# Nonequilibrium Defect-Unbinding Transition: Defect Trajectories and Loop Statistics

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In a Ginzburg-Landau model for parametrically driven waves, a transition between a state of ordered and one of disordered spatiotemporal defect chaos is found. To get insight into the breakdown of the order, the defect trajectories are tracked in detail. Since the defects are created and annihilated in pairs, the trajectories form loops in space-time. The probability distribution functions for the size of the loops and the number of defects involved in them undergo a transition from exponential decay in the ordered regime to a power-law decay in the disordered regime. These power laws are also found in a simple lattice model of randomly created defect pairs that diffuse and annihilate upon collision.

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For pattern-forming systems far from thermodynamic equilibrium that exhibit spatiotemporal chaos, one of the important problems is how to characterize these spatially disordered and temporally chaotic states. A conspicuous feature of many of them are spatially localized defects such as the dislocations found in stripelike convection-roll patterns in Rayleigh-Bénard or electroconvection (e.g., [1,2]). A tantalizing question is whether the spatiotemporal chaos or the breakdown of order can be described in terms of these defects.

Early on in the investigation of pattern-forming systems it has been recognized that near onset dislocations in stripe patterns are mathematically closely related to defects in the equilibrium $xy$-model in two dimensions, which describes, e.g., magnetic systems in which the spins are confined to lie in a plane [3]. Both systems are described by a single complex order parameter $A$, which gives the magnitude and wave vector of the stripe pattern and the magnitude and orientation of the local magnetization, respectively. In terms of $A$ the dislocations are given by locations of vanishing magnitude, $|A| = 0$.

A fascinating phase transition studied extensively in the $xy$-model is the Kosterlitz-Thouless transition, which is associated with the unbinding of defect pairs [3,4]. The analogy between these defects and those in stripe patterns motivated early efforts to identify related phenomena also in pattern-forming systems such as Rayleigh-Bénard convection [5]. No clear signature of such phenomena were found, however. This is in part related to the fact that the phase transitions occur at finite temperature and are intimately related to the relevance of fluctuations, whereas in macroscopic systems such as Rayleigh-Bénard convection the effect of (thermal) noise is negligible in most situations [6]. The recent observations of spatiotemporal chaos in various types of convection experiments (e.g., [1,7,8]) have renewed the interest in connections between phase transitions and nonequilibrium transitions with the notion that the chaotic dynamics may to some extent mimic the fluctuations of the thermal systems.

Various aspects of the role of defects in spatiotemporal chaos have been investigated. The single-defect probability distribution function has been measured in electroconvection [9] and found to agree quite well with results based on the single complex Ginzburg-Landau equation (CGLE) and on a simple diffusive model [10]. In binary-mixture convection the defects have been used to reconstruct the full wave pattern [8]. The dynamical relevance of dislocations has been demonstrated best thus far in work that extracted the contribution of each dislocation to the total fractal dimension of the (extensively) chaotic attractor of the CGLE [11].

The spatiotemporally chaotic states found in pattern-forming systems typically arise from ordered states through some transition when a control parameter is changed. An interesting question is what actually happens when the order of the pattern breaks down. In analogy with the melting of two-dimensional crystals [3,12] one may expect that defects in the pattern may play an important role.

In this Letter, we present results for a transition between two spatiotemporally chaotic states in a Ginzburg-Landau model for parametrically excited waves [13]. While one state is disordered in space, the other retains a stripelike order despite the chaotic creation and annihilation of defect pairs. We characterize the breakdown of order in terms of the defect dynamics and find that the transition to the disordered state is associated with what one may call an unbinding of pairwise created defects. Tentative results for this unbinding transition have been presented earlier [13,14].

  

We consider a Ginzburg-Landau model for parametrically excited small-amplitude waves in a two-dimensional axially anisotropic system [15,16],

$$\partial_t A + s\partial_x A = (d\nabla^2 + a + c|A|^2 + g|B|^2)A + bB^*, \quad (1)$$

$$\partial_t B - s\partial_x B = (d\nabla^2 + a + c|B|^2 + g|A|^2)B + bA^*, \quad (2)$$

as it applies, for instance, to electroconvection in nematic liquid crystals [2]. In terms of the complex amplitudes $A$ and $B$, the waves are given by $A(x,y,t)\exp(i\omega_f\tilde{t}/2 - iq_c\tilde{x}) + B(x,y,t)\exp(i\omega_f\tilde{t}/2 + iq_c\tilde{x}) + \text{c.c.} + \text{h.o.t.}$ Here $(\tilde{x},\tilde{y},\tilde{t})$ and $(x,y,t)$ are fast and slow spatial and temporal variables, respectively. With $a \equiv a_r + ia_i$, the traveling waves arise at $a_r = 0$ in a Hopf bifurcation with frequency $\omega_H$ and wave number $q_c$. For $c_r < 0$ the bifurcation is supercritical and the waves exist for $a_r > 0$. The system is periodically forced parametrically at close to twice the Hopf frequency, $\omega_f \approx 2\omega_H$. In (1) and (2), this induces a time-independent resonant interaction term of magnitude $b$ between the amplitudes of the counterpropagating waves [15,16]. For $a_r < 0$ and $b^2 > a_r^2 + a_i^2$ standing waves are excited parametrically that are phase locked to the forcing. In the simulations we use periodic boundary conditions in both directions and solve (1) and (2) pseudospectrally with a fourth-order integrating-factor Runge-Kutta scheme.

Numerical simulations of (1) and (2) show two distinct regimes of spatiotemporal chaos for the parametrically excited waves: a conventional regime in which the spatial correlation function decays rapidly in an essentially isotropic way and a regime of spatiotemporal chaos that exhibits a strikingly ordered state in which the correlation function reveals a stripelike order [14] that is also apparent in individual snapshots [13]. The transition between the two states is discontinuous as indicated by a jump in the average number of defects.

In order to get insight into the role of the defect dynamics in this order-disorder transition, we track each defect from its creation to its annihilation. Figure 1 presents an example of the resulting space-time diagram in the regime with persistent spatial order. The $y$-location of each defect with positive topological charge (i.e., along a contour encircling the defect the argument of $A$ changes by $+2\pi$) is shown as a solid square while the $y$-location of the defects with negative charge are shown as dots. The trajectories of almost all the defect pairs form simple loops in space-time. Thus, while for topological reasons in any system defects are always annihilated in pairs of opposite charge, here the annihilating defects have also been created together. It is in this sense that we consider them to be *bound pairs*.

The preservation of stripelike order in the ordered regime can then be understood intuitively, since the dynamics of defects in simple defect loops affect only a very small portion of the system and, moreover, render the system almost unchanged after their disappearance. In some cases the space-time loops involve two (see arrow in Fig. 1) or possibly three defect pairs. Then the area of the system that is perturbed by the defects is larger, but after their annihilation the system is still left in essentially the same state as before.

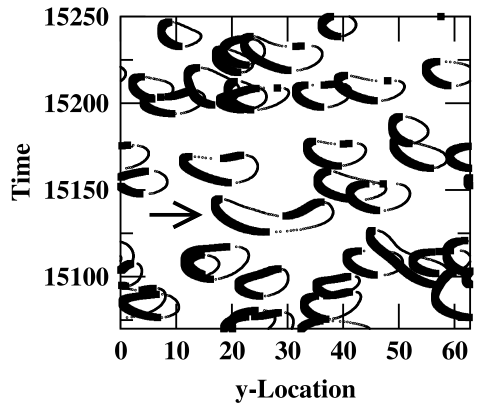


FIG. 1. Space-time diagram of defect trajectories for $a = 0.25$, $c = -1 + 4i$, $d = 1 + 0.5i$, $s = 0.2$, $g = -1 - 12i$, and $b = 2$. Squares and dots denote defects of opposite topological charge.

The orientation and position of the stripe pattern is affected significantly only between the defects. At first one may therefore expect that the destruction of order requires that the defects in a pair have to *unbind* and separate arbitrarily far from each other. However, it would also be sufficient if the defects in a given pair are annihilated by defects from two other pairs, which in turn are annihilated by further defect pairs, generating a chain of events whose trajectory in space-time is a large loop that spans the whole system. Our simulations show that in fact even in the disordered regime most defects are annihilated by their "own" partner and most loops are small compared to the system size. Thus, to distinguish the two regimes we consider more detailed measures such as the distribution of defect loops as a function of their size.

Since the relevant information turns out to be in the relatively rare, large loops, care has to be taken to identify annihilation and creation processes reliably and distinguish them from situations in which a defect simply moved relatively far in one time step. In our defect-tracking scheme we recursively check the distances between all defects $\mathcal{D}_i(t)$ at time $t$ from all defects $\mathcal{D}_i(t + \Delta t)$ at time $t + \Delta t$. If for two defects of equal charge this distance is smaller than some threshold value $\delta_1^{(n)} = n \cdot \delta_1$, they qualify as a single "continuing defect" that has moved from one position to the other. It can happen that with this criterion a given defect $\mathcal{D}_k(t)$ has more than one possible continuation defect $\mathcal{D}_j(t + \Delta t)$. Then among the possible continuation defects the one closest to $\mathcal{D}_k(t)$ is assigned to be its continuation. Defects that are not continuing defects are candidates for annihilation and creation events. Among those, two defects of opposite charge and closer than a second threshold $\delta_2^{(n)} = n \cdot \delta_2$ are identified as a pair that was annihilated (or created) in this time step. This analysis is then repeated with increased values for the thresholds, $\delta_i^{(n+1)} = (n + 1) \cdot \delta_i$, until all defects have been assigned.

Figure 2 shows our results for the relative frequency of loops consisting of at least $n$ defect pairs. These results (and those in Figs. 3 and 4) are based on 8000 time steps ($dt = 0.5$) with an average number of 7000 defects at any given time in the disordered regime. In the ordered regime ($b \geq 0.7$) very few loops contain more than five defect pairs and the distribution decays essentially exponentially. In the disordered regime ($b \leq 0.625$), however, the number of loops with many defects is greatly increased and the decay of the distribution function is only algebraic with an exponent of $\alpha \approx 1.5$.

Since the defect motion essentially affects only the (vaguely defined) part of the system between the defects, a better indicator for the expected loss of order are the spatial extents $\Delta x \equiv x_{\max} - x_{\min}$ and $\Delta y \equiv y_{\max} - y_{\min}$ of the defect loops in the $x$- and $y$-directions, respectively. Here $x_{\min,\max}$ and $y_{\min,\max}$ refer to the minimal and maximal values of $x$ and $y$ in any given loop. Note that these values need not be obtained at the same time. Thus, in principle, a small loop could still yield large $\Delta x$ or $\Delta y$ if it traveled.

Similar to Fig. 2, Fig. 3 shows the relative frequency of loops with size in the $x$-direction larger than $\Delta x$. In the ordered regime the decay is again very rapid and there are essentially no loops with $\Delta x$ larger than ten, which is of the order of one wavelength. This may indicate some pinning of the defects by the pattern in that it may restrict their motion to a predominantly climbing motion. In the disordered pattern, on the other hand, the loops reach the size of the system. In a simple interpretation these events would be associated with a persistent change in the average wave vector of the pattern. Again, the distribution functions are exponential in the ordered regime and exhibit a power law in the disordered regime with exponent $\beta \approx 3$. The distinction between the regimes is not quite as striking in the spatial extent $\Delta y$ in the $y$-direction. There, even in the ordered regime the loops can reach a size of $\Delta y \approx 100$, while the loops in the disordered regime extend to sizes of $\Delta y \approx 1000$. The distribution is still exponential in the ordered regime and appears to be power law in the disordered regime. However, the measured exponent increases from about 2.8 to 4 as $b$ is increased from 0.4 to 0.625.

The duration $\Delta t$ of the loops is also of interest and the corresponding relative frequencies are shown in Fig. 4. The exponential and power-law character of the distributions are quite clear in the respective regimes with the exponent of the power-law $\gamma \approx 2.7$.

To give further support for the existence of power laws in the distribution functions in the disordered regime and to get more insight into their origin, we have investigated a simple two-dimensional lattice model of the defect dynamics, which is based on the observation that the single-defect statistics in the disordered regime show the same signature as those of the defect chaos in the CGLE. This type of distribution has been shown to arise if the defects behave as random walkers that are annihilated upon colliding with any other defect of opposite charge [10].

The results of our implementation of the simple lattice model are shown in Fig. 5. With a probability $p$, random walkers of opposite charge are created pairwise at the same randomly chosen site of a square lattice. They interact only with walkers of opposite charge and annihilate upon contact. Figure 5 shows the loop statistics for these walkers in a system of size $L = 1600$ and a probability of creation $p = 0.000\,016$ (thick lines) and $p = 0.0001$ (thin lines). All measured quantities, i.e., number of defects in a loop and the spatial as well as the temporal extent of the loops, show power-law behavior for large loops. The simplicity of the lattice model suggests that the power laws are expected to arise in a much wider class of spatiotemporally

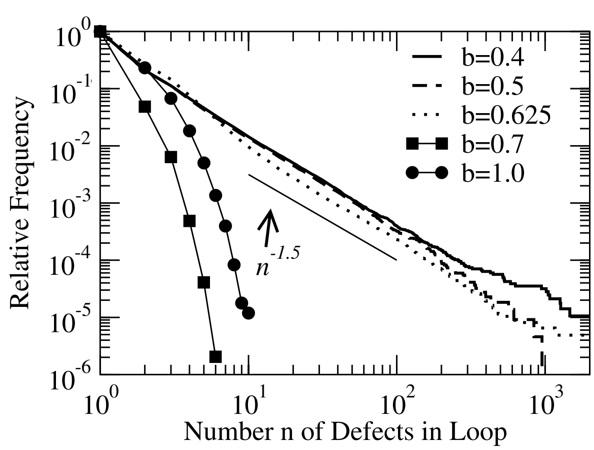


FIG. 2. Relative frequency of loops made up of at least $n$ defect pairs. Parameters as in Fig. 1 except for $b$. System size $L = 1088$ in the disordered regime; $L = 272$ and $L = 136$ for $b = 0.7$ and $b = 1.0$, respectively.

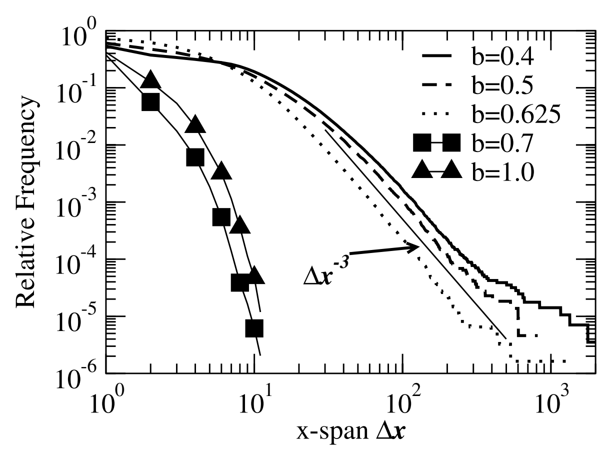


FIG. 3. Relative frequency of loops with spatial extent in the $x$-direction at least $\Delta x$. Parameters as in Fig. 2.

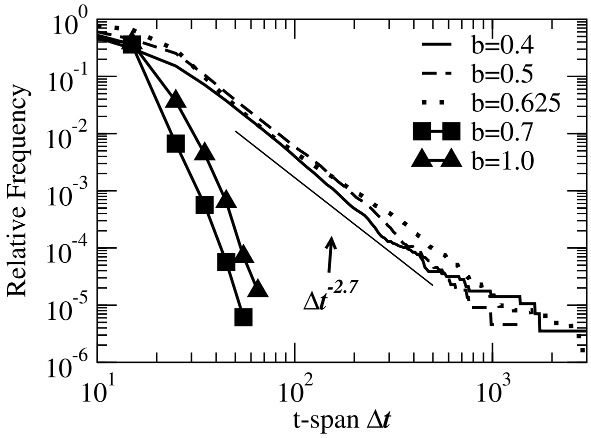


FIG. 4. Relative frequency of loops with lifetime at least $\Delta t$. Parameters as in Fig. 2.

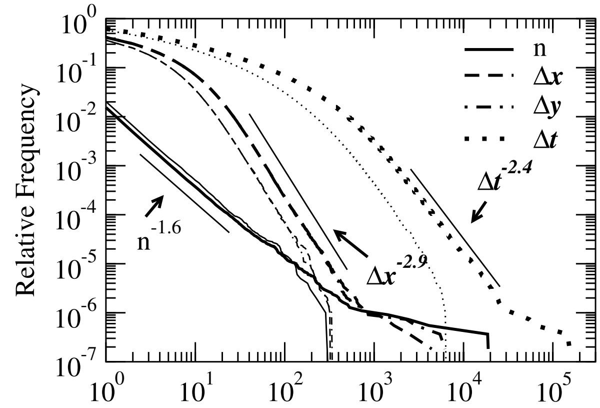


FIG. 5. Simulations of the lattice model of size $L = 1600$. Thick lines denote $p = 0.000\,016$, thin lines $p = 0.0001$.

chaotic systems including the CGLE. The exponents are measured to be $\alpha = 1.6$, $\beta = 2.9$, and $\gamma = 2.4$, respectively. Thus, even the values of the exponents agree quite well with those obtained in the simulations of (1) and (2).

In conclusion, using numerical simulations of two coupled complex Ginzburg-Landau equations describing parametrically excited waves in two dimensions, we have addressed the general problem of how the motion of defects can be related to the breakdown of order in a spatial pattern. The persistent creation and annihilation of defects in itself need not be sufficient to destroy the order as illustrated by the spatially periodic correlation function found in the chaotic but ordered regime [14] (cf. [13]). Our study of the transition from this ordered state to a disordered state with an (almost) isotropically decaying correlation function shows that the breakdown of order is closely connected with certain details of the dynamics and interaction of the defects. Following the trajectories of all defects in the system, we have determined the statistics of the loops formed in space-time by chains of creation and annihilation events of oppositely charged defects. We have found that the order-disorder transition is signified by an orders-of-magnitude increase in the number of loops that extend over large parts of the system, which we associate with a type of unbinding of defect pairs. More precisely, the decay of the loop distribution functions changes from exponential to algebraic in that transition. The algebraic decay is also found in a simple lattice model of diffusing and annihilating defects, with the exponents agreeing quite well with those found in the Ginzburg-Landau equations. This suggests that power laws may be the signature of the disordered states and that the same power laws may occur in a wider class of disordered defect-chaotic states including those of the single complex Ginzburg-Landau equation [17] and possibly also in strongly nonlinear states that are not described by weakly nonlinear theories.

The single-defect statistics obtained in the disordered state and in the lattice model have also been found in experiments in electroconvection [9] and in thermal convection in an inclined layer [18]. It would be exciting to study also the loop distribution functions in these systems.

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