Spatiotemporal Chaos of Self-Replicating Spots in Reaction-Diffusion Systems

Hongli Wang and Qi Ouyang*
Department of Physics, Peking University, Beijing 100871, China
Center for Theoretical Biology, Peking University, Beijing 100871, China
The Beijing-Hong Kong-Singapore Joint Center for Nonlinear and Complex Systems (PKU), Beijing 100871, China
(Received 25 May 2007; published 20 November 2007)

The statistical properties of self-replicating spots in the reaction-diffusion Gray-Scott model are analyzed. In the chaotic regime of the system, the spots that dominate the spatiotemporal chaos grow and divide in two or decay into the background randomly and continuously. The rates at which the spots are created and decay are observed to be linearly dependent on the number of spots in the system. We derive a probabilistic description of the spot dynamics based on the statistical independence of spots and thus propose a characterization of the spatiotemporal chaos dominated by replicating spots.

DOI: 10.1103/PhysRevLett.99.214102 PACS numbers: 05.45.Jn, 05.40.−a, 82.40.Ck

Spatiotemporal chaos (STC) refers to the state where a high-dimensional dynamical system is temporally chaotic and spatially irregular [1]. Although pattern formation in nonequilibrium systems has been extensively investigated in the past decades, STC is as yet not well understood and is the focus of current experimental and theoretical research. One of the central challenges in this field is the origin of STC. Several mechanisms for the transition to these states have been proposed, such as the Ruelle-Takens scenario [2], sequences of bifurcations via quasiperiodicity or temporal chaos [3], instabilities of spiral wave patterns [4], and others.

Another important problem in the study of STC is to find the characterizations of the disordered states. Beyond the simple description of correlation functions, macroscopic approaches that describe STC on large spatial and temporal scales have been derived for a few systems [5,6]. For many STCs that arise in a wide range of pattern-forming systems, the dynamics of a pattern is dominated by defects, such as vortices or dislocations, which nucleate and annihilate perpetually. The defects are a feature of the disordered state, and the dynamics of defects can be used to characterize the spatiotemporally chaotic state [7–13]. Description of a stochastic master equation and the probability distribution for the number of defects have been derived. The complex STCs were thus represented by the relatively simple dynamics of defects.

In this Letter, we consider the STC of self-replicating spots in reaction-diffusion systems where a pattern is dominated by spots [14]. The self-replicating spot [15–23] is a phenomenon visually similar to biological cell division. The spots consist of localized regions where the concentrations of reactants differ from the background field. They grow to a critical size and split in two, which can then grow and divide again. On the other hand, the spots interact with each other; they can decay to the background when they feel too crowded. The asymptotic pattern is characterized by perpetual and indefinite creation and annihilation of spots, a typical spatiotemporally chaotic behavior [See Fig. 1(a)]. It has been found that such replication of spots is generic in a broad class of reaction-diffusion systems and was observed in well-controlled experiments [15,21] and studied in the Gray-Scott model [16–20], the four-species reaction-diffusion model for the ferrocyanide-iodate-sulfate reaction [21], the FitzHugh-Nagumo model [22], and others [23].

Our goal here is to characterize the STC of self-replicating spots by looking into the statistical properties of the spots that dominate the chaotic pattern in the reaction-diffusion Gray-Scott model. We find that the rates at which the spots are created and decay are linearly dependent on the number of spots in the system. We derive a probabilistic description for the spot dynamics based on observed creation and annihilation rates, and we present theoretical results that agree with our numerical findings on the base of the assumption of statistical independence of spots.

Model and methodology.—Patterns of replicating spots have been studied most often with the Gray-Scott model [24]. The kinetic reaction-diffusion equations for the model can be written as [14]

$$\frac{\partial u}{\partial t} = -uv^2 + F(1-u) + D_u \nabla^2 u, \tag{1}$$

$$\frac{\partial v}{\partial t} = uv^2 - (F+k)v + D_v \nabla^2 v, \tag{2}$$

where u and v represent the concentration of species U and V, respectively. F and k are control parameters. The system has a trivial homogeneous state ($u = 1$, $v = 0$, referred to as the red state), which is always linearly stable. Two additional steady states can be created through a saddle-node bifurcation, the stable one of which is referred to as the blue state and can lose it stability through Hopf and Turing bifurcations.

The self-replicating pattern in the Gray-Scott model was first described by Pearson [14], who also reported a rich variety of other spatiotemporal patterns by making small changes in the control parameters F and k. Dependent on the parameters, the replicating spots can form steady states

 © 2007 The American Physical Society

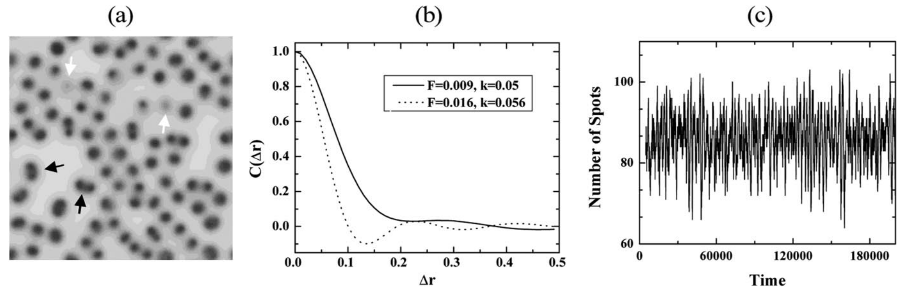

FIG. 1. (a) Spatiotemporal chaos of self-replicating spots in the Gray-Scott model. In the gray-scale snapshot, black represents the lowest value of u. Spot splitting is indicated by black arrows; white arrows are for spots that are being annihilated. (b) Spatial correlation functions calculated from chaotic patterns of self-replicating spots. (c) The number of spots as a function of time. $F = 0.016$, $k = 0.056$ for (a) and (c).

where the spots consist of a hexagonal pattern, or typically result in chaotic states in which the spots compete for territory. The spot multiplication process [16,18,20] and pattern formation [25] in this system have been studied in detail. The transition to STC has also been investigated from the global bifurcation viewpoint [26]. Instead, here we are interested in the statistical dynamics of STC of self-replicating spots in the chaotic regime.

The numerical simulation of the system evolution is performed by direct integration of Eqs. (1) and (2) with a finite-difference algorithm. Periodic boundary conditions have been applied. The spatial domain consists of a 200×200 lattice with mesh space $h = 0.01$. The initial conditions employed throughout this paper consist of a localized square pulse of size 20×20 that perturbs the homogeneous red state. We fix the diffusion coefficients to the values $D_u = 2.0 \times 10^{-5}$, $D_v = 1.0 \times 10^{-5}$. Before data are analyzed, the system has been integrated for 40 000 time steps (step $dt = 0.1$) in order for the transient to die out.

In $F - k$ space, the parameter values we use fall in the STC region of self-replicating spots, i.e., pattern ε in Pearson's paper [14]. The region locates lower than but very close to the lower branch of the saddle-node bifurcation curve $F_{\rm sn} = (1 - 8k \pm \sqrt{1 - 16k})/8$. Slightly over the lower branch, Turing instability of the blue state arises in a narrow region stretching along the saddle-node curve. When $D_u/D_v = 2$, this region falls almost entirely within the region where the system also exhibits a Hopf instability [25].

Results.—A snapshot from the evolution of a spatiotemporal chaos of self-replicating spots is illustrated in Fig. 1(a). The map is coded with the gray scales of the concentration of u field. Spots in the pattern are localized regions of low u value and high v value, which are generated from the trivial steady state, i.e., the background with $u = 1.0$ and $v = 0.0$. They are readily recognized numerically by determining the locations of minima in the u field and/or maxima in the v field. The spots can undergo division or decay, as demonstrated in Fig. 1(a) with black or white arrows. In the chaotic regime, they are constantly created by spot multiplications, move fast, and decay into the background. The processes occur continuously and indefinitely, and the spatiotemporal pattern looks like a chaotic "soup" of spots. Notice that in this system, spots do not merge together because they are repulsive.

For the irregular patterns, we calculated the spatial autocorrelation function $C(\Delta r) = \langle [u(r,t) - \langle u \rangle] \times [u(r + \Delta r, t) - \langle u \rangle] \rangle_{r,t}$, where $\langle\rangle_{r,t}$ signifies the average over the space and time, and $\langle u \rangle$ is the average of u field. Figure 1(b) depicts $C(\Delta r)$ for the patterns obtained with different parameters. The correlations decay exponentially with short characteristic length scales, demonstrating spatial incoherence in the system. In Fig. 1(c), the number n of spots in the pattern of Fig. 1(a) is shown as a function of time. The fluctuations in $n(t)$ provide further evidence of the existence of STC mediated by spots. From the time series $n(t)$, a mean value $\langle n \rangle$ of 85.9 is obtained with a standard deviation of $\sigma = 6.2$ for the fluctuations. Figure 2 depicts the probability distribution function for the number of spots n obtained from simulations.

As the spots compete with each other, the creation and decay rates are dependent on the total number of spots in the system. Figure 3 shows the rates under parameters $F = 0.016$ and $k = 0.056$. They are obtained by counting the

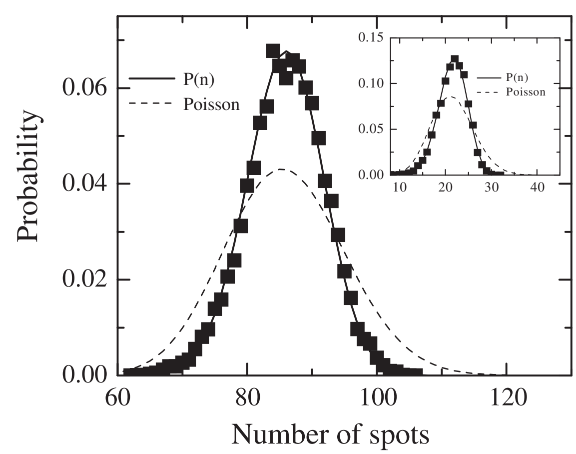

FIG. 2. Probability distribution function for the number of spots computed from time series $n(t)$ (squares) and from theory of Eq. (6) (solid line). Parameters as in Fig. 1(a). The dashed line is the Poisson distribution. For the inset, $F = 0.014$, $k = 0.053$, simulated with a 100×100 lattice.

current number of spots at time t and those being created and vanishing in a subsequent short time interval and are then averaged over long time of evolution. We observe that both the creation and annihilation rates are linearly dependent on the total number n of spots in the system. The multiplication rate decreases while the decay rate increases as a function of the number of spots. For different parameters, the linear dependence of the rates on n also hold. The observed creation rate $\Xi_+(n)$ and annihilation rate $\Xi_-(n)$ are therefore approximately given by

$$\Xi_+(n) = c_0 + c_1 n, \tag{3}$$

$$\Xi_-(n) = a_0 + a_1 n. \tag{4}$$

For the rates in Fig. 3, these values are found to be $c_0 = 1.007$, $c_1 = -0.0077$, $a_0 = 0.162$, $a_1 = 0.0021$. The coefficients depend on the parameters F and k. As we explore the $F - k$ parameter space where the system exhibits the disordered states of spots, the relation of Eqs. (3) and (4) always holds. For instance, under parameter values $F = 0.009$, $k = 0.05$, the line of creation rate has a positive slope ($c_1 > 0$) and both rates grow linearly with the number of spots ($a_1 > 0$). Whatever parameter values in the regime of spot chaos are taken, the multiplication rate is always higher than the annihilation rate when the spot density is low and background space is available, while the latter surpasses the former when there is insufficient space with too many spots in the system. From these observations, we conclude that the linear dependence of Ξ_+ and Ξ_- on $n(t)$ is characteristic of the STC of self-replicating spots.

To establish a quantitative connection between the observed creation or annihilation rates and the spot number distribution function, we consider a simple probabilistic description for spot dynamics that is an extension of the model for defect-mediated turbulence [7]. As the average distance between the spots is larger than the correlation length in the pattern, it can be assumed that the spots in the system are statistically independent entities, and the spot dynamics follows a discrete birth-death Markov stochastic process with the transition rates $\Xi_+(n)$ and $\Xi_-(n)$. In the statistical stationary state of detailed balance, the probability distribution function $P(n)$ of finding a number of n spots in the system satisfies the master equation of the simple recursion,

$$P(n) = \frac{\Xi_+(n-1)}{\Xi_-(n)} P(n-1). \tag{5}$$

Based on the observed creation and annihilation rates of Eqs. (3) and (4), the above recursive relation leads to the following distribution function:

$$P(n) = P(0) \prod_{j=0}^{j=n-1} \frac{c_0 + c_1 j}{a_0 + a_1(j+1)}, \tag{6}$$

where $P(0)$ is determined by the normalization condition.

Figure 2 illustrates the probability distribution function $P(n)$ of Eq. (6) with the coefficients determined from the creation and annihilation rates of Fig. 3. It matches closely the distribution derived directly from numerical simulations.

The above probabilistic description is based on the assumption that the spots are statistically independent; i.e., the spots in the chaotic patterns are uncorrelated. This assumption is supported by the power spectrum calculated from the time series $n(t)$ of spots. If the fluctuations in $n(t)$ arise from independent random events, the power spectrum $S(f) = |\frac{1}{T} \int_0^T dtn(t) \exp[-i2\pi ft]|^2$ would have a Lorentzian shape [11], i.e, $S(f) \propto f^{-\gamma}$ with $\gamma = 2.0$. Figure 4 shows that for not too small frequencies, the power spectrums for spots have Lorentzian shape with the values of exponent γ very close to 2.0 for different parameters. This indicates that the spots are uncorrelated and statistically independent. The result we find here for patterns of self-replicating spots is in contrast with previous findings for defect-mediated turbulence in the Willamowski-Rössler model and in a recent experiment of catalytic surface reaction [11] where the power spectrum has a non-Lorentzian shape and the defects exhibit short-range correlations.

Conclusion and Discussion.—For spatiotemporally chaotic systems that are dominated by special entities in the pattern, such as defects in defect-mediated turbulence or replicating spots of disordered states, it is possible to obtain a reduced description for the complex dynamics by building low dimensional phenomenological models for the objects that feature the disordered pattern. In this Letter, we have analyzed the statistical properties of self-replicating spots that dominate the spatiotemporal chaos in the Gray-Scott model. The multiplication and annihilation rates of the spots as functions of the total spots in the system have been obtained. We found that as there are sufficient space and low number of spots in the system, the multiplication rate is faster than that of the annihilation,

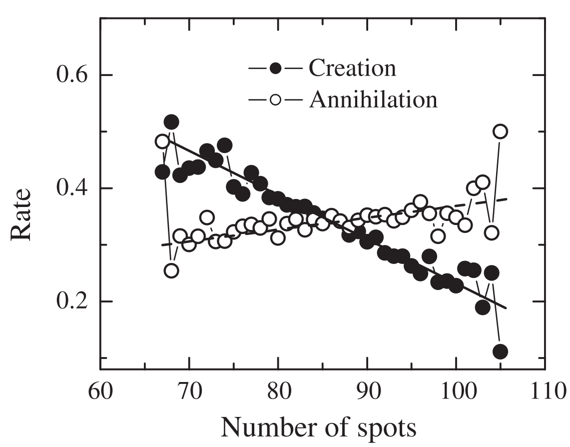

FIG. 3. The creation rate (black dots) and annihilation rate (open circles) as functions of the number of spots in the pattern. Parameters: $F = 0.016$, $k = 0.056$.

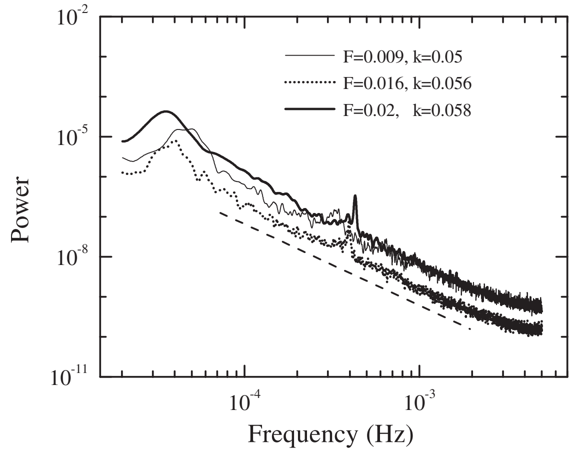

FIG. 4. Power spectrum $S(f)$ of the time series of spot number $n(t)$ vs the frequency f for different parameters. The dashed line is to guide the eye and scales as $f^{-\gamma}$ with $\gamma = 2.0$.

while the former is surpassed by the latter as the system contains a sufficiently high number of spots. Both rates exhibit linear dependence on the number of spots in the pattern. The processes of spot multiplication and decay are found to be statistically independent, and the spot dynamics can be described as a discrete Markovian random walk. Based on the observed linear dependence of the rates on n, we derived a theoretical probability distribution function for the number of spots that agrees well with numerical simulations. The disordered states of replicating spots, which have been found to be common in a broad class of reaction-diffusion systems, are therefore characterized with the reduced description of spots.

The spot dynamics of spot-mediated STC in the Gray-Scott model we considered here is similar to the defect dynamics in defect-mediated turbulence [7–13] that have been previously studied theoretically and experimentally. Both the defects and spots have been assumed to follow stochastic random walks. Because of different instability mechanisms of these disordered states, the detailed dynamics of spots and defect is distinct. The main difference comes from the creation and decay rates. For defects of vortices [7] or dislocations [9], the nucleation of defect is independent of n. The annihilation rate can be best approximated with a rate proportional to n^2 [7] or follows a combined quadratic and linear dependence on n [13]. For penta-hepta defect chaos [10], the defect is no longer created constantly but follows a quadratic polynomial rate $c_0 + c_1 n + c_2 n^2$. The defects decay also with the rate $a_1 n + a_2 n^2$. For chaos of replicating spots that we reported here, both rates of replicating and decay of spots depend linearly on n (see Fig. 3). Accordingly, the distribution function for replicating spots is different from those of defects. Besides these, defects have been reported to typically have short-range correlations [8,11,13], while the spots in the Gray-Scott arose from independent random events as indicated by the Lorentzian shape power spectrum.

The work is supported by the National Basic Research Program of China (973 Program) (No. 2007CB814800) and the Natural Science Foundation of China (No. 10774008).

*To whom all correspondence should be addressed: qi@pku.edu.cn.

[1] M. C. Cross and P. C. Hohenberg, Rev. Mod. Phys. **65**, 851 (1993); T. Bohr, M. H. Jensen, G. Paladin, and A. Vulpiani, *Dynamical Systems Approach to Turbulence* (Cambridge University Press, Cambridge, 1998).
[2] D. Ruelle and F. Takens, Commun. Math. Phys. **20**, 167 (1971).
[3] Z. Qu, J. N. Weiss, and A. Garfinkel, Phys. Rev. Lett. **78**, 1387 (1997); F. Brochard, E. Gravier, and G. Bonhomme, Phys. Rev. E **73**, 036403 (2006).
[4] Q. Ouyang and J. M. Flesselles, Nature (London) **379**, 143 (1996).
[5] V. Yakhot, Phys. Rev. A **24**, 642 (1981); S. Zaleski, Physica D (Amsterdam) **34**, 427 (1989).
[6] G. D. Granzow and H. Riecke, Phys. Rev. Lett. **77**, 2451 (1996).
[7] L. Gil, J. Lega, and J. L. Meunier, Phys. Rev. A **41**, 1138 (1990).
[8] M. Hildebrand, M. Bär, and M. Eiswirth, Phys. Rev. Lett. **75**, 1503 (1995).
[9] K. E. Daniels and E. Bodenschatz, Phys. Rev. Lett. **88**, 034501 (2002); Chaos **13**, 55 (2003).
[10] Y. N. Young and H. Reicke, Phys. Rev. Lett. **90**, 134502 (2003).
[11] J. Davidsen and R. Kapral, Phys. Rev. Lett. **91**, 058303 (2003);
[12] H. Wang, Phys. Rev. Lett. **93**, 154101 (2004).
[13] C. Beta, A. S. Mikhailov, H. H. Rotermund, and G. Ertl, Europhys. Lett. **75**, 868 (2006).
[14] J. E. Pearson, Science **261**, 189 (1993).
[15] K. J. Lee, W. D. McCormick, Q. Ouyang, and H. L. Swinney, Science **261**, 192 (1993).
[16] W. N. Reynolds, J. E. Pearson, and S. Ponce-Dawson, Phys. Rev. Lett. **72**, 2797 (1994); W. N. Reynolds, S. Ponce-Dawson, and J. E. Pearson, Phys. Rev. E **56**, 185 (1997).
[17] N. Parekh, V. R. Kumar, and B. D. Kulkarni, Phys. Rev. E **52**, 5100 (1995).
[18] Y. Nishiura and D. Ueyama, Physica D (Amsterdam) **130**, 73 (1999).
[19] M. R. Roussel and J. Wang, Phys. Rev. Lett. **87**, 188302 (2001).
[20] C. B. Muratov and V. V. Osipov, Eur. Phys. J. B **22**, 213 (2001).
[21] K. J. Lee and H. L. Swinney, Phys. Rev. E **51**, 1899 (1995).
[22] C. Elphick, A. Hagberg, and E. Meron, Phys. Rev. E **51**, 3052 (1995).
[23] C. B. Muratov and V. V. Osipov, Phys. Rev. E **54**, 4860 (1996).
[24] P. Gray and S. K. Scott, Chem. Eng. Sci. **39**, 1087 (1984).
[25] W. Mazin, K. E. Rasmussen, E. Mosekilde, P. Borckmans, and G. Dewel, Math. Comput. Simul. **40**, 371 (1996).
[26] Y. Nishiura and D. Ueyama, Physica D (Amsterdam) **150**, 137 (2001).