}_0$. Then, expressions (2.5) and (2.6) are transformed into

$$\mathbf{B}_{2} = 2\hat{\mathbf{D}} \frac{\partial^{2} \mathbf{X}_{1}}{\partial r \partial R_{x}} + \hat{\mathbf{D}} \frac{\partial^{2} \mathbf{X}_{1}}{\partial R_{y}^{2}} + \mathbf{M}_{0} \mathbf{X}_{1} \mathbf{X}_{1}$$

$$+ \mathbf{Q} \left(\frac{\partial \mathbf{X}_{1}}{\partial r} \right)^{2} + \mathbf{Q} \mathbf{X}_{1} \frac{\partial^{2} \mathbf{X}_{1}}{\partial r^{2}} , \qquad (2.17)$$

$$\mathbf{B}_{3} = -\frac{\partial \mathbf{X}_{1}}{\partial T} + \mathbf{J}_{1} \mathbf{X}_{1} + \hat{\mathbf{D}} \frac{\partial^{2} \mathbf{X}_{1}}{\partial R_{x}^{2}} + 2\hat{\mathbf{D}} \frac{\partial^{2} \mathbf{X}_{2}}{\partial r \partial R_{x}} + \hat{\mathbf{D}} \frac{\partial^{2} \mathbf{X}_{2}}{\partial R_{y}^{2}}$$

$$+ 2\mathbf{M}_{0} \mathbf{X}_{1} \mathbf{X}_{2} + \mathbf{N}_{0} \mathbf{X}_{1} \mathbf{X}_{1} \mathbf{X}_{1} + 2\mathbf{Q} \frac{\partial \mathbf{X}_{1}}{\partial r} \frac{\partial \mathbf{X}_{2}}{\partial r}$$

$$+ 2\mathbf{Q} \frac{\partial \mathbf{X}_{1}}{\partial r} \frac{\partial \mathbf{X}_{1}}{\partial R_{x}} + \mathbf{Q} \left(\frac{\partial \mathbf{X}_{1}}{\partial R_{y}} \right)^{2} + \mathbf{Q} \mathbf{X}_{1} \frac{\partial^{2} \mathbf{X}_{2}}{\partial r^{2}}$$

$$+ \mathbf{Q} \mathbf{X}_{2} \frac{\partial^{2} \mathbf{X}_{1}}{\partial r^{2}} + 2\mathbf{Q} \mathbf{X}_{1} \frac{\partial^{2} \mathbf{X}_{1}}{\partial r \partial R_{x}} + \mathbf{Q} \mathbf{X}_{1} \frac{\partial^{2} \mathbf{X}_{1}}{\partial R_{y}^{2}} , \qquad (2.18)$$

 $^{^1}$ The cubic amplitude equation represents the solvability condition for the third order of expansion [11], $\mathbf{U}^*\mathbf{B}_3^1=0$, where \mathbf{U}^* is the left eigenvector of the matrix \mathbf{L}_0 , and the superscript 1 on \mathbf{B}_3 points out that only the contributions with the first harmonics are retained.

and in the case of a two-component system described by equations

$$\frac{\partial u}{\partial t} = F_1(u, v) + D_{11}\Delta u + Q_{11}\nabla(u\nabla u) ,$$

$$\frac{\partial v}{\partial t} = F_2(u, v) + D_{22}\Delta v + Q_{22}\nabla(v\nabla v) ;$$
(2.19)

the procedure discussed in Section 2.1 gives a result that coincides with Eqn (2.14) upon substitution $D_{11} \rightarrow \hat{D}_{11}$. Here, $\hat{D}_{11} = D_{11} + Q_{11}u_0$ and $\hat{D}_{22} = D_{22} + Q_{22}v_0$, where u_0 and v_0 satisfy equalities $F_1(u_0, v_0) = F_2(u_0, v_0) = 0$. Expressions for computing the coefficients η and g can be found in Ref. [9].

3. Conclusion

The Newell–Whitehead–Segel equation presented in this paper was obtained with the help of the standard nonlinear analysis, which emphasizes its general character as the method to analyze instabilities and pattern formation in reaction–diffusion systems. The attention to a system with nonlinear diffusion is motivated by the use of similar systems in current research [17, 18] on pattern formation. Notice that the influence of nonlinear diffusion contributes to making the emergence of Turing patterns easier than in classical linear diffusion [18], which may have practical implications for conducting experimental research.

Acknowledgments

The author is indebted to V K Vanag for the introduction to the subject. This study was supported by the Russian Foundation for Basic Research (grant No. 13-01-00333A).

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