

The Generation of Dissipative Quasi-Particles near Turing's Bifurcation in Three-Dimensional Reaction-Diffusion Systems

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Abstract. In order to model pattern formation processes in a dc driven semiconductor-gas discharge system on a phenomenological level, we investigate a three-component reaction-diffusion system of 1-activator-2-inhibitor-type. The solutions of this system show localized moving and stationary structures which interact by scattering, annihilation or more complex scenarios. Because of this particle-like behaviour the structures are called *dissipative quasi-particles*. This work deals with the generation mechanism of dissipative quasi-particles related to Turing's destabilisation of homogeneous states. Two- and three-dimensional simulations are shown and in the two-dimensional case compared with experimental results.

1 Introduction

Nature shows a rich variation of patterns and structures, with famous examples related to mammalian coat patterns [1]. Since Turing in 1952 established a reaction-diffusion system to model the morphogenesis of embryos [2], a lot of experiments has been conducted to systematically investigate pattern formation resulting from the interaction of these two basic mechanisms. Examples include spreading depression waves in chicken retina [3], the Belousov-Zhabotinsky reaction [4] and the oxidation of CO on platinum coated surfaces [5].

In our group layered semiconductor devices [6–8], direct current [9–11] and alternating current gas discharge systems [12,13] are being studied, which exhibit a huge variety of pattern formation scenarios. In particular, in the case of DC gas discharge systems and semiconductor devices empirical bifurcation sequences could be successfully described [7,14]. Two-component reaction-diffusion systems have been used to model basic patterns such as Turing-like spatial periodic structures [15], localized stationary filaments and their interaction [16]. In this context a third component with inhibiting characteristics has been introduced to provide a robust access to experimentally observed moving filaments both with theoretical and numerical methods [17,18]. These examples refer to two-dimensional reaction-diffusion experiments. But three-dimensional systems like the excitation waves observed within the heart muscle [19] or three-dimensional chemical Turing patterns [20] aren't unusual as well. There are other dissipative systems where particles are capable to organize themselves, for example superconducting ceramic particles in an electrical direct current tension field, which form macroscopic balls [21].

This motivates the investigation of the three-component equations on three-dimensional domains. As a fundamental pattern we find particle-like structures which solve the three-dimensional reaction-diffusion system. These so-called dissipative quasi-particles may be stationary, but were also found to move and interact for certain parameter ranges. Simple collision processes merely change the particles' trajectories and can be captured by means of a reduced dynamics approach [22].

The aim of this work is to describe structure formation processes beyond the regime of conserved numbers of particles. Here we find annihilation of quasi-particles [18,23] as well as generation of new ones both from the scratch and via the formation of intermediate compound states, which separate into new quasi-particles through symmetry breaking.

2 The Reaction-Diffusion System

2.1 The Three-Component Reaction-Diffusion System

We start by presenting the full three-component system of partial differential equations under investigation. Based on these equations we will discuss two limit cases. The first case describes a reduced dynamics exploiting the particle-like character of localized solutions. It is included to familiarize the reader with the concept of dissipative quasi-particles.

The second case is a two-component limit, that is of sufficient complexity to include Turing's bifurcation of a homogeneous reference state with respect to finite wavelength perturbations. We will employ this destabilizing mechanism in order to generate new quasi-particles from the scratch.

Consider the following equations:

$$\begin{array}{rcl}
 \dot{u} & = & D_u \Delta u + \lambda u - u^3 - \kappa_3 v - \kappa_4 w + \kappa_1, \\
 \tau \dot{v} & = & D_v \Delta v + u - v, \\
 \theta \dot{w} & = & D_w \Delta w + u - w,
 \end{array} \tag{1}$$

$\underbrace{\quad}$
 rate of
change

$\underbrace{\quad}$
 diffusions
terms

$\underbrace{\quad}$
 reaction terms

According to the reaction terms we refer to the system as a 1-activator-2-inhibitor system, because, for small values of u , this (auto-catalytic) component, the activator, enhances the production of u , v and w . The remaining components v and w , on the other hand, inhibit the activator's growth as well as their own.

The speciality of this reaction-diffusion system depends on the inhibitors v and w . These favor moving localized structures (quasi-particles) if one of the inhibitors is slow (say τ is large), and the other has a large diffusion length (say D_w is large). In this case the inhibitor v controls the propagation of the quasi-particle in the direction of motion, while the inhibitor w stabilizes the shape of the solution transverse to the direction of motion [16].

2.2 The Limit Case of Reduced Dynamics

In the limit case $\theta \rightarrow 0$ and $D_v \rightarrow 0$ the dynamics of quasi-particles can be analytically described for $\tau \simeq \frac{1}{\kappa_3}$ [22,24]. According to these results, stable stationary quasi-particles exist only for $\tau \leq \frac{1}{\kappa_3}$. They will start to move if τ is increased beyond this point of bifurcation. Close to the branching point, the velocity c_0 is given by

$$c_0 = \kappa_3^{\frac{3}{2}} \sqrt{\frac{\tau - \frac{1}{\kappa_3}}{Q}}. \quad (2)$$

The constant $Q = \langle \bar{u}_{xx}^2 \rangle / \langle \bar{u}_x^2 \rangle$ is computed from the activator component \bar{u} of the corresponding stationary quasi-particle. Note, that for the sake of simplicity we assumed rotational symmetry for this stationary solution.

To describe the interaction of two quasi-particles in this limit case, we have to deal with two degrees of freedom per quasi-particle and dimension: These are the position \mathbf{p} and a quantity α , which is proportional to the velocity if the particle is far away from others. Thus the interaction dynamics reduces to a system of ordinary differential equations:

$$\begin{aligned} \dot{\mathbf{p}}_1 &= \kappa_3 \alpha_1 - F(d) (\mathbf{p}_2 - \mathbf{p}_1), \\ \dot{\alpha}_1 &= \kappa_3^2 \left(\tau - \frac{1}{\kappa_3} \right) \alpha_1 - \kappa_3 Q |\alpha_1|^2 \alpha_1 - F(d) (\mathbf{p}_2 - \mathbf{p}_1), \end{aligned} \quad (3)$$

Here $F(d)$ represents an interaction term, that depends on the distance $d = |\mathbf{p}_1 - \mathbf{p}_2|$ and is computed numerically making use of the shape of the stationary solution $(\bar{u}, \bar{v}, \bar{w})$ [22].

Since comparison between the reduced dynamics (3) and three-dimensional numerical solutions shows an excellent fit [23], the reduced dynamics is used to obtain initial conditions $\mathbf{p}_i(t=0)$ and $\alpha_i(t=0)$ for complex interaction processes before starting three-dimensional simulations (Fig. 1).

2.3 The Generation of Quasi-Particles via Turing-Bifurcation

If one deals with quasi-particles in the framework of a particle formalism, the number a particles involved is free but strictly conserved. To investigate the equally interesting process of particle generation we have choose a different approach. Experimentally, the generation of quasi-particles has been observed, for instance, in direct current gas discharge systems [25], where the scenario is as follows: The supply voltage is slowly increased until a first quasi-particle in form of a current filament arises in front of a homogeneous background. This filament causes a higher total current flow, which reduces the voltage available at the discharge gap due to the voltage drop over a global load resistor. If the supply voltage is further increased, the process is repeated at a new random position, more and more filaments appear until the domain is filled.

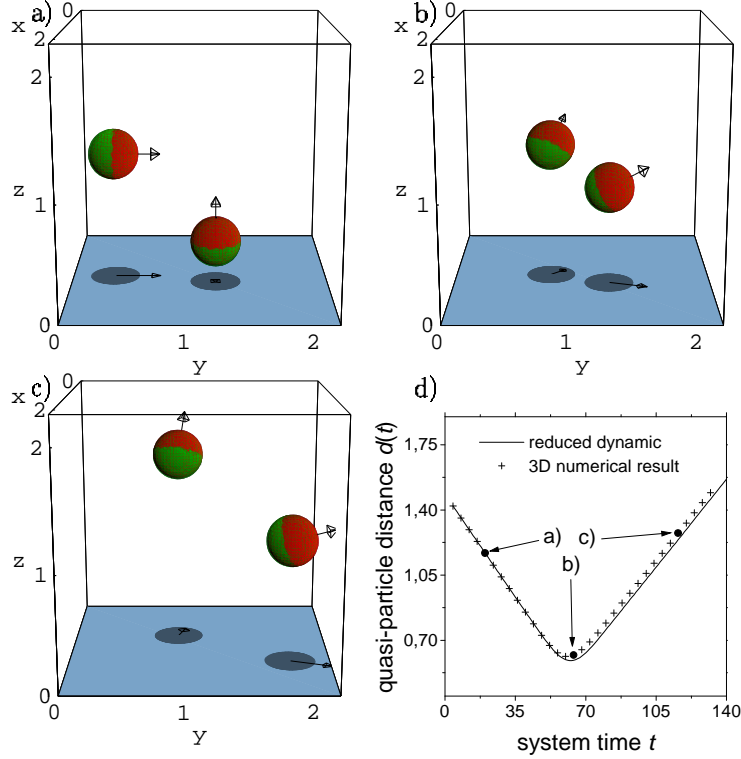


Fig.1. Pictures (a)-(c) show the scattering of two quasi-particles. Red indicates the activator's iso-surface $u(x, y, z) = -1.0$ and green the slow inhibitor's iso-surface $v(x, y, z) = -1.0$. Diagram (d) compares the quasi-particle distances computed from the full numerical solution and from the reduced dynamics (3). Parameters: $D_u = 4.67 \cdot 10^{-3}$, $D_v = 0$, $D_w = 0.01$, $\lambda = 5.67$, $\kappa_1 = -1.126$, $\kappa_3 = 1$, $\kappa_4 = 3.33$, $\tau = 1.03$, $\theta = 0.01$, $\mathbb{G} = 2.25 \times 2.25 \times 2.25$, $\Delta x = 0.028$, $\Delta t = 1 \cdot 10^{-3}$

This feedback mechanism can be modeled by means of the three-component reaction-diffusion system (1) if we use a finite domain \mathbb{G} and consider the limit case of an infinitely fast reacting and well diffusing second inhibitor w , i.e. $\theta \rightarrow 0$ and $D_w \rightarrow \infty$. As a consequence, the third reaction-diffusion equation (1) can be removed in favor of an integral over the activator u . Thus the three-component reaction-diffusion equation becomes a two-component reaction-diffusion equation with additional global feedback:

$$\begin{aligned} \dot{u} &= D_u \Delta u + \lambda u - u^3 - \kappa_3 v + \kappa_1 - \kappa_4 \frac{1}{\|\mathbb{G}\|} \int_{\mathbb{G}} u \, dV, \\ \tau \dot{v} &= D_v \Delta v + u - v, \end{aligned} \quad (4)$$

where the integral term is normalized to the domain size $\|\mathbb{G}\|$. With regard to the direct current gas discharge system the activator u matches the current

flow and the inhibitor v represents the (inverted) voltage. The bistability of the characteristic curve of the gas is modeled by the cubic term $\lambda u - u^3$ of the activator equation, while the change of the supply voltage is obtained by variations of parameter κ_1 . The feedback via the global load resistor corresponds to the integral term $\kappa_4/\|\mathbb{G}\| \int_{\mathbb{G}} u \, dV$.

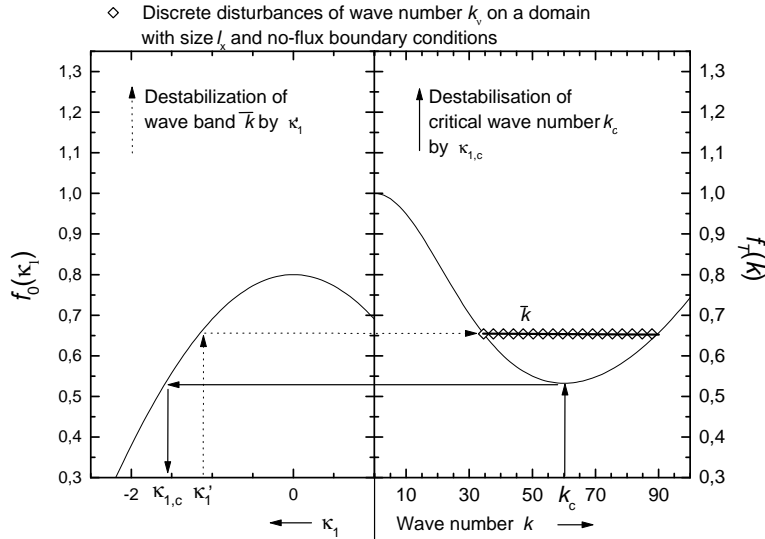


Fig.2. Violation the stability condition (6) by $\kappa_1' > \kappa_{1,c}$ on a one-dimensional domain $\mathbb{G} = [0, l_x]$. This Turing-destabilisation excites perturbations with discrete wave numbers k_ν . Parameters as in (8)

In order to investigate the generation of quasi-particles in the two-component reaction-diffusion system (4) close a Turing-bifurcation one starts with a stable homogeneous state $u_0 = v_0$, with $\Delta u_0 = \Delta v_0 = 0$ and $\dot{u}_0 = \dot{v}_0 = 0$. Here $u_0(\kappa_1)$ is a solution of the cubic equation

$$\kappa_1 = u_0 (\kappa_3 + u_0^2 - \lambda + \kappa_4) . \quad (5)$$

Perturbation theory with respect to small disturbances e^{ikx} shows that the system $u_0(\kappa_1)$ will be stable against perturbations with wavelength k if the condition

$$\underbrace{\lambda - 3(u_0(\kappa_1))^2}_{=: f_0(\kappa_1)} < \underbrace{\kappa_3(1 + D_v k^2)^{-1} + D_u k^2}_{=: f_T(k)} \quad (6)$$

is fulfilled. In this case amplitudes of disturbances with wavelength k decrease in the course of time. If κ_1 is increased in order to violate equation (6), perturbations with wave numbers k within the wave band \bar{k} will be destabilized. Zero-flux boundary conditions on a cuboid domain \mathbb{G} with size $l_x \times l_y \times l_z$ selects discrete

wave numbers

$$|\mathbf{k}_{\nu,\eta,\xi}| = \left(\frac{\pi\nu}{l_x}, \frac{\pi\eta}{l_y}, \frac{\pi\xi}{l_z} \right) \quad \text{with } |\mathbf{k}_{\nu,\eta,\xi}| \in \bar{k} \quad \text{and } \nu, \eta, \xi \in \mathbb{N} \quad (7)$$

from the continuous wave band \bar{k} . If there is a small amplitude attractor close to the reference state, the system is likely to find this solution. If, on the other hand, such a stable small amplitude solution does not exist, as for instance in the case of subcritical bifurcations, large amplitude structures such as quasi-particles will be formed. However, this generation process can't continue infinitely, because the activator integral increases with increasing number of quasi-particles which leads to an effective reduction of κ_1 . This results in a re-stabilization of the system. Thus a homogeneous system can be transformed into a structured one filled with a number of quasi-particles by means of a generation cascade triggered by an initial Turing-bifurcation.

3 Numerical Results

3.1 Strategy and Numerical Methods

In order to generate quasi-particles a homogeneous system or a system with one stable quasi-particle is destabilized by increasing κ_1 above a critical value $\kappa_{1,c}$ (see Fig. 6). For homogeneous systems this is the Turing-bifurcation point. For a structured domain the critical value is much smaller than the Turing-bifurcation point and can be predicted from stability analysis of one-dimensional radially symmetric quasi-particle solutions [26]. In any case, if a homogeneous or a structured system is treated close a bifurcation point, perturbations will be excited but their amplitudes will grow only very slowly. For that reason the reaction-diffusion equations (4) have to be integrated numerically with high discretisation in time and space over a long time interval. In order to reduce the numerical effort it is important to estimate parameters for the 3-d generation mechanism by means of two-dimensional problems and get a detailed understanding of the process.

Solutions of the two-component reaction diffusion system have been computed using a finite difference scheme with a fixed discretisation length Δx on two- and three-dimensional domains and zero-flux boundary conditions. The fixed discretisation length Δx enables the perturbation modes of a destabilized homogeneous system to grow all over the domain, which would be suppressed by variable discretisation lengths. Due to advantages in stability and accuracy properties we implemented the Crank-Nicholson scheme for the time discretisation. The resulting discrete reaction-diffusion system is solved iteratively whereby a successive-overrelaxation method provides a reasonably fast convergence.

Parallelism of the system is achieved by dividing the domain in sub-domains with equal size and boundaries as small as possible. Each processor of the parallel computer solves the set of equations on one domain and synchronizes itself after each iteration with his neighbors using the Message Parsing Interface (MPI).

Performance investigations of the parallel solution algorithm have been carried out validating that the algorithm shows a satisfactory scale-up [27].

The quasi-particle generation problem was studied on the Cray T3E of the High Performance Computing Center Stuttgart (HLRS). A two-dimensional system with a 100×100 discretisation typically runs on 32 processors for about one hour per node. Simulations of three-dimensional systems with a $100 \times 100 \times 100$ discretisation need up to 10 hours per node on 128 processors.

3.2 Interaction between global feedback and generation of quasi-particles

First, we discuss the generation cascade in the framework of a two-dimensional system (4) using the following parameters:

$$\begin{aligned} D_u &= 6 \cdot 10^{-5}, D_v = 6 \cdot 10^{-4}, \lambda = 0.8 \\ \kappa_1 &= -1.575, \kappa_3 = 1, \kappa_4 = 5 \\ \tau &= 1.0, \Delta t = 0.05, \Delta x = 0.01, l_x = 1.0. \end{aligned} \tag{8}$$

Starting with a stable homogeneous state parameter κ_1 is changed to a value slightly above the critical value $\kappa_{1,c} = -1.575$. The Turing-destabilization excites perturbations, with small amplitudes (Fig. 3, row 1). This leads to the formation of one localized quasi-particle (Fig. 3, row 2). Additional quasi-particles appear next to the first one and the activator u between two adjacent particles decreases because of their combined inhibiting influence (Fig. 3, row 3). The growing number of particles results in an increasing activator integral, effectively reducing κ_1 . Finally, the term $\kappa_1 - \kappa_4 / \|\mathbb{G}\| \int_{\mathbb{G}} u \, dV$ drops below a critical value and the system is re-stabilized: The generation of quasi-particles stops. In a second phase, the distances between the quasi-particle change slightly and slowly, thereby the final structure of the quasi-particle-cluster is obtained. This results from the over- and undershooting at the quasi-particle tails, the so-called oscillating tails, which are typical for the parameter range where this generation mechanism is observed. The movement arises from the fact, that each quasi-particle tries to center itself on top of the oscillatory tails of its neighbors [16].

Beyond that, we found that the number of quasi-particles generated during the cascade depends nonlinearly on κ_1 (Fig. 4). This goes along with a nonlinear relation between the number of quasi-particles and the activator integral $\|\mathbb{G}\|^{-1} \int_{\mathbb{G}} u \, dV$. The ultimate cause is the finite size of the domain; note that this finiteness is essential in this context in order to introduce a global feedback. If the particle cluster generated during the cascade almost fills the available space, ignition of new filaments becomes more difficult. Instead, the particles tend to develop higher amplitudes. This leads to a higher per particle contribution to the feedback integral. As a consequence, fewer particles have to be generated in order to stabilize the system.

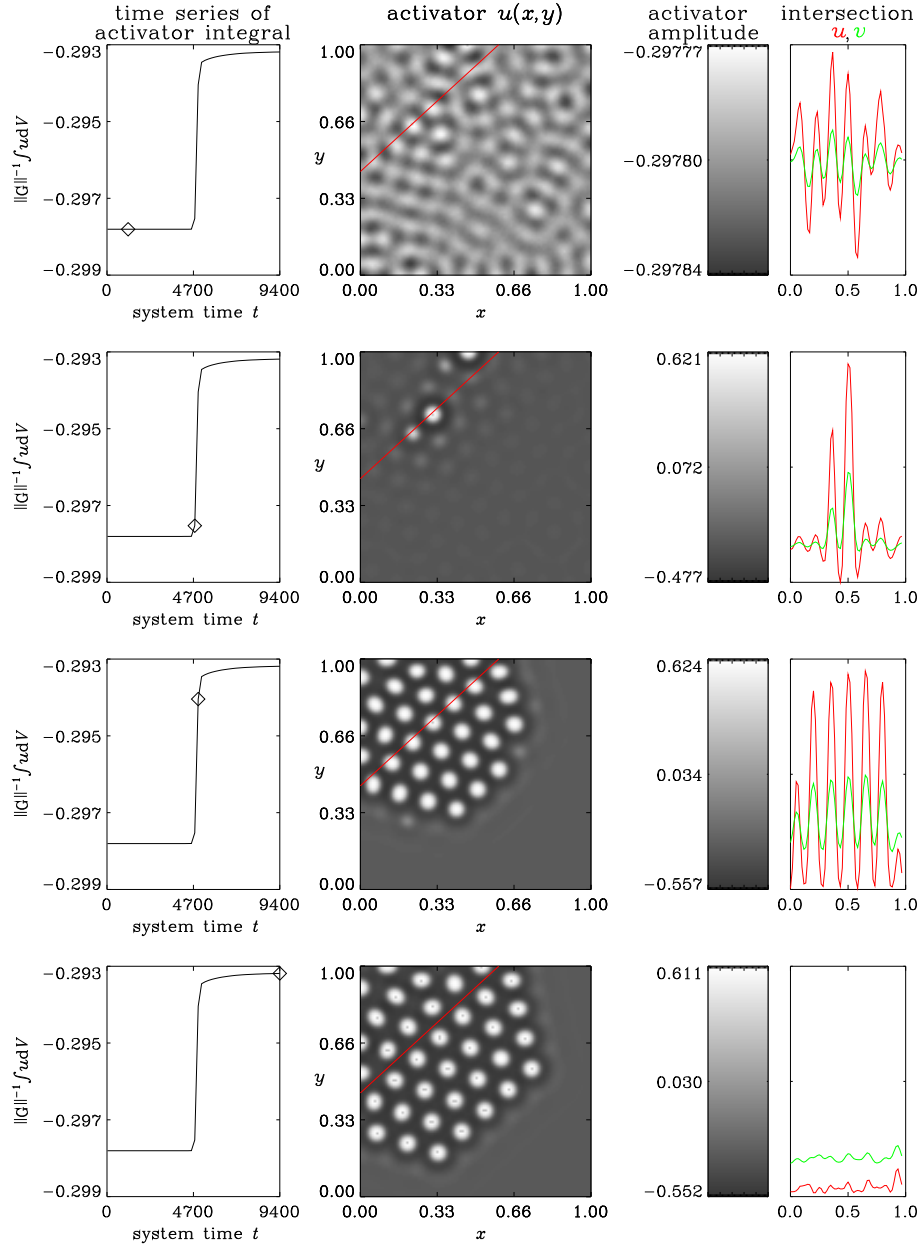


Fig.3. Turing destabilisation of a homogeneous two-dimensional system. Each **row** shows a snap shot at the moment which is indicated by a diamond within the first diagram. Growing perturbation amplitudes (**row 1**) finally ignite a quasi-particle (**row 2**). Next to this first structure, more quasi-particles are generated (**row 3**). The increase of the activator integral re-stabilizes the system and the generation process is stopped. The cluster of quasi-particles rearranges slightly because each quasi-particle tries to center itself on top of the oscillatory tails of its neighbors (**row 3** and **4**). Parameters as in (8)

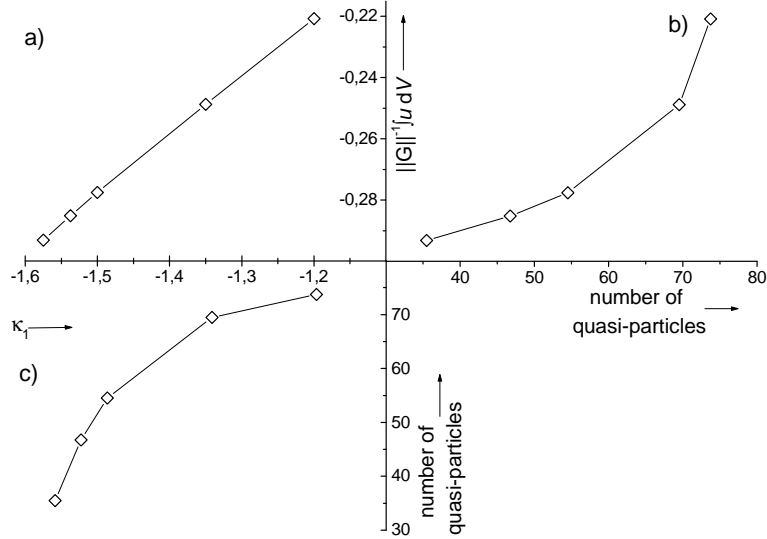


Fig.4. The interaction of global feedback and generation of quasi-particles. The results of the displayed simulation series were obtained by destabilizing a homogeneous system (8) through $\kappa_1 > \kappa_{1,c} = -1.60$ (Fig. 2). Diagram (a) shows that the activator integral $\|\mathbb{G}\|^{-1} \int u \, dV$ depends linearly on κ_1 : A stronger destabilization needs a higher feedback in order to re-stabilize the system. In diagram (b) the number of quasi-particles which were generated in order to achieve this re-stabilization of the system is plotted against the activator integral of the stabilized system. The dependency between these quantities is strongly nonlinear and starts with a large offset: Even for values of κ_1 (c) slightly beyond the bifurcation point $\kappa_{1,c}$ a large number of quasi-particles is needed to re-stabilize the structure. Therefore, the investigated model system is not able to reproduce the step by step generation of quasi-particle clusters, that was observed in the experiment

3.3 Reproduction of experimental self-completion scenario

Astrov and Logvin showed in 1997 [11] that extended structures of current filaments in DC driven planar semiconductor-gas discharge systems arise via a self-completion scenario. They observed that a single stable current filament is destabilized due to an increase of the feeding voltage resulting in the generation of another current filament which re-stabilizes the system. A further increase generates the next filament and so on. The process can be continued until the system is filled up with filaments.

They also presented a semi-phenomenological model of activator-inhibitor type with global feedback which suggests that the Turing mechanism triggers the generation process as discussed above. In contrast to the experiment, however, their model system just needs one increase of the feeding voltage to generate a whole cluster of filaments. This may be ascribed to inhomogeneities of the experimental system interrupting the generation cascade at an early stage, which aren't considered within the model.

Our two-component reaction-diffusion system (4) models the same experimental system [14] using totally different reaction terms, but shows the same generation mechanism (Fig. 5) as in the experiment and in the Astrov-Logvin model. This implies that the self-completion scenario through Turing destabilization is a generic feature of two-component reaction-diffusion systems with global feedback.

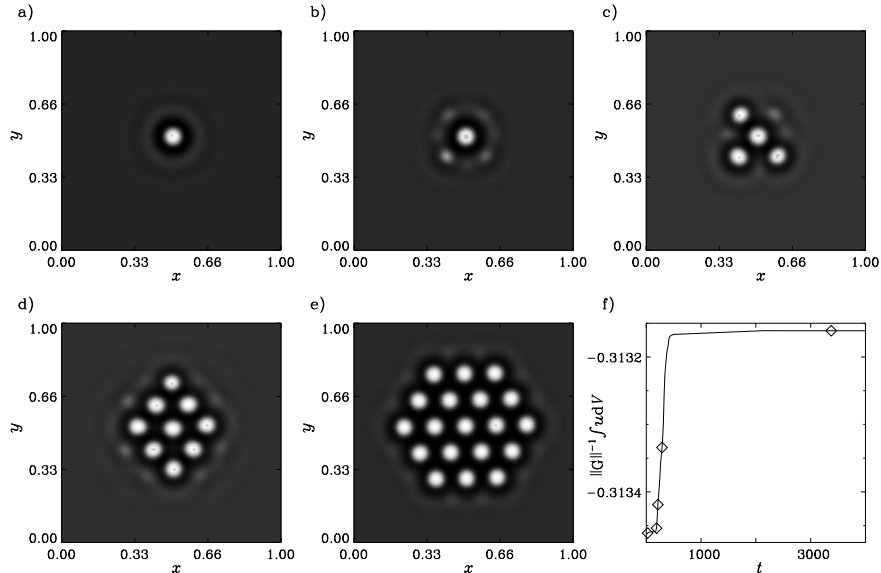


Fig.5. Self-completion scenario starting from a single quasi-particle. Parameter like (8) with $\kappa_1 = -14.4$ and $\kappa_4 = 45.0$. Diagrams (a)-(e) show gray-scale images of the activator $u(x, y)$ at different moments t , which are indicated by diamonds in diagram (f) showing the time series of the activator integral $\|\mathbb{G}\|^{-1} \int u dV$. The destabilization of the quasi-particle depicted in (a) results in the generation of a quasi-particle cluster (c)-(e) which increases the activator integral (f) and re-stabilizes the system. Note that this cluster is much smaller than the smallest cluster obtained for homogeneous initial conditions.

3.4 The Generation of Quasi-Particles in three-dimensional Systems

Because three-dimensional Turing patterns have been observed in chemical systems [20] we investigate the Turing destabilization of two-component reaction-diffusion systems (4) on three-dimensional domains. Concerning this we mentioned before that the dynamics of the system slow down near the bifurcation point $\kappa_{1,c}$. Simulations show that in particular the ignition of the first quasi-particle requires a vast amount of time.

This is why we, typically, started cascade runs in three dimensions from a single stationary quasi-particle (Fig. 7, column 1) as opposed to a homogeneous initial state.

Analytical results with respect to the stability of quasi-particles are hard to obtain and typically restricted to simplifying limit cases. One such limit exploits the separation of length scales that can be enforced by choosing $D_v \gg D_u$. Though this limit provides some insight as to how a filamentary structure is stabilized, it suffers from the fact that Turing's bifurcation (which is based on similar scales) is systematically excluded. Nevertheless, it is well-known from separated scales studies, and also true beyond this limit, that localized structures may be destabilized due to shape instabilities. The most important of these instabilities is related to a dumb-bell shaped deformation which tends to split the particle. Such a mode is, of course, possible only for dimensions higher than one.

Numerical analysis shows that for the parameters specified above single particles on large three-dimensional domains are unstable with respect to this mode. Hence, the 3-d generation cascade should more complex than in the previous 2-d design. This is, indeed, the case. In addition to Turing-like adjacent ignitions, the particles are pulled apart by the dumb-bell mode (Fig. 7, column 2), which leads to a cluster of worm-like patterns (Fig. 7, column 3).

Concerning the destabilisation of homogeneous three-dimensional initial states we used only small systems with domains $[0; 0.3]^3$ and 30^3 grid points.

As in the two-dimensional case (Fig. 5) the homogeneous system could be transferred into a structured state (Fig. 6). In these simulations the dumb-bell modes are quenched by the small domain size and cannot be observed.

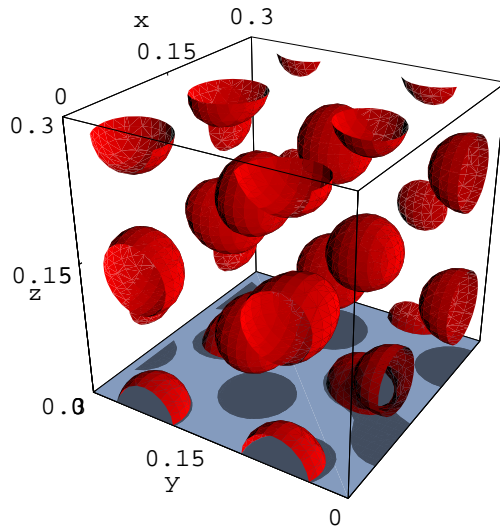


Fig.6. Three-dimensional Turing structure represented by an activator iso-surface. Parameters as in (8) but $l_x = 0.3$, $\kappa_1 = 13.35$ and $\mathbb{G} = 30 \times 30 \times 30$

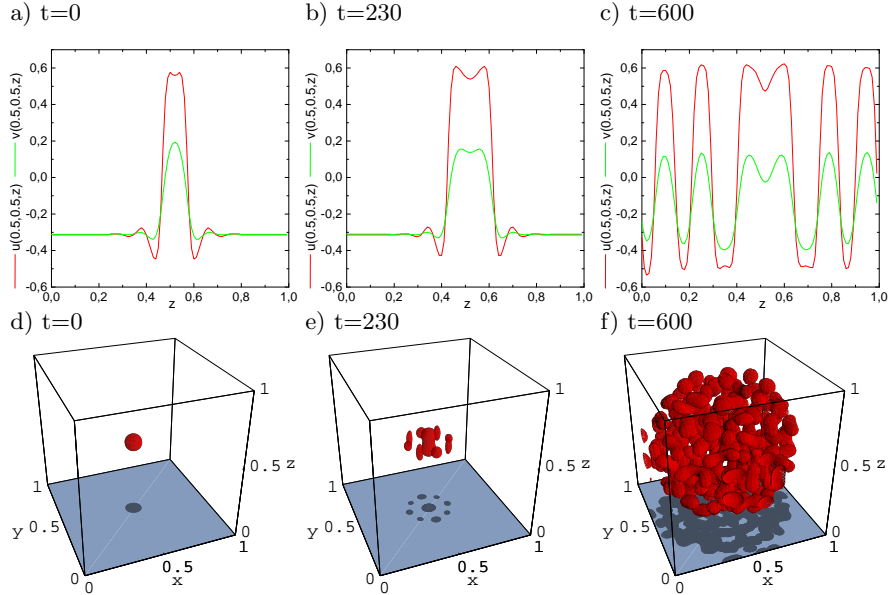


Fig.7. Destabilisation of a three-dimensional quasi-particle. Diagrams (a)-(c) show intersections at $x = 0.5$ and $y = 0.4$ at different moments t , pictures (d)-(f) show iso-surfaces $u(x, y, z) = 0.5$. Parameters as in (8) but $\kappa_1 = 14.0$ and $\kappa_4 = 45.0$. (a), (d) The quasi-particle is unstable with respect to adjacent ignitions and dumb-bell modes. (b), (e) Therefore it is pulled apart and new particles are generated in the $x \times y$ plane. (c), (f) The newly generated quasi-particles are also pulled apart, and the domain fills with worm-like structures.

4 Conclusion and Outlook

In this paper we present recent results on the generation of dissipative quasi-particles in three-component reaction-diffusion systems. Inspired by experimental set-ups with global feedback based for instance on a global load resistor, we consider the limit case of a strongly diffusing, fast third component. This leads to a two-component integro-differential system resembling the experimental situation.

We found that there are different generation mechanisms, two of which we describe in some detail. The first should be associated to the famous Turing bifurcation and can be interpreted as an ignition of new filamentary structures in the vicinity of already existing structures. Due to their (superimposed) oscillating tails, these old patterns determine the position of the new structures - up to remaining symmetries.

In particular we demonstrated that an ignition cascade in the above sense is capable to transform a homogeneous state into a structured one. This supports the conjecture that such cascades are the generic mechanism to generate multi-filament states as they are observed after spontaneous self-organization in various

experiments as for instance in the DC-driven gas-semiconductor discharge system discussed in the text [11].

As a typical feature of these cascades we remark, that in general it is no problem to create a cluster of quasi-particles but it is much more difficult to generate small numbers.

In the context of a three-dimensional system we discuss a more complex structure formation process combining the Turing-related ignition mechanism with a shape instability that tends to split existing structures.

We finish with the remark that there are completely different processes that lead to the generation of new quasi-particles in the context of traveling patterns:

Simulations with traveling quasi-particles show that new structures may arise from superimposed oscillatory tails of two quasi-particles which come close to each other. Other simulations reveal that two quasi-particles may form a [23] transient toroidal compound state upon collision. This torus finally breaks up into two new quasi-particles (Fig. 8, [27]). With different simulation parameters this compound state should end up in more than two new quasi-particles.

These “dynamic” mechanisms are natural effects in the context of traveling localized structures. Together with interactions leading to super-structures (quasi-particle molecules) [22,26] and annihilation phenomena [18], the generation processes provide a fascinating approach to multi-filament ensembles with fluctuating numbers of particles.

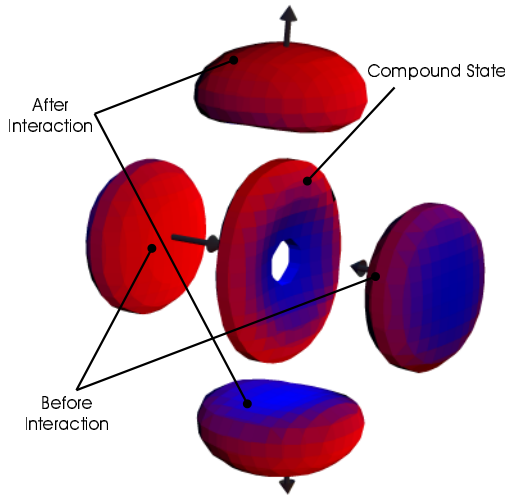


Fig.8. Merging of two quasi-particles [27]. A compound state is formed which breaks up into new quasi-particles. The picture shows activator iso-surfaces $u(x, y, z) = 0.8$, which are coloured with the inhibitor concentration v . Red indicates a big ratio u/v , blue a small one. Parameter: $D_u = 1.5 \cdot 10^{-4}$, $D_v = 1.86 \cdot 10^{-4}$, $D_w = 9.6 \cdot 10^{-3}$, $\lambda = 2.0$, $\kappa_1 = -6.92$, $\kappa_3 = 1$, $\kappa_4 = 8.5$, $\tau = 48.0$, $\Delta t = 0.002$, $\Delta x = 120^{-1}$, $l_x = [0, 1.0] \times [0, 1.33] \times [0, 1.0]$

Acknowledgment

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