A Non-Equilibrium 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 spatio-temporal defect chaos is found. To characterize the two different chaotic states and to get insight into the break-down of the order, the trajectories of the defects are tracked in detail. Since the defects are always 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.

Very early in the investigation of pattern-forming systems far from thermodynamic equilibrium it has been recognized that dislocations in stripe patterns near onset are mathematically closely related to defects in the equilibrium xy-model since both systems are described by a single complex order parameter \( A \) in terms of which the dislocations are given by locations of vanishing magnitude \( |A| = 0 \). One of the fascinating phase-transition phenomena studied extensively in the xy-model is the K\"{u}ppers-Lortz transition, which is associated with the unbinding of defect pairs \( \bigcirc \). This motivated early efforts to identify related phenomena also in pattern-forming systems like Rayleigh-B\"{e}nard convection \( \bigcirc \). A direct analogy between these systems does not hold, however, for a number of reasons. Most significantly, the phase transitions occur at finite temperature and are intimately related to the relevance of fluctuations, whereas in macroscopic systems like Rayleigh-B\"{e}nard convection the effect of (thermal) noise is negligible in most situations \( \bigcirc \). Moreover, in the absence of noise there are no persistent dynamics in the Ginzburg-Landau with real coefficients that describes the equilibrium system.

More recently, spatio-temporal chaos in pattern-forming systems has found considerable attention. A number of variations of convection experiments have revealed various different types of spatio-temporal chaos like spiral-defect chaos (e.g. \( \bigcirc \)), domain chaos triggered by the K\"{u}ppers-Lortz instability (e.g. \( \bigcirc \)), dislocation-dominated chaos in binary-mixture convection \( \bigcirc \) and in electroconvection \( \bigcirc \). Extensive theoretical investigations have focussed on the complex Ginzburg-Landau equation (CGLE) for the complex amplitude of oscillations arising in a Hopf bifurcation (e.g. \( \bigcirc \)). In contrast to the Ginzburg-Landau equation describing the xy-model the coefficients in the CGLE are complex and make this system non-variational.

Various results have been obtained for the dynamics of defects in spatio-temporally chaotic systems. In binary-mixture convection progress has been made to reconstruct the full wave pattern from the locations of the dislocations \( \bigcirc \). The probability distribution function for the number of dislocations has been measured in electroconvection \( \bigcirc \) and found to agree quite well with results based on the complex Ginzburg-Landau equation and on a simple diffusive model \( \bigcirc \). The dynamical relevance of dislocations has been demonstrated best so far in work that succeeded in extracting the contribution of each dislocation to the total fractal dimension of the (extensively) chaotic attractor of the CGLE \( \bigcirc \).

The spatio-temporally 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 \( \bigcirc,13 \) one may expect that defects in the pattern may play an important role. In this Letter we present results for a transition between two spatio-temporally chaotic states in a Ginzburg-Landau model for parametrically excited waves \( \bigcirc \). While one state is disordered in space, the other retains a stripe-like order despite the chaotic creation and annihilation of defect pairs. We characterize the break-down 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 the pairwise created defects. Tentative results for this unbinding transition have been presented earlier in \( \bigcirc,14 \).

To illustrate the possible role of the defect dynamics in the break-down of order, Fig.1 presents a space-time diagram of the defect dynamics in the regime with persistent spatial order. The \( y \)-location of each defect with positive topological charge is shown as a solid circle while the \( y \)-location of each defect with negative charge is shown as a dot. The trajectories of almost all of the defect pairs form simple loops in space-time. Thus, while in any given system defects are always annihilated in pairs of opposite charge, in the ordered regime the annihilating defects have also been created together. It is in this sense that we consider them to be bound pairs. The preservation of the stripe-like order in this regime can then be understood intuitively, since the dynamics of defects in such 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.

The orientation and position of the stripe pattern is affected significantly only between the defects. Therefore, one may 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 may 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. Simulations show that in fact even in the disordered regime most defects are annihilated by their ‘own’ partner forming a simple loop and most loops are small compared to the system size. Thus, if a distinction between the two regimes can be made based on defect trajectories it must involve more subtle aspects like the distribution of defect loops as a function of their size. Using a detailed statistical analysis of the defect dynamics we show in the following that indeed the statistical properties of the defect loops in space-time are qualitatively different in the two regimes.

We consider a Ginzburg-Landau model for parametrically excited waves in an axially anisotropic system in which at the bifurcation point the waves travel only along the $x$-axis,

\[ \begin{align*}
\partial_t A + s \partial_x A &= d \nabla^2 A + a A + b B + c |A|^2 A + g |B|^2 A, \\
\partial_t B - s \partial_x B &= d \nabla^2 B + a^* B + b^* A + c^* |B|^2 B + g^* |A|^2 B.
\end{align*} \tag{1} \tag{2} \]

Here $A$ and $B$ are the complex amplitudes of right- and left-traveling waves. All the coefficients except for the group velocity $s$ and the parametric forcing $b$ are complex. The traveling waves arise in a Hopf bifurcation at $a_r \equiv Re(a) = 0$. For $c_r < 0$ the bifurcation is supercritical and the waves exist for $a_r > 0$. The parametric forcing is applied at close to twice the Hopf frequency. It therefore induces a resonant interaction between the counter-propagating waves at linear order $\mathcal{O}(k)$. For $a_r < 0$ and $b^2 > a^2 + a^2$ standing waves are excited parametrically that are phase-locked to the forcing. These waves correspond qualitatively to the waves excited in Faraday experiments. In all of the simulations we use periodic boundary conditions in both directions and solve the system pseudo-spectrally with a fourth-order Runge-Kutta scheme using an integrating factor for the linear derivative terms.

Numerical simulations of (1,2) show two distinct regimes of spatio-temporal 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 spatio-temporal chaos which exhibits a strikingly ordered state in which the relevant information turns out to be in the 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 defects of equal and of opposite charge. If in consecutive time steps two defects of equal charge are closer than some threshold value $d_i = n \cdot \delta_i$ they qualify as a single defect that has moved from one to the other position. If more than two defects fall into this category the closest defects are taken to be ‘continuing’ defects. 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 $d_2 = n \cdot \delta_2$ are identified as a pair that was annihilated (or created) in this time step. After one step of this analysis the same analysis is repeated with new, increased values for the thresholds, $d_i^{(n+1)} = (n+1) \cdot \delta_i$, until all defects have been assigned.

Fig. 2 shows the relative frequency of loops consisting of at least $n$ defect pairs. The results in figs. 1 and 3 are based on 8000 timesteps ($dt = 0.5$) 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 5 defect pairs and the distribution de-
cays 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 \(\alpha \approx 1.5\).

![Figure 2](image-url)  
**FIG. 2.** Relative frequency of loops made up of at least \(n\) defect pairs. Parameters as in fig. 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.

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 (vaguely defined) part of the system between the defect pairs. Parameters as in fig.1 except for \(b\).

![Figure 3](image-url)  
**FIG. 3.** Relative frequency of loops with spatial extent in the \(x\)-direction at least \(\Delta x\). Parameters as in fig.2.

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 10, 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, a noticeable number of loops is of the order of the system size \(L = 1088\) and even larger (i.e. wrapping around the system due to the periodic boundary conditions). In a simple interpretation these events would be associated with a persistent change in the average wavevector 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. 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.

![Figure 4](image-url)  
**FIG. 4.** Relative frequency of loops with lifetime at least \(\Delta t\). Parameters as in fig.2.

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 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. Fig. 5 shows the loop statistics for these walkers in a system of size $L = 1600$ and a probability of creation $p = 0.000016$ (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 spatio-temporally 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 exponents agree quite well with those obtained in the simulations of (12).

In conclusion, using numerical simulations of two coupled complex Ginzburg-Landau equations we have investigated the break-down of order in a transition from a non-equilibrium, chaotic stripe phase to a disordered phase. To get insight into the way the order breaks down we have analyzed the trajectories of the dislocations in the pattern. In particular, we have determined the statistics of the loops formed in space-time by chains of creation and annihilation events of oppositely charged defect pairs. The order-disorder transition is related to a significant increase in the number of loops that extend over the whole system, which we associate with the unbinding of defect pairs. More precisely, the decay of the loop distribution function 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. The agreement between the Ginzburg-Landau equations and the lattice model suggests that the power laws may be found in a wider class of defect-chaotic systems and in particular also in the single complex Ginzburg-Landau equation.

The single-defect statistics obtained in the disordered state and in the lattice model have also been found in experiments in electroconvection [12] and in thermal convection in an inclined layer [18]. It would be exciting to study also the loop distribution functions in these systems. The amount of detailed data necessary to determine the loop statistics represents presumably a challenging task in the current set-ups.

The simplicity of the lattice model suggests that the power laws may also be amenable to an analytic approach. A further interesting question is whether the lattice model can be extended to obtain also a transition from power-law to exponential decay. Introducing an attractive interaction between the defects would seem to be a natural choice. It is not clear whether the interaction should be short- or long-range.

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![Fig. 5. Simulations of the lattice model. Thick lines denote $p = 0.000016$, thin lines $p = 0.0001$. $L = 1600$.](image)

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