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Spatiotemporal patterns in the Bär model induced by concentration-dependent diffusivities

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Abstract

We investigate the effects of diffusivity on pattern formation in the excitable 2D Bär model with periodic boundary conditions. Our work generalizes previous findings of Roussel and coworkers in 1D and focusses on the turbulent states, including the spiral breakdown process. Diffusion coefficients ($D(u)$) quadratically dependent on the activator concentration were studied. Inhibition of the spiral instability was found with a negative linear coefficient in the concentration dependence of $D(u)$. At a given value of ε the inhibition can be complete for nonflux boundary conditions while a delay of the instability occurs in systems with periodic boundary conditions. Positive quadratic coefficients in the concentration dependence of $D(u)$ strongly modify the defect statistic in the chaotic zone.

1. Introduction

Spatiotemporal patterns such as target patterns, spiral waves, and turbulence have been observed in excitable media and modeled by reaction–diffusion equations. In particular, the onset of turbulent behavior has received a great deal of theoretical and experimental attention [1–4].

Though pattern formation has been studied mainly considering a constant diffusion coefficient, this is indeed an exceptional situation. In surface chemical reactions for example, this case corresponds to a noninteracting adsorbate that occupies just one lattice site in an array of equivalent lattice sites. Intermolecular forces, substrate-mediated interactions, and even blocking of adjacent sites by adsorbates are all factors that may cause the surface diffusion coefficients to vary with coverage [5,6]. Other nontrivial coupling modes have also been invoked [7,8].

Other systems also have transport coefficients that strongly depend on the local concentrations: active transport through ionic channels in the cell, glucose-dependent glucose transport, autocatalytic proton transport, proton-dependent peptide transport, and even processes in population dynamics [9–11].

Roussel and coworkers studied the concentration-dependent diffusivities on a two-variable Gray–Scott excitable media model in one spatial dimension [5,12]. Their work showed that these dependences can induce a transition from self-replicating behavior to stationary patterns with no change in the relative diffusivity between the activator and the inhibitor.

In the 1D-Bär model with nonflux boundary conditions, the existence of a stabilization effect of the backfiring has been reported [6].

Following the studies performed by Roussel and coworkers in Ref. [6], we analyze the Bär model in 2D, with periodic boundary conditions. We propose diffusion coefficients dependent on the local concentration of the activator and investigate their effects on pattern formation.

Our study focusses on the turbulent states, including the spiral breakdown process. In early studies turbulent states have been characterized by performing defect statistic, and variations in the average value of defects (μ) and in its variance (σ) have been related to changes in the medium excitability. Quite recently it has been shown that defect statistic

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is also dependent on the dimension of the dynamic system and on the existence of noise [13,14]. In the present work, we show that defect statistic is also altered by the characteristics of the transport process. This result applies to the case of diffusivities strongly dependent on the activator concentration and has not been reported before.

The development of turbulent states is a relevant issue in many biological problems [15–18]. It is now widely accepted that ventricular arrhythmias are due to the existence of spiral waves of electrical activity in the heart muscle. The evolution from this state to ventricular fibrillation implies a transition from a state dominated by spirals to a chaotic or turbulent state. The elucidation of the influence of the transport processes on the development of the chaotic states is relevant in the study of this type of transitions.

The present work is organized as follows: in Section 2 we describe the model and details of our calculations. Section 3 summarizes our results, and Section 4 our conclusions.

2. The model

The well-known model developed by Bär et al. is written as

$$\frac{\partial u}{\partial t} = \nabla(D\nabla u) - \frac{1}{\varepsilon}u(u-1)(u-\frac{v+b}{a}), \tag{1}$$

$$\frac{\partial v}{\partial t} = f(u) - v, \tag{2}$$

where u is the activator, v is the inhibitor, and $f(u)$ is given by

$$f(u) = \left\{\begin{array}{ll} 0 & u < \frac{1}{3} \\ 1.0 - 6.75u(u-1)^2 & \frac{1}{3} \leqslant u \leqslant 1 \\ 1 & u > 1 \end{array}\right\}. \tag{3}$$

The Bär model has been well characterized in earlier studies, assuming homogeneous media and constant diffusion coefficients [2]. The decisive parameters of the model are b (which is the excitation threshold) and ε (which is the relationship of the time scales of the fast (activator, u) and the slow (inhibitor, v) variables). The system presents a saddle-node bifurcation at $b = 0$ and two unstable fixed points. The medium is excitable for small positive b and $a < 1 + b$. In two spatial dimensions, a variety of wave forms are generated as the two decisive parameters b and ε are varied. For $a = 0.84$ and $b = 0.07$, the system exhibits steadily rotating spirals in the range $0.01 < \varepsilon < 0.06$. At $\varepsilon = 0.06$ spirals undergo a transition to meandering and for $\varepsilon > 0.07$ they break and the system exhibits turbulence due to breakup and autoreplication of spirals.

Turbulent regimes have been described in terms of topological defects, which are local zeros of the order parameter and correspond to the case of u and v assuming their unstable fixed point values in the reaction term of Eq. (1). The structure of the spatiotemporally chaotic states has been described by means of the statistic of the topological defects, i.e., analyzing the dependence of the mean value and the variance of the number of topological defects on ε. It has been shown then that initially almost fixed, rotating defects gradually lose their rotational motion, until this degree of freedom is eventually transformed into an entirely translational motion or diffusive mode. As ε increases, the systems undergo a transition from a 'hard-disk liquid' state to a 'point gas' state [2].

For $a = 0.84$ and $b = 0.07$, the system has a saddle point at $\varepsilon = 0.19$ and a Hopf bifurcation at $\varepsilon = 0.2245$.

Now we consider the influence of concentration-dependent diffusion coefficients on pattern formation. Specifically, we consider that the local diffusion coefficient depends on the activator u, and therefore, $D(u)$ may vary in time and space due to the spatiotemporal variation of u. We assume that

$$D(u) = D_u^0\left[1 + k_u u(x,t) + k_{uu}(u(x,t))^2\right], \tag{4}$$

where $D_u^0 = D_u(0)$, k_u and k_{uu} are constants.

The effect of a linear dependence of D_u on u, on the wave stability in the Bär model, has been previously studied in 1D [6], with nonflux boundary conditions. In the present work, we explore the influence, on the turbulent states, of a quadratic dependence of D_u on u, in 2D, with periodic boundary conditions. Our calculations explore part of the $(k_u, k_{uu}, \varepsilon)$-parameter space, with $a = 0.84$ and $b = 0.07$.

Simulations were performed in a two-dimensional 256×256 point grid with periodic boundary conditions. We used an Euler integration scheme for both the reaction and the diffusion terms. For the latter a nine-point stencil with $\Delta x = \Delta y = 0.196$ was used. The integration time step was chosen in each case to ensure mathematical stability. Results were checked to be independent of the integration step for sufficiently small values of Δt.

3. Results

We started our investigations by extending the previous studies in 1D performed by Roussel et al. [6] to 2D. This involves exploring the subspace $(k_u, 0, \varepsilon)$, where we consider both negative and positive values of k_u.

In 1D with nonflux boundary conditions, the existence of a stabilization effect of the backfiring has been reported. Negative values of k_u stabilize the wave instability that produces the backfiring. In Ref. [6] the induction time, measured as the time required for a secondary peak to appear from a given initial condition, was measured as a function of k_u to quantify the stabilization effect. The first splitting was used to eliminate effects due to crowding, which become significant at later times [6].

In 2D a spiral instability leads to the spiral breakdown, and we verified a stabilization effect in our simulations with periodic boundary conditions, with negative values of k_u (not shown here for brevity). Roussel and coworkers have reported the existence of a threshold value of k_u (at a given value of ε) below which the inhibition is complete. This threshold cannot be found in our simulations with periodic boundary conditions, the spiral breakdown always occurs for sufficiently long times. By performing 2D simulations with nonflux boundary conditions, we verified that this fact is due to the nature of the boundary conditions: complete inhibition exists in systems with nonflux boundary conditions, and a delay of the instability occurs in systems with periodic boundary conditions.

As in Ref. [6] we did not find instability inhibition for constant diffusion coefficient $D < 1$, i.e., the inhibition of the instability is a consequence of the spatial modulation of the diffusion coefficient, which makes the amount of activator supplied by diffusion insufficient to overcome the negative dynamic influence of the inhibitor in the back of the wave.

Then we studied the chaotic zone, and turbulent states were characterized by determining the variation of both the mean value (μ) and the variance (σ) of the number of topological defects in the medium, with ε. For the 2D Bär model with constant diffusion, the chaotic states were previously characterized, and a transition, was found with the increase of ε, characterized by a loss of rotational motion and an increase in the translational mobility of defects. Because both μ and σ depend on the size of the system, the intrinsic variable σ^2/μ is preferable to characterize the spatiotemporal state of the system. σ^2/μ tends to zero approaching the spiral instability, while toward the Hopf bifurcation it approaches unity [2].

The above-described transition was called a 'liquid–gas transition'. In the present simulations, we have similarly characterized the chaotic states by means of μ and σ^2.

As shown in Fig. 1a, both μ and σ increase as k_u decreases. However, by comparing Fig. 1a with Fig. 1b (which shows the changes in μ and σ with constant $D \neq 1$) it can be seen that these phenomena are due to the decrease of the diffusion coefficient alone rather than to its spatial variation.

Finally, we note that the liquid–gas transition is not modified by the diffusion coefficient linearly dependent on u-concentration. This regime is indeed modified by the quadratic dependence of the diffusion coefficient $D(u)$ on u (Eq. (4)) as is shown below.

Though both positive and negative values for k_{uu} were considered, we only report here the results for $k_{uu} > 0$. Pattern formation with $k_{uu} > 0$ is less sensitive to the initial conditions, and the discussion can be realized in terms of a phase diagram in the (b, ε)-parameter space, as in the original Bär model (Eqs. (1)–(3)). In order to rationalize the observed behavior we chose the specific values $D_u^0 = 1$, $-k_u = k_{uu} = \text{const}$, with $0 < \text{const} < 4$. Therefore $D(u) \geqslant 0$ reaches its minimum value for $u = 1/2$ and $D(u) = 1$ for $u = 0$ and $u = 1$. Pattern formation was studied then as a function of ε and k_{uu}. We found that states of spirals, meandering, and chaos are still observed, though there is a clear modification of the phase space.

Fig. 2 shows the spiral breakdown initiation as a function of k_{uu} and ε. The spiral breakdown starts at higher values of ε as k_{uu} increases (and $k_u = k_{uu}$ decreases), i.e., the inhibition of the spiral instability is progressively inhibited. As in the linear case with periodic boundary conditions, the inhibition is not complete but just delayed.

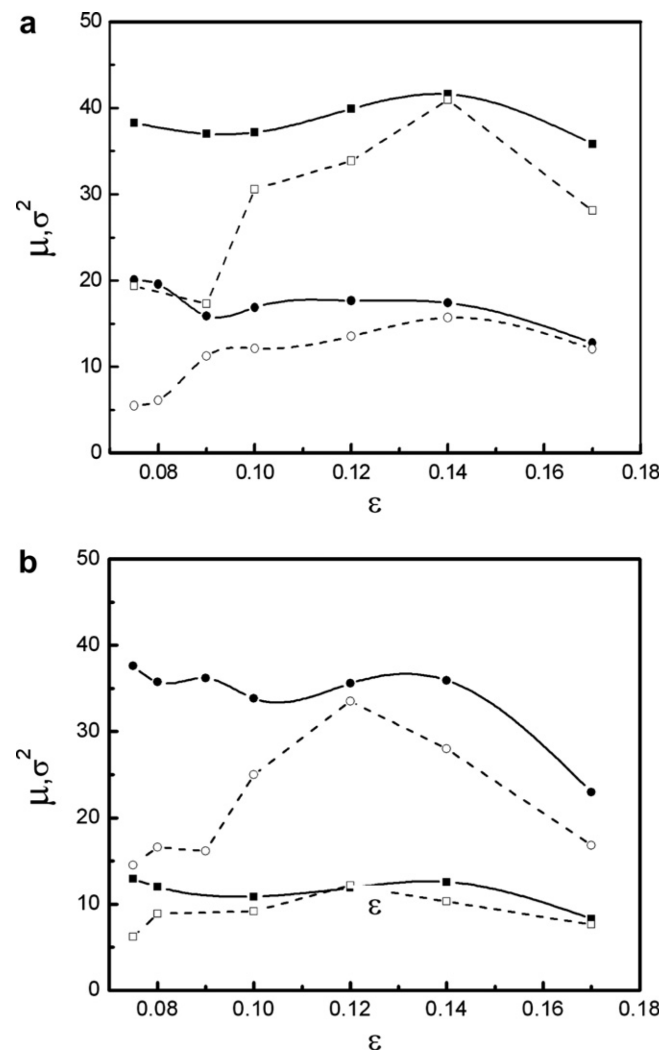

Fig. 1. Statistic of defects in the Bär model with: (a) linearly dependent $D(u)$ on u (i.e., $k_{uu} = 0$), (b) constant $D \neq 1$ (for comparison purposes). In both figures μ and σ^2 are represented by filled and open symbols respectively. (a) Circles stand for the case $D(0) = 1.0$, $k_u = 0.0$ and squares stand for the case $D(0) = 1.0$, $k_u = -1$; (b) circles stand for the case $D(0) = 0.5$, $k_u = 0.0$, and squares stand for the case $D(0) = 1.5$, $k_u = 0.0$. Other parameters were: $a = 0.84$, $b = 0.07$. Periodic boundary conditions were used. Both μ and σ^2 were calculated over a total of 5000 frames sampled every 0.95 s.

Chaotic states show significant differences with respect to the original Bär model. Both μ and σ^2 rapidly increase with epsilon, and the movement of defects becomes restricted in space, i.e., degrees of freedom are strongly inhibited. All these features are shown in Figs. 3 and 4 for the particular case $-k_u = k_{uu} = 4$, which is the maximum value of k_{uu} that ensures mathematical stability. The high σ^2 value found in this case when we compare it with the original Bär model implies a high rate of creation and destruction of defects. Also the translational move-

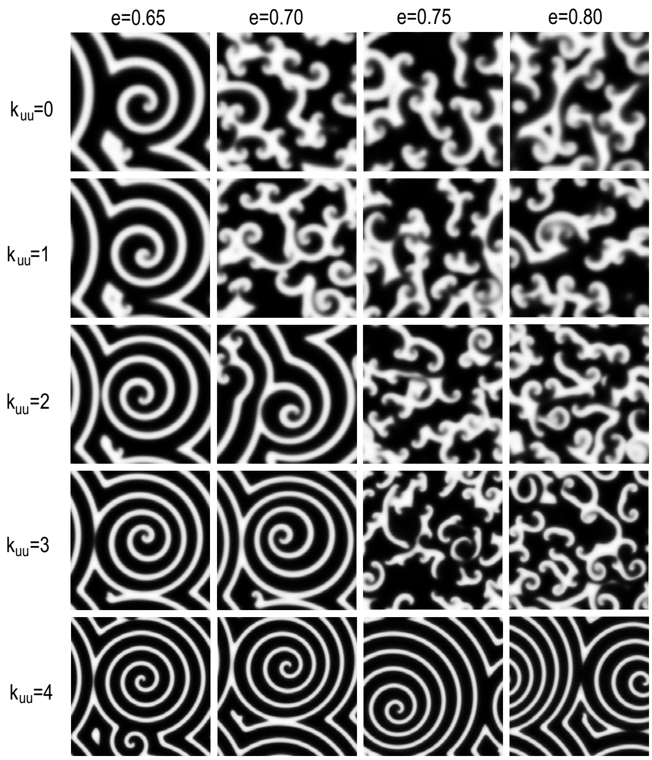

Fig. 2. Patterns as a function of ε and k_{uu} in the Bär model ($a = 0.84$, $b = 0.07$ and periodic boundary conditions) with $D(u) = 1 + k_u u + k_{uu} u^2$ ($k_u = -k_{uu}$).

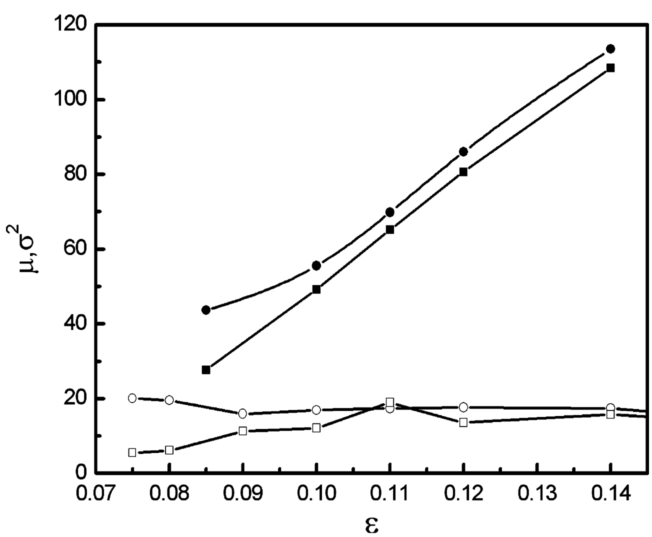

Fig. 3. Statistic of defects in the Bär model with ($a = 0.84$, $b = 0.07$ and periodic boundary conditions) $D(u) = 1 - 4u + 4u^2$. Circles: μ vs. ε, squares: σ^2 vs. ε. Open symbols correspond to the original Bär model and have been included for comparison purposes. Both μ and σ^2 were calculated over a total of 5000 frames sampled every 0.95 s.

ment of defects should be highly correlated with each other. Fig. 5 shows that μ monotonically increases with k_{uu}. The lower the k_{uu} value, the higher the minimum of $D(u)$ (see Eq. (4)), and the movement of defects becomes more localized.

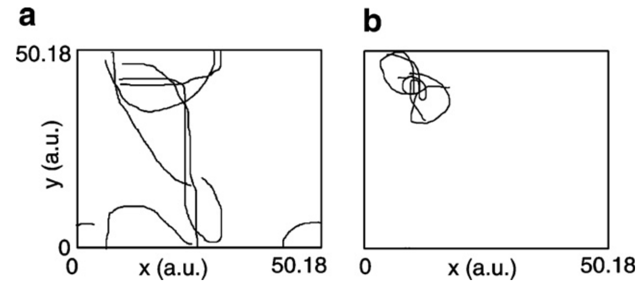

Fig. 4. Trajectory of some topological defects over 0.95 s in a system with: (a) constant $D = 1$ and (b) $D(u) = 1 - 4u + 4u^2$. $a = 0.84$, $b = 0.07$, $\varepsilon = 0.14$. Periodic boundary conditions were used. Lattice size: $\Delta x \times L = 0.196 \times 256 = 50.18$.

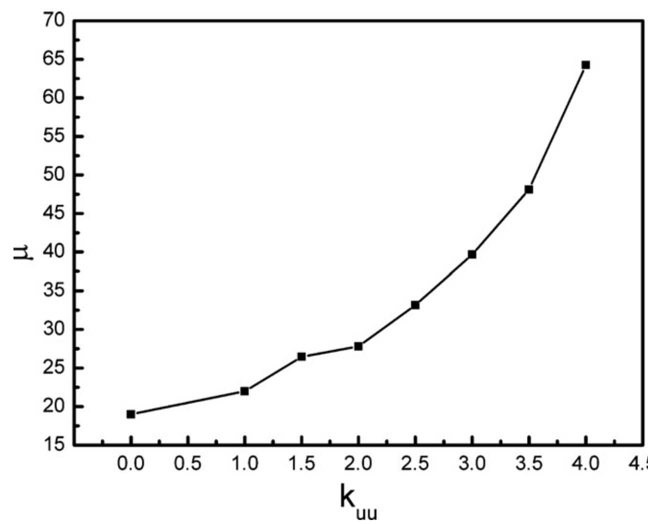

Fig. 5. μ vs. k_{uu} for $D(u) = 1 + k_u u + k_{uu} u^2$ ($k_u = -k_{uu}$), $a = 0.84$, $b = 0.07$, $\varepsilon = 0.10$. Periodic boundary conditions were used. μ was calculated averaging a total of 5000 frames sampled every 0.95 s.

The calculation of the mean value and the variance of the number of defects has been proposed as a means of characterizing the excitability of a given system. This result suggests, however, that both μ and σ also depend on the transport properties of the medium.

4. Conclusions

In the present work, we studied the effect of the concentration-dependent diffusion coefficient on the spatiotemporal behavior of the Bär model. We generalize previous findings of Roussel and coworkers in 1D [6].

The main results of our work can be summarized as follows:

(i) Inhibition of the spiral instability can be found with a negative linear coefficient in the concentration dependence of the diffusion coefficient (k_u). At a given value of ε, complete inhibition exists (for a given threshold value of k_u) in systems with nonflux boundary conditions, and a delay of the instability occurs in systems with periodic boundary conditions.

(ii) Linear dependences of the diffusion coefficient on concentration do not qualitatively modify the chaotic zone.

(iii) A quadratic dependence with the coefficients $k_u = -k_{uu}$ strongly inhibits the spiral instability, bringing the initiation of the spiral breakdown to higher values of ε. Also the chaotic zone is strongly altered. Both μ and σ show a positive dependence on ε, which is stronger than in the original Bär model. The translational movement of defects is strongly inhibited, while the rate of both defect-creation and defect-destruction processes increases.

Defect statistic has been extensively studied as a means of characterizing the excitability of a given system. It has been argued that the quantification of the mean value and the variance of the number of defects could be used to estimate the excitability of the system, i.e., the ε value in the Bär model.

Our work suggests that a local modulation of the transport properties of the medium should equally modify the turbulent states in excitable media. These modifications have not been reported so far and appear as a consequence of a second-order modulation of the diffusion coefficient dependence on the activator concentration. In surface reactions, the concentration dependence of the diffusivities is often dramatically nonlinear, as is certainly the case in biological applications due to highly nonlinear responses of the transporters to local concentrations. The existence of turbulent states of electrical activity in the heart muscle is related to the appearance of ventricular fibrillation, a severe cardiac condition that normally evolves from ventricular arrhythmias throughout a spiral breakdown scenario.

The present study contributes to the elucidation of the influence of transport processes on the development of chaotic states [19].

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