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Defect-mediated turbulence and transition to spatiotemporal intermittency in the Gray-Scott model

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In this paper, we show that the Gray-Scott model is able to produce defect-mediated turbulence. This regime emerges from the limit cycle, close or far from the Hopf bifurcation, but always right before the Andronov homoclinic bifurcation of the homogeneous system. After this bifurcation, as the control parameter is further changed, the system starts visiting more and more frequently the stable node of the model. Consequently, the defect-mediated turbulence gradually turns into spatiotemporal intermittency. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4896848]

The Gray-Scott model is known to produce spatiotemporal chaos due to the interplay between a stable state and a limit cycle. This chaos takes the form of spatiotemporal intermittency. Here, we show that the limit cycle alone can produce spatiotemporal chaos of the defect-mediated type, when having equal diffusivities for both species. The transition from defect-mediated turbulence to spatiotemporal intermittency is gradual.

Spatiotemporal chaos is often seen in reaction-diffusion systems. In many situations, this chaotic state is characterized by defects, *in extenso* by breaks in the phase of the system where the amplitude becomes zero.[1] Such defect-mediated turbulence has been observed in the Belousov-Zhabotinsky reaction[2] as well as in the Oregonator model for that reaction,[3] and in a surface reaction[4] as well as in a model for surface reactions.[5] It has also been observed in other theoretical systems such as the FitzHugh-Nagumo[6] and the Brusselator[7] models, and in the complex Ginzburg-Landau equation (CGLE).[1,8] These models[3,5–8] are all non-chaotic in the homogeneous limit, but this feature is not mandatory: The Willamosky-Rössler system does present chaos for well-mixed systems, and defect turbulence is seen in this case as well.[9]

The Gray-Scott model[10] represents the set of reaction $A + 2B \rightarrow 3B$, $B \rightarrow C$, and is one of the most studied systems in pattern formation. Spatiotemporal chaos has been observed for this system.[11] For equal diffusion coefficients of A and B, it was shown to be due to the interplay between a limit cycle and a stable steady state, a mechanism that is generic for spatiotemporal intermittency.[12] Other forms of spatiotemporal chaos are known for this system when differential diffusion is considered.[13]

Here, we show that the Gray-Scott model can show defect-mediated turbulence when the diffusion coefficients of both species are equal, and we analyze the properties of this regime as well as its interplay with the spatiotemporal intermittency. The rest of the paper is organized as follows: First, we present the model with the parameters we use, and we define the measures we take in the system to assess its dynamics. We then describe the regime of defect-mediated turbulence and show that in this regime the stable node does not play a role. We finally show how, by changing one of the parameters, we change to the regime of spatiotemporal intermittency, where the system actually alternates between defect-mediated turbulence and the stable steady state. This change is gradual so that initially the system visits the stable state very rarely and, as the parameter changes, these visits become more frequent.

The Gray-Scott model reads[10]

$$\frac{\partial a}{\partial t} = 1 - a - \mu a b^2 + D_a \nabla^2 a,$$
$$\frac{\partial b}{\partial t} = b_0 - \phi b + \mu a b^2 + D_b \nabla^2 b.$$

It represents the reaction-diffusion kinetics of the above-mentioned reactions, in the presence of two sources of reactants: a and b stand, respectively, for the concentrations of A and B. We consider here one-dimensional domains with no-flux boundary conditions. We use equal diffusivities for a and b ($D_a = D_b$), no feeding term for the autocatalyst ($b_0 = 0$) and a decay rate constant $\phi = 5$. The control parameter is thus μ, which tunes the rate of conversion of A into B by the cubic autocatalytic reaction. Under these conditions, the system has three steady states: a stable node S^n at ($a = 1$, $b = 0$), a saddle S^s at (a^-, b^-), and a focus S^f at (a^+, b^+), with

$$a^{\pm} = \frac{1 \mp \sqrt{1 - 4\phi^2/\mu}}{2},$$
$$b^{\pm} = \frac{1 \pm \sqrt{1 - 4\phi^2/\mu}}{2\phi}.$$

The focus can give rise to oscillations under the form of a limit cycle, which is found for $\mu_A < \mu < \mu_H$, where $\mu_H = \phi^4/(\phi - 1)$ is a Hopf bifurcation point[11] and μ_A stands for a homoclinic (Andronov) bifurcation, due to a collision between the limit cycle and the saddle point.

We will use several relevant measures to assess the dynamical behavior of this system. Since the spatiotemporal

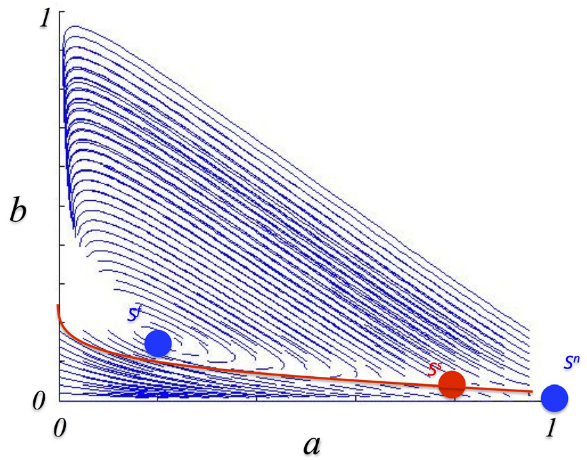

FIG. 1. Basins of attraction in the Gray-Scott model for $\mu = 155$ and $\phi = 5$. Below the red line, the system goes towards the node S^n. The saddle is marked as S^s.

intermittency implies that some regions of the system fall into S^n, we measure the distance between the local composition of the system and the point (1, 0), which we define as $l_n = ((a-1)^2 + b^2)^{1/2}$. Defect-mediated turbulence is characterized by a zero amplitude of the oscillation around the unstable focus,[14] so we also measure the distance $l_f = ((a-a^+)^2 + (b-b^+)^2)^{1/2}$. We also measure the distance to the saddle point, $l_s = ((a-a^-)^2 + (b-b^-)^2)^{1/2}$.

As we are interested in intermittency, it is convenient to know in which basin of attraction of the homogeneous system (either that of the limit cycle or that of S^n) each point of the spatially extended system is. To do so, we introduce a Boolean variable X, such that $X = 0$ when the local composition is above the separatrix of the homogeneous dynamics, and is 1 otherwise (see Figure 1). This measure can be used even after the Andronov bifurcation, as long as the saddle point exists.

With these tools in hand, we first consider a situation for which the limit cycle and the stable node coexist.[15] For $\mu = 155$, we observe a form of spatiotemporal chaos for which the distance l_f to the focus sometimes reaches zero, whereas the distance towards S^n is always large (Figure 2(a)).

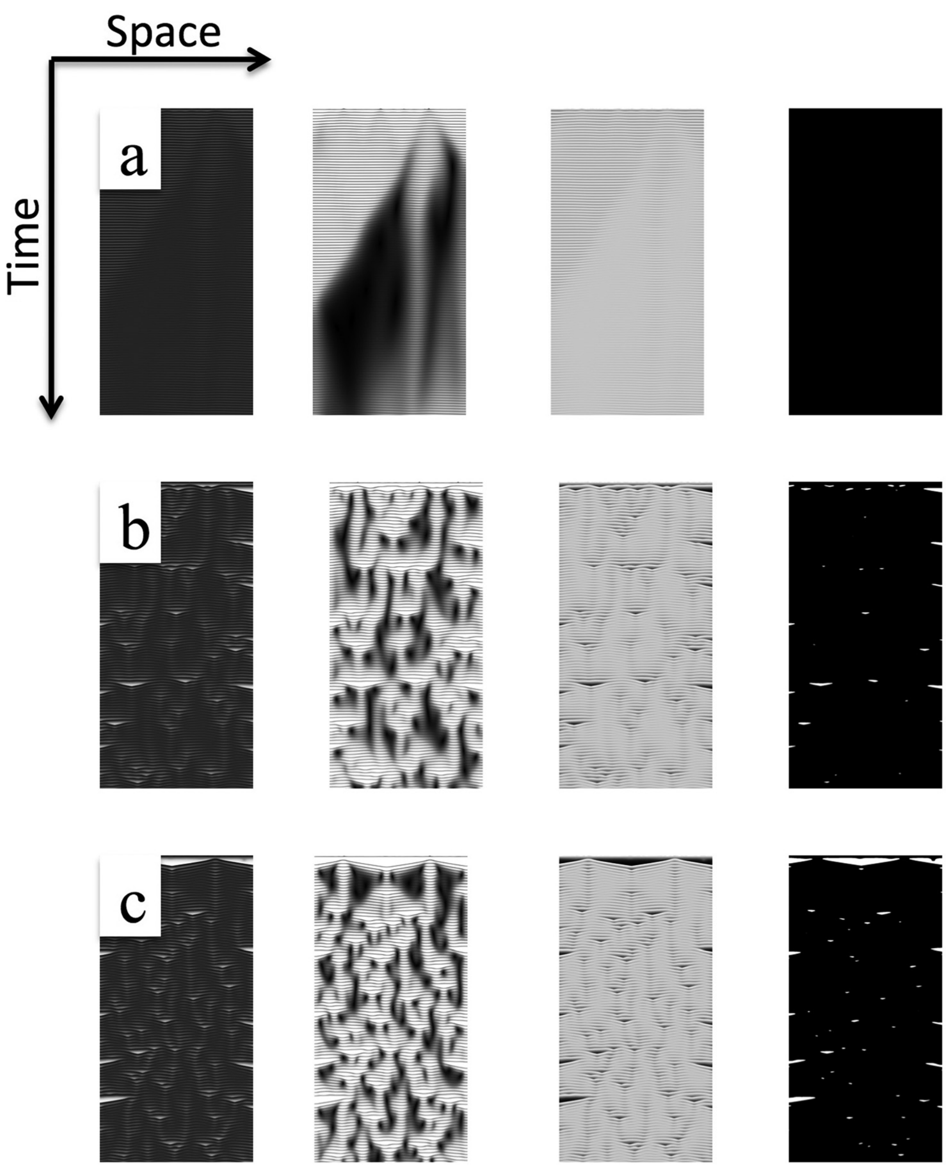

FIG. 2. Space-time plots for $\mu = 155$ (a), 151 (b), and 149 (c), showing the concentration of a (first column), *amplitude* (second column), distance to (1, 0) (third column), and the basins of attraction (fourth column). The size of the space-time plots is 100 space units $\times$ 200 time units. For the first three columns, black corresponds to a low value. For the fourth column, black represents the system being in the basin of attraction of the limit cycle, while white stands for the system being in the one of S^n.

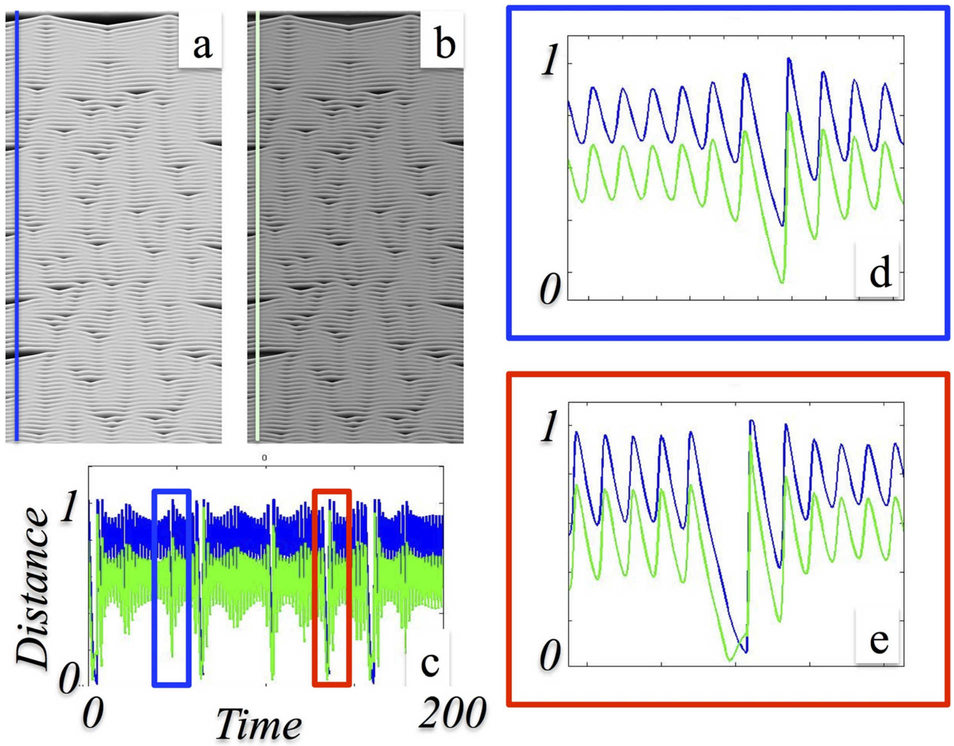

FIG. 3. Space-time plots for $\mu = 149$, showing the distance to (1, 0) (a) and to the saddle point (b). Size of space-time plots is 100 space units $\times$ 200 time units, with black corresponds to a low value. (c) Time traces for the lines in blue and light green in (a) and (b), respectively. (d) and (e) Enlargement of the boxes marked in (c).

Moreover, we see that here the system remains entirely within the neighborhood of the limit cycle. The chaotic dynamics that we observe is thus not spatiotemporal intermittency, as usually observed in the Gray-Scott model, but defect-mediated turbulence. In a sense, one could say that the system behaves "as if" the limit cycle were the only low-dimensional attractor in the system and from which chaos can emerge.

This raises the question of the transition from such defect-mediated mechanism to the traditional spatiotemporal

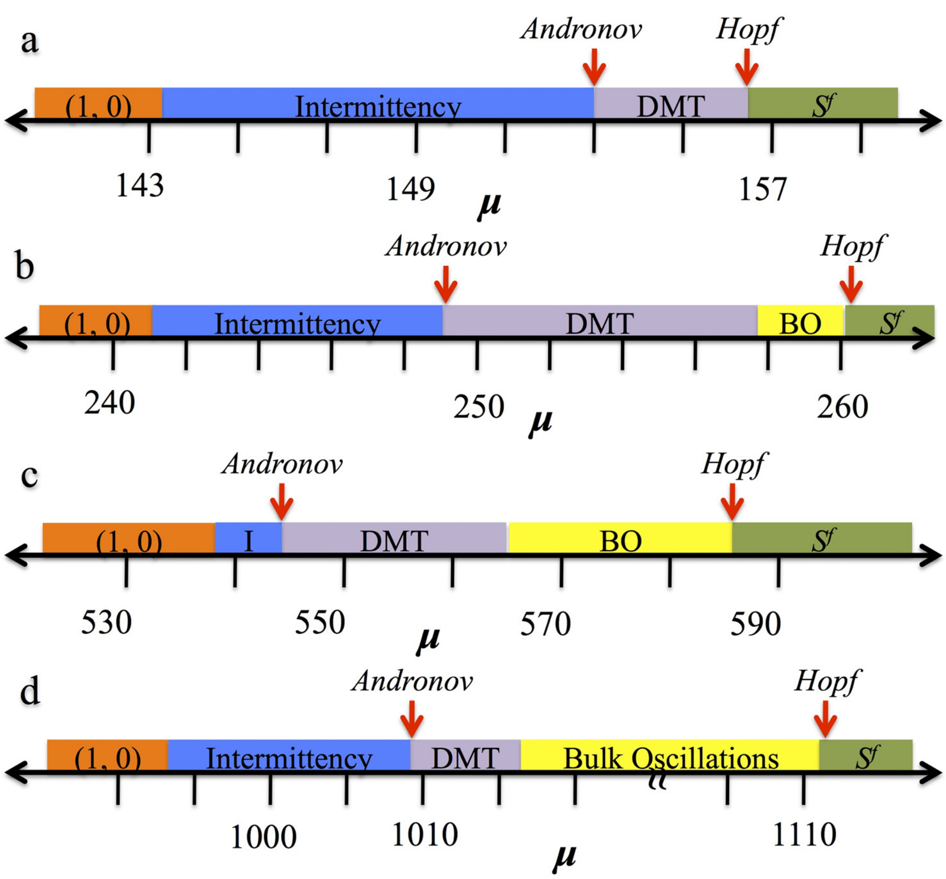

FIG. 4. Phase diagrams for $\phi = 5$ (a), $\phi = 6$ (b), $\phi = 8$ (c) and $\phi = 10$ (d).

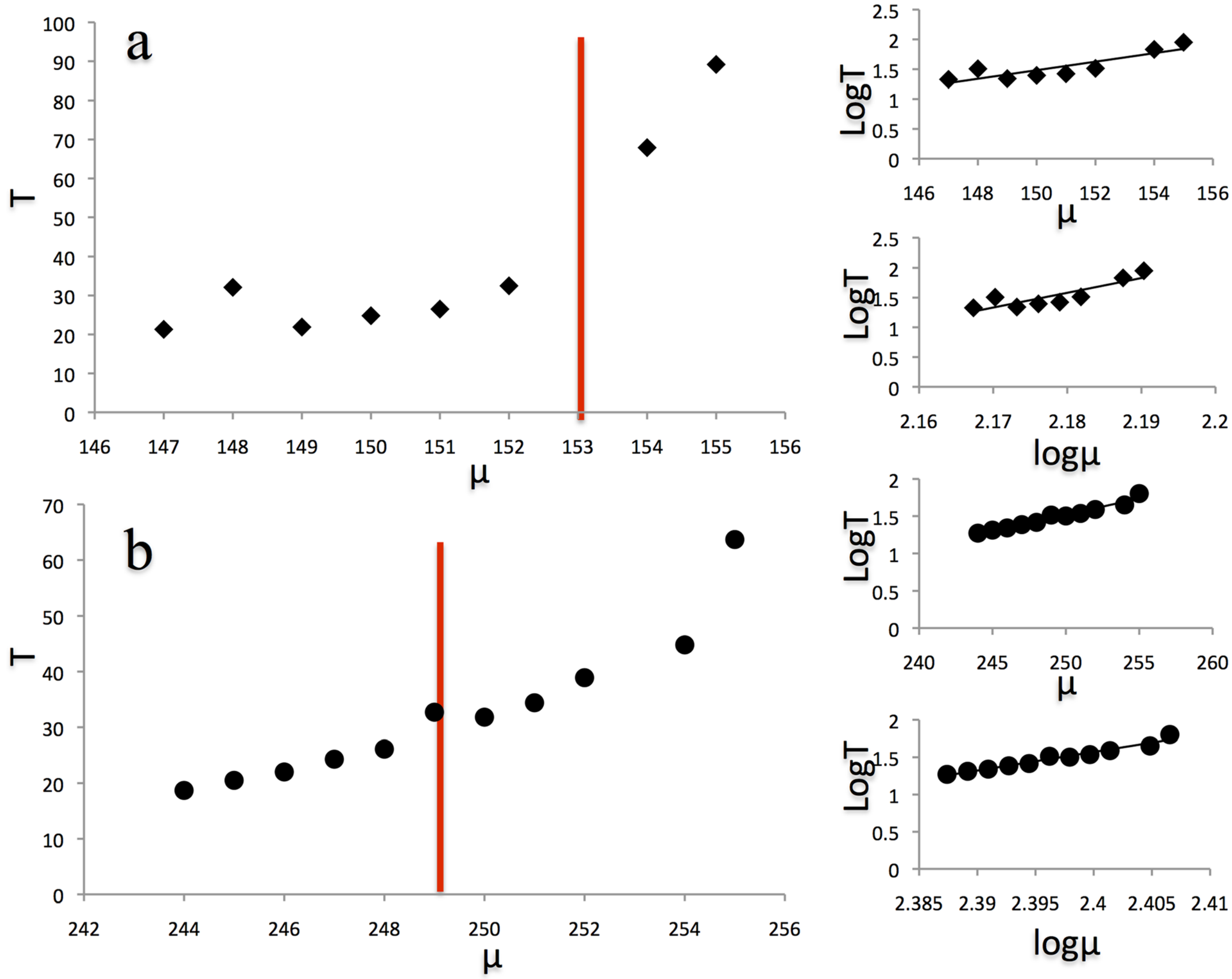

FIG. 5. Statistics for the time spent in a defect (T) over 1000 time units for $\phi = 5$ (a) and $\phi = 6$ (b) at different values of μ, and the red line shows where the Andronov homoclinic bifurcation occurs. Insets show the logarithm of the time spent at the defect vs μ (top) and vs log μ (bottom). For $\phi = 5$, the fits are $\log T = 0.071(\mu) - 9.253$ (with $R^2 = 0.758$) and $\log T = 24.79\log(\mu) - 52.48$ (with $R^2 = 0.753$). For $\phi = 6$, the fits correspond to to $\log T = 0.043(\mu) - 9.350$ (with $R^2 = 0.962$) and $\log T = 24.96\log(\mu) - 58.33$ (with $R^2 = 0.961$).

intermittency. To assess this problem, we decrease gradually the control parameter μ. For $\mu = 153$, we reach the Andronov homoclinic bifurcation, which means that the limit cycle should, in principle, disappear. We still observe however the same type of defect-mediated turbulence, but on very rare occasions, the system now reaches S^n. This observation corresponds to an intermittent behavior, as the system alternates between the two basins of attraction. For $\mu = 151$, the

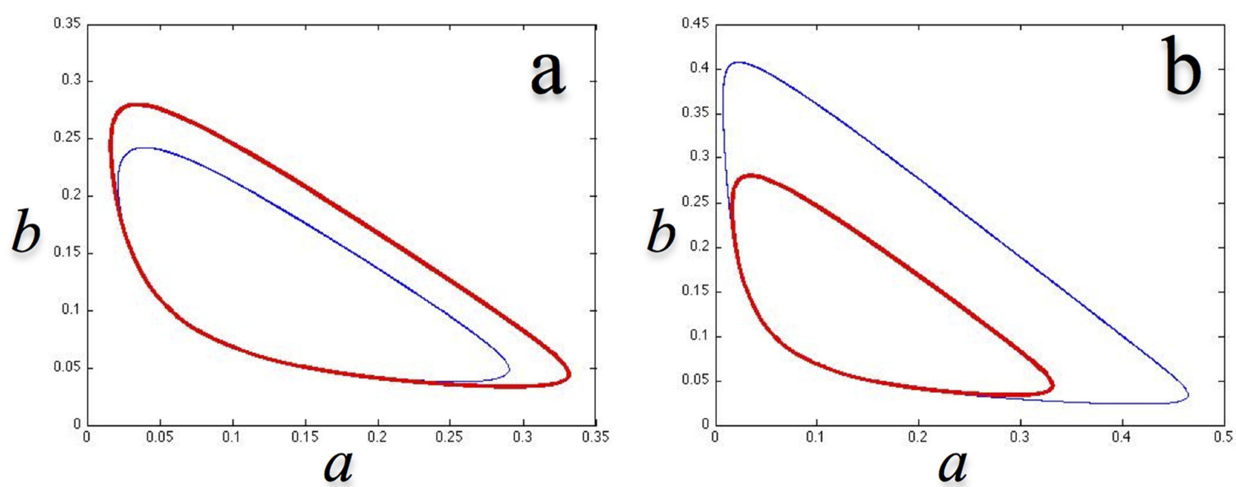

FIG. 6. Limit cycles for $\phi = 10$ and (a) $\mu = 1020$ (red) and 1030 (thin blue) and (b) $\mu = 1020$ (red) and 1010 (thin blue).

frequency of *visits* to S^n increases (Figure 2(b)), as does the frequency of *amplitude* reaching 0. For $\mu = 149$, we see (Figure 2(c)) that the amplitudes l_f and the distance l_n often reach 0. Consequently, the system alternates constantly between the (previous) basins of attraction, and the dynamics can be qualified as being "fully" intermittent. It should be also noted that the distances l_n and l_s are usually synchronized during the defect-mediated turbulence (as shown in Figure 3), the system being closer to the saddle than to the node. This synchronization changes when the system falls into S^n, since the system passes through the saddle point first (Figure 3(d)).

The different observed behaviors are summarized in Figure 4(a). We see that the Hopf bifurcation ($\mu_H = 156.25$) is close to the homoclinic bifurcation ($\mu_A \approx 153$). To assess how the distance between these two bifurcation points affects the dynamics, we now investigate the system at different values of ϕ. For $\phi = 10$, the Hopf bifurcation occurs at $\mu_H = 1111.11$, whereas the Andronov bifurcation takes place at $\mu_A \approx 1009$. In this case, we see again that before (but close to) the Andronov bifurcation, the system displays defect-mediated turbulence. After that bifurcation, it additionally presents *visits* to the (1, 0) state (Figure 4(d)). However, the defect domain is now separated from the Hopf bifurcation by a region of stable bulk oscillations, indicating that the defect-mediated regime can be found close as well as far from the Hopf point. Intermediate values of $\phi = 6$ and $\phi = 8$ are shown in Figures 4(b) and 4(c), respectively. These results confirm our observation that the defect-mediated regime always occurs close to the Andronov bifurcation point. Note that the saddle-node bifurcation at which the saddle point vanishes occurs at low values of μ (for $\phi = 5$, $\mu_s = 100$, whereas for $\phi = 10$, $\mu_s = 400$) and is not what causes the disappearance of the intermittency in favor of the (1,0) point.

We have extracted and analyzed several statistical quantities related to the defects in order to further characterize the defect-mediated and the intermittent states. We observed that the number of defects in the system varies as time goes by, but that the time-averaged value does not depend appreciably on μ for a fixed value of ϕ: There are usually between 2 and 3 defects for 100 space units. However, the time spent by each point of the system in a defect strongly increases with μ, as illustrated in Figure 5 for $\phi = 5$ and $\phi = 6$. These curves can be fitted with both an exponential and a power law. As the insets of Figure 5 show, the correlation coefficient is essentially the same for the semi logarithmic and the logarithmic plots, so that we cannot really discriminate between these two laws. We note that the statistics do not change abruptly when the Andronov homoclinic bifurcation is crossed, a further indication that the transition to spatiotemporal intermittency is gradual.

How can we understand, at least qualitatively, the appearance of defect-mediated turbulence? In order to see what is different between the dynamics of the homogenous system before and after the appearance of spatiotemporal chaos, we plot in Figure 6(a) the limit cycle at $\phi = 10$ and $\mu = 1030$ and 1020 (in the region of bulk oscillations) and in Figure 6(b) the limit cycle at $\phi = 10$ and $\mu = 1010$ and 1020 (in the region of defect-mediated turbulence). We see that in Figure 6(a) there is but a small modification of the size of the limit cycle, while in Figure 6(b) the same change in the parameter produces a large increase of this size. This situation is similar to what is seen for the Oregonator model,[3] for which the domain where spatiotemporal chaos occurs separates small amplitude oscillations (close to the Hopf bifurcation) and large amplitude oscillations (away from the Hopf bifurcation). The extreme variability of the amplitude with respect to small parametric changes seems to be the main reason behind the emergence of chaos in the Oregonator. We believe that, similarly, the system can be "excited" locally from a small limit cycle towards a big one, and that this excitation can make that part of the system pass extremely close to (and eventually go through) the unstable focus, which acts as a defect.

In summary, we have found a regime of defect-mediated turbulence in the Gray-Scott model in which the presence of the stable node S^n does not play a role towards the formation of spatiotemporal chaos. This behavior is observed far from the Hopf bifurcation and, despite the chaotic behavior, the system always remains within the basin of attraction of the limit cycle generated by the unstable focus S_f. Decreasing the control parameter μ makes the limit cycle of the homogeneous problem collide with the saddle point (*via* a homoclinic bifurcation). At this point, the extended system shows, on top of the defect-mediated turbulence, very rare jumps to the node S^n. As the parameter μ is further decreased, these excursions become more frequent and one observes the type of chaos reported thus far in the literature. Note that the excursions to the stable node always pass through the saddle point.

An analytical assessment of the behavior of the defects and of their statistics would certainly bring a crucial additional understanding of their origin and properties. We expect that such a study could be done in the limit where the Hopf and the Andronov bifurcation are close, or if they merge. It is well-known that near a Hopf bifurcation, a system can be represented by amplitude equations that take the form of the CGLE.[1] Such amplitude equations have, for example, been derived previously for the Gray-Scott model.[12] It is also known that the CGLE can sustain defect-mediated turbulence.[8] The transition from defect-mediated turbulence to spatiotemporal intermittency should be seen and could be investigated with a CGLE-like equation that accommodates the presence of multiple steady states.

On a more general note, we can conclude that having a stable state coexisting with a limit cycle does not imply having spatiotemporal intermittency. Similarly, having defects in an oscillatory behavior does not exclude the possibility of having spatiotemporal intermittency as well.

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[1]B. I. Shraiman, A. Pumir, W. Van Saarloos, P. C. Hohenberg, H. Chaté, and M. Holen, Phys. D **57**, 241–248 (1992).
[2]Q. Ouyang and J. M. Flesselles, Nature **379**, 143 (1996).
[3]I. Berenstein and C. Beta, J. Chem. Phys. **135**, 164901 (2011).
[4]C. Beta, A. S. Mikhailov, H. H. Rotermund, and G. Ertl, Europhys. Lett. **75**, 868–874 (2006).

[5]K. Krischer, M. Eiswirth, and G. Ertl, J. Chem. Phys. **96**, 9161 (1992); D. Krefting and C. Beta, Phys. Rev. E **81**, 036209 (2010).
[6]M. Bär, M. Hildebrand, M. Eiswirth, M. Falke, H. Engel, and M. Neufeld, Chaos **4**, 499 (1994).
[7]Q. Zhuang, X. Gao, Q. Ouyang, and H. Wang, Chaos **22**, 043133 (2012).
[8]P. Coullet, L. Gil, and J. Lega, Phys. Rev. Lett. **62**, 1619 (1989).
[9]J. Davidsen and R. Kapral, Phys. Rev. Lett. **91**, 058303 (2003).
[10]P. Gray and S. K. Scott, Chem. Eng. Sci. **39**, 1087–1097 (1984).
[11]J. H. Merkin, V. Petrov, S. K. Scott, and K. Showalter, Phys. Rev. Lett. **76**, 546 (1996); R. Wackerbauer and K. Showalter, *ibid.* **91**, 174103 (2003).
[12]M. Argentina and P. Coullet, Phys. A **257**, 45–60 (1998).
[13]Y. Nashiura and D. Ueyama, Phys. D **150**, 137–162 (2001).
[14]M. Bertram and A. S. Mikhailov, Phys. Rev. E **63**, 066102 (2001).
[15]I. Berenstein and C. Beta, Phys. Rev. E **86**, 056205 (2012).