Localized structures in 3KRD system

Localized structures in reaction-diffusion systems

Svetlana Gurevich

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Outline

Introduction

- Reaction-Diffusion Systems
- Experimental system in question
- Possible Model Systems

Localized structures in 3KRD system

- Phenomenological 3KRD model
- Stationary Turing structures
- Localized structures and their stability

Reaction-Diffusion Systems

 $\partial_t \mathbf{u} = \mathbf{D} \nabla^2 \mathbf{u} + \mathbf{R}(\mathbf{u})$

- $\mathbf{u} = \mathbf{u}(\mathbf{r}, \mathbf{t}) = (u_1, u_2, \dots, u_n)^T$ -a vector of concentration variables, $\mathbf{r} \subset \mathbb{R}^m$, m = 1, 2, 3;
- ∇^2 the Laplace operator;
- $\mathbf{R}(\cdot)$ a local reaction kinetics;
- D- a diagonal diffusion coefficient matrix;

1937:

• R. Fisher The wave of advance of advantageous genes;

• A. N. Kolmogorov, I. G. Petrovsky,

N. Piskunoff A study of the equation of dissusion with increase in the quantity of matter, and its application to a bilological problem;

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• Y. B. Zeldovich, D. A. Frank-Kamenetsky A theory of thermal propagation of flame;

$$\partial_t u = d^2 u_{xx} + u(1-u)(u-\alpha), \ \alpha \in (0,1)$$

1952:

• A. M. Turing The chemical basis of morphogenesis

$$\begin{split} \partial_t u &= D_u \nabla^2 u + f(u,v), \\ \partial_t v &= D_v \nabla^2 v + g(u,v) \end{split}$$

1952:

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$$\begin{split} \partial_t u &= D_u \nabla^2 u + f(u,v), \\ \partial_t v &= D_v \nabla^2 v + g(u,v) \end{split}$$

Belousov-Zhabotinsky reaction, other autocatalytic and oscillatory chemical reactions, different musters on animal's skin, nerve pulse transmission, bacteria growth processes, structures, observed in semiconductors or gas-discharge systems,

Reaction-Diffusion Systems: 3K and more

$$\partial_t u_\alpha = D_\alpha \nabla^2 u_\alpha + R_\alpha(u)$$

a model of blood clotting, population dynamics, ecology, photosensitive Belousov-Zhabotinsky reaction ,glycolysis, a model of CO oxidation on Pt(110), a model of Dictyostelium amoebae, patterns arising in gas-discharge system.....



Localized structures in 3KRD system

Experimental set-up

Planar dc gas-discharge system with high-ohmic electrode:



- $d = 0.1 2 \,\mathrm{mm};$
- Gases: N₂, He, Ar;
- $p \approx 30 400 \, \text{hPa};$
- Semiconductor: GaAs
- $d_c = 0.5 1.5 \,\mathrm{mm};$
- $\rho_{\rm SC} \approx 10^7 10^8 \,\Omega \,\cdot {\rm cm};$
- $U_0 = 1 5 \,\mathrm{kV}$

Examples of observed patterns

stripes

hexagons



targets

spots



chains









Localized structures in 3KRD system

Possible Model Systems

The current patterns are 3D objects, evolving on the time scale of $1\,\text{ms}-1\,\text{s}$



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- fluid based models, (e.g., drift-diffusion): $\tau_e \approx 10 \, \mathrm{ns}$;
- particle based models (PIC): $\approx 10^{-12}$ s;



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direct numerical simulation is very time-consuming or even impossible

an appropriate reduced discharge models should be developed or qualitative models should be used

Localized structures in 3KRD system

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Localized structures in 3KRD system

- Phenomenological 3KRD model
- Stationary Turing structures
- Localized structures and their stability

Phenomenological three-component RD model

$$\partial_t u = D_u \Delta u + f(u) - \kappa_3 v + \kappa_1 - \frac{\kappa_2}{\|\Omega\|} \int_{\Omega} u dr,$$

$$\tau \partial_t v = D_v \Delta v + u - v;$$

 $u = u(\mathbf{r}, t)$ -is related to the avalanche multiplication of charged carriers in the discharge gap;

 $v = v(\mathbf{r}, t)$ -the voltage drop at the semiconductor plate; κ_1 - is connected with the normalized applied voltage; κ_2 - describes a normalized internal resistance of the voltage source.

Localized structures in 3KRD system

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Phenomenological three-component RD model

$$\partial_t u = D_u \Delta u + f(u) - \kappa_3 v - \kappa_4 w + \kappa_1 - \frac{\kappa_2}{\|\Omega\|} \int_{\Omega} u dr,$$

$$\tau \partial_t v = D_v \Delta v + u - v,$$

$$\theta \partial_t w = D_w \Delta w + u - w;$$

Localized structures in 3KRD system

Phenomenological three-component RD model

$$\partial_t u = D_u \Delta u + f(u) - \kappa_3 v - \kappa_4 w + \kappa_1,$$

$$\tau \partial_t v = D_v \Delta v + u - v,$$

$$\theta \partial_t w = D_w \Delta w + u - w;$$

 $u = u(\mathbf{r}, t), v = v(\mathbf{r}, t), w = w(\mathbf{r}, t), \mathbf{r} \subset \mathbb{R}^2, f(u) = \lambda u - u^3, D_u, D_v, D_w, \lambda, \tau, \theta, \kappa_3, \kappa_4 \ge 0$

Localized structures in 3KRD system

Turing instability

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The idea (Turing, 1952):
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- The homogeneous solution of the system is stable in absence of diffusion;
- A difference in diffusion constants of components could be enough to destabilize the homogeneous solution;
- Another control parameter can be used (in our case we choose κ₁ as the control parameter)

Localized structures in 3KRD system

Stationary Turing patterns





Localized structures in 3KRD system

Stationary solutions



Localized structures in 3KRD system

Linear stability analysis

• The system in general form: $\partial_t \mathbf{u} = \mathfrak{L} \mathbf{u}$;

Localized structures in 3KRD system

Linear stability analysis

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- Equation for perturbation $\widetilde{\mathbf{u}} = \mathbf{u} \mathbf{u_s}$:

$$\partial_t \widetilde{\mathbf{u}} = \mathfrak{L}'(\mathbf{u}_s) \widetilde{\mathbf{u}} + \frac{1}{2!} \mathfrak{L}''(\mathbf{u}_s) \widetilde{\mathbf{u}} \widetilde{\mathbf{u}} + \frac{1}{3!} \mathfrak{L}'''(\mathbf{u}_s) \widetilde{\mathbf{u}} \widetilde{\mathbf{u}} \widetilde{\mathbf{u}} + \cdots,$$

Localized structures in 3KRD system

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Localized structures in 3KRD system

Linear stability analysis

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- Linearized system: $\partial_t \widetilde{\mathbf{u}} = \mathfrak{L}'(\mathbf{u_s})\widetilde{\mathbf{u}}$;
- Eigenvalue problem: $\mathfrak{L}'(\mathbf{u}_s)\mathcal{F} = \lambda \mathcal{F};$

Localized structures in 3KRD system

Linear stability analysis

• Neutral stability: $\lambda = 0$, $\mathcal{G}_{\mathbf{r}} = \partial \mathbf{u}_{\mathbf{s}} / \partial \mathbf{r}$, r = (x, y);

Localized structures in 3KRD system

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$$\mathbf{u_s}(\mathbf{r} + \boldsymbol{\epsilon}) = \mathbf{u_s}(\mathbf{r}) + \boldsymbol{\epsilon} \frac{\partial \mathbf{u_s}}{\partial \mathbf{r}} + O(\boldsymbol{\epsilon}^2).$$

Localized structures in 3KRD system

Linear stability analysis

• Neutral stability: $\lambda = 0$, $\mathcal{G}_{\mathbf{r}} = \partial \mathbf{u}_{\mathbf{s}} / \partial \mathbf{r}$, r = (x, y);

$$\mathbf{u_s}(\mathbf{r}+\epsilon) = \mathbf{u_s}(\mathbf{r}) + \epsilon \frac{\partial \mathbf{u_s}}{\partial \mathbf{r}} + O(\epsilon^2).$$

• $\widetilde{\mathbf{u}} \sim \widetilde{\mathbf{u}}_{\mathbf{n}} e^{in\phi}$:

$$\lambda_n \widetilde{\mathbf{u}}_n = \mathfrak{L}'_p \widetilde{\mathbf{u}}_n,$$



Localized structures in 3KRD system







Localized structures in 3KRD system

Properties of the operator $\mathfrak{L}'(\mathbf{u}_s)$

$$\mathcal{L}'(\mathbf{u_s}) = \begin{pmatrix} D_u \triangle + \lambda - 3\bar{u}^2 & -\kappa_3 & -\kappa_4 \\ \frac{1}{\tau} & \frac{D_v \triangle - 1}{\tau} & 0 \\ \frac{1}{\theta} & 0 & \frac{D_w \triangle - 1}{\theta} \end{pmatrix}$$
$$\mathcal{L}'(\mathbf{u_s}) \neq \mathcal{L}'^{\dagger}(\mathbf{u_s})$$

Localized structures in 3KRD system

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$$\begin{split} & \mathcal{L}'(\mathbf{u_s}) \neq \mathcal{L}'^{\dagger}(\mathbf{u_s}) \\ & \mathcal{L}'(\mathbf{u_s}) = ML(\mathbf{u_s}), \end{split}$$

where

$$M = M^{\dagger} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/\kappa_3 \tau & 0 \\ 0 & 0 & -1/\kappa_4 \theta \end{pmatrix},$$

and

$$L = L^{\dagger} = \begin{pmatrix} D_u \triangle + \lambda - 3u_s^2 & -\kappa_3 & -\kappa_4 \\ -\kappa_3 & -\kappa_3 D_v \triangle + \kappa_3 & 0 \\ -\kappa_4 & 0 & -\kappa_4 D_w \triangle + \kappa_4 \end{pmatrix}.$$

Localized structures in 3KRD system

Properties of the operator $\mathfrak{L}'(\mathbf{u}_s)$

• Two eigenvalue problems:

$$\begin{split} \mathfrak{L}'(\mathbf{u}_{\mathbf{s}})\mathcal{F} &= \lambda \mathcal{F}, \qquad \mathfrak{L}'^{\dagger}(\mathbf{u}_{\mathbf{s}})\mathcal{F}^{*} = \bar{\lambda} \mathcal{F}^{*}, \\ \mathfrak{L}'(\mathbf{u}_{\mathbf{s}})\overline{\mathcal{F}} &= \bar{\lambda}\overline{\mathcal{F}}, \qquad \mathfrak{L}'^{\dagger}(\mathbf{u}_{\mathbf{s}})\overline{\mathcal{F}}^{*} = \lambda \overline{\mathcal{F}}^{*}. \end{split}$$

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$$\begin{split} &\langle \overline{\mathcal{F}}^* | \mathcal{F} \rangle = 0 \quad \text{if} \quad \lambda \neq \bar{\lambda}, \qquad \overline{\mathcal{F}}^* = M^{-1} \mathcal{F}, \\ &\langle \mathcal{F}^* | \overline{\mathcal{F}} \rangle = 0 \quad \text{if} \quad \lambda \neq \bar{\lambda}, \qquad \mathcal{F}^* = M^{-1} \overline{\mathcal{F}}. \end{split}$$



Localized structures in 3KRD system

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• If λ is real (e.g., $\lambda = 0$):

$$\mathcal{G}_r^* = M^{-1}\mathcal{G} = \begin{pmatrix} \frac{\partial \mathbf{u}_s}{\partial \mathbf{r}} \\ -\kappa_3 \tau \frac{\partial \mathbf{v}_s}{\partial \mathbf{r}} \\ -\kappa_4 \theta \frac{\partial \mathbf{w}_s}{\partial \mathbf{r}} \end{pmatrix}$$

However, in this case $\langle \mathcal{G}_r^* | \mathcal{G} \rangle \neq 0$.

Localized structures in 3KRD system

Stability diagramm



Localized structures in 3KRD system

Order of bifurcations

• Limit case: $\tau = 0, \theta = 0, D_v = 0$



Localized structures in 3KRD system

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- Limit case: $\tau = 0, \theta = 0, D_v = 0$
- Eigenvalue problem with eigenvalue λ and eigenfunction $\mathcal{F} = (f_u, f_v, f_w)^T$:

$$\lambda f_u = D_u \triangle f_u + (f'(u_s) - \kappa_3) f_u - \kappa_4 f_w$$
$$D_w \triangle f_w + f_u - f_w = 0$$



Localized structures in 3KRD system

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• In the limit case the operator $\mathfrak{L}'(\mathbf{u_s})$ is Hermitian. All λ 's are real.

Localized structures in 3KRD system

Order of bifurcations

• Let us now consider $\tau > 0$:

$$\mu f_u = D_u \triangle f_u + (f'(u_s) - \kappa_3) f_u - \kappa_4 f_w$$

$$\tau \mu f_v = f_u - f_v$$

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Localized structures in 3KRD system

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$$\tau \mu f_v = f_u - f_v$$
$$0 = D_w \triangle f_w + f_u - f_w$$

$$\left(\mu - \frac{\kappa_3 \tau \mu}{\tau \mu + 1} \right) f_u = D_u \triangle f_u + (f'(u_s) - \kappa_3) f_u - \kappa_4 f_w$$
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Localized structures in 3KRD system

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$$0 = D_w \triangle f_w + f_u - f_w$$

$$\lambda = \mu - \frac{\kappa_3 \tau \mu}{\tau \mu + 1}$$
$$\mu_{1,2} = \frac{\lambda \tau - 1 + \kappa_3 \tau}{2\tau} \pm \sqrt{\frac{\lambda}{\tau} + \left(\frac{\lambda \tau - 1 + \kappa_3 \tau}{2\tau}\right)^2}$$
$$f_{v1,2} = \frac{1}{1 + \tau \mu_{1,2}} f_u$$

Localized structures in 3KRD system

Order of bifurcations

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$$f_{v1,2} = \frac{1}{\tau \mu_{1,2}} f_u$$

•
$$\mu = 0 \Rightarrow \lambda = 0;$$

Localized structures in 3KRD system

Order of bifurcations

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$$\mu = 0 \Rightarrow \lambda = 0;$$

- For some $\lambda < 0$ μ is complex;
- Bifurcation point:

$$\tau_c = \frac{1}{\lambda + \kappa_3};$$

Localized structures in 3KRD system

Order of bifurcations

$$\lambda = \mu - \frac{\kappa_3 \tau \mu}{\tau \mu + 1}$$
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$$\lambda = 0 \Rightarrow \mu_{1,2} = \left\{0, \frac{\kappa_3 \tau - 1}{\tau}\right\} \Rightarrow f_{v1,2} = f_u.$$

Localized structures in 3KRD system

Order of bifurcations

$$\lambda = \mu - \frac{\kappa_3 \tau \mu}{\tau \mu + 1}$$
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- $\lambda = 0 \Rightarrow \mu_{1,2} = \left\{0, \frac{\kappa_3 \tau 1}{\tau}\right\} \Rightarrow f_{v1,2} = f_u.$
- Propagator mode: Generalized eigenfunction

$$\mathfrak{L}'(\mathbf{u_s})\mathfrak{L}'(\mathbf{u_s})\mathcal{P}_{\mathbf{r}} = 0 \Rightarrow \ \mathfrak{L}'(\mathbf{u_s})\mathcal{P}_{\mathbf{r}} = \mathcal{G}_{\mathbf{r}}$$

Localized structures in 3KRD system

Breathing DSs

• Destabilization via the mode n = 0:





Localized structures in 3KRD system

Breathing DSs



Localized structures in 3KRD system

Amplitude equation

The idea:

• Two-scale expansion in the vicinity of bifurcation point,

$$\begin{split} \theta &= \theta_c: \ \widetilde{\mathbf{u}} = A e^{i\omega t} \mathcal{F}_c + c.c. + r \\ \theta &= \theta_c + \varepsilon: \ \widetilde{\mathbf{u}} = A(t) e^{i\omega t} (\mathcal{F}_c + \varepsilon \mathcal{F}_{\varepsilon}) + c.c. + r; \end{split}$$

Amplitude equation is a normal form of a Hopf bifurcation;

 Complex coefficients can be immediately evaluated if the solitary stationary solution is known;

$$\partial_t A = \varepsilon a_1 A + a_2 A |A|^2,$$

$$a_1 = \frac{\langle \mathcal{L}'_{\varepsilon}(\mathbf{u_s})\mathcal{F}_c | \mathcal{F}_c^* \rangle}{\langle \mathcal{F}_c | \mathcal{F}_c^* \rangle}, \qquad a_2 = \frac{\langle \mathcal{L}''_c(\mathbf{u_s})\mathcal{F}_c \mathcal{F}_c \overline{\mathcal{F}}_c | \mathcal{F}_c^* \rangle}{2\langle \mathcal{F}_c | \mathcal{F}_c^* \rangle}.$$

Localized structures in 3KRD system

Amplitude equation



Localized structures in 3KRD system

Moving DSs

• Destabilization via the mode n = 1:



Localized structures in 3KRD system

Moving DSs

• Destabilization via the mode n = 1:





Localized structures in 3KRD system

Moving DSs: Drift-Bifurcation

Fredholm alternative:

$$\mathfrak{L}'(\mathbf{u_s})\mathcal{P}_{\mathbf{r}} = \mathcal{G}_{\mathbf{r}} \Leftrightarrow \langle \mathcal{G}_{\mathbf{r}}^* | \mathcal{G}_{\mathbf{r}} \rangle = 0$$

Localized structures in 3KRD system

Moving DSs: Drift-Bifurcation

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• Bifurcation point:

$$\tau_{c,x} = \frac{1}{\kappa_3} - \theta \frac{\kappa_4}{\kappa_3} \frac{\langle w_{s,x}^2 \rangle}{\langle u_{s,x}^2 \rangle}$$

Localized structures in 3KRD system

Moving DSs: Drift-Bifurcation

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• Propagation velocity:

$$c^{2} = \frac{\kappa_{3}}{\tau_{c,x}^{2}} \frac{\langle u_{s,x}^{2} \rangle}{\langle u_{s,xx}^{2} \rangle} \left(\tau - \tau_{c,x}\right)$$

Localized structures in 3KRD system

Drift-Bifurcation due to a change of shape



Localized structures in 3KRD system

Drift-Bifurcation due to a change of shape



Localized structures in 3KRD system

Breathing and moving DSs







Localized structures in 3KRD system





Localized structures in 3KRD system

Breathing and moving DSs



Localized structures in 3KRD system

Breathing DSs with oscillatory tails



Localized structures in 3KRD system

Breathing DSs with oscillatory tails

