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Defects and traveling-wave states in nonequilibrium patterns with broken parity

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A class of elementary defects of one-dimensional periodic patterns found far from equilibrium is described. They are "spatiotemporal grain boundaries" between regions in which the parity symmetry of the cellular pattern is broken in the opposite of two senses. The defect cores act as sources or sinks of traveling waves and cellular structures by means of a periodic phase instability closely related to "phase slips" in superconducting wires. An explanation for observations of annihilating collisions between two finite domains of opposite broken parity follows from these results.

Nonequilibrium systems as distinct as a layer of fluid heated from below and a moving solid-liquid interface often exhibit periodic patterns in space and time.[1] Whether in Rayleigh-Bénard convection or in directional solidification, many long-wavelength properties of these patterns are consistent with a general class of dynamics based solely on symmetry considerations.[2] In particular, the existence of a discrete translational symmetry as well as reflection symmetry (parity) is a common feature in experiments, and underlies many such theoretical treatments. However, several recent experiments[3-7] on one-dimensional pattern-forming systems, in the contexts of solidification, viscous fingering, and convection, are consistent with the notion[8,9] that these periodic "cellular" structures may undergo a secondary instability at which the parity symmetry of the pattern is broken.

A one-dimensional pattern $U(x,t)$ with a region of broken parity (asymmetry) may be resolved into symmetric and antisymmetric components, U_S and U_A, respectively,

$$U(x,t)=S(x,t)U_S(x+\phi(x,t)) + A(x,t)U_A(x+\phi(x,t))\,, \qquad (1)$$

where S and A are real amplitudes and $\phi(x,t)$ is the phase of the pattern. The amplitude $A(x,t)$ serves as the order parameter of the broken parity, vanishing outside the region of asymmetry. Now, in one-dimensional systems, there is, in general, a *twofold degeneracy* of broken-parity states, corresponding to the two possible signs of A. In addition, an important consequence of basic symmetry considerations[8] is that the breaking of parity leads to a *propagation of the pattern* in a direction determined by the sign of A. There are thus two possible directions of propagation of the pattern. Motivated primarily by recent experiments,[3,5] we study here patterns in which the two states coexist, the junction between them being an elementary defect[10] of broken-parity states; it is an example of a spatiotemporal grain boundary.

Important evidence of a parity-breaking transition is the observation[3] of slowly spreading domains of asymmetric cells (originally termed "solitary modes") that move across the periodic interface. Their properties are suggestive of those of nucleated inclusions of a dynamically more stable asymmetric state. It is observed[3,4] that when two domains of different length, moving in opposite directions, collide, they leave behind a single inclusion propagating in the direction of the longer one, whose length is approximately the difference between the two. This remarkable rule of length subtraction is quite unlike that associated with solitary waves, and emphasizes the strongly dissipative nature of the dynamics in these systems. Figure 1 is a graphical representation of such a collision, obtained from numerical solution of a model described below; Fig. 1(a) showing the envelope function $A(x)$, Fig. 1(b) showing the interface pattern, reconstructed from considerations appropriate to directional solidification. As in experiment, the annihilation shown leads to the *creation of new symmetric cells* in the region of the collision, where the amplitude A exhibits a local kink shape crossing through zero. In a space-time portrait like Fig. 1, it is clear that the creation of a new cell is a "space-time dislocation." Figure 2 illustrates a permanent grain boundary between traveling-wave states, the junction (where $A=0$) being the site of the periodic space-time dislocations.

In this paper we propose a mathematical description of the dynamics of spatiotemporal grain boundaries in patterns with broken parity and suggest the existence of an important connection between such boundaries and the dynamics of collisions of localized asymmetric regions. We find that a consistent description of the creation of new cells in both of these contexts requires an important coupling between the symmetric and antisymmetric components into which the pattern is resolved. In brief, we know on rather general grounds that it is most natural to consider the dynamics of a parity-symmetric pattern U_S in terms of a complex amplitude $B=S\exp(i\phi)$, the resulting dynamics of B bearing a strong resemblance to the time-dependent Ginzburg-Landau (TDGL) theory of a complex superconducting order parameter. The proposed coupling of a *scalar field* A to B is then like that found in the TDGL description of a superconductor in an electric

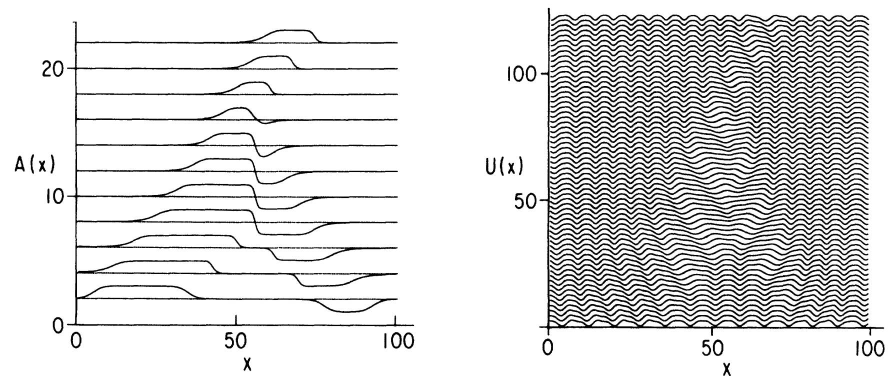

FIG. 1. Partially annihilating collision between inclusions of broken parity of opposite sense. (a) The antisymmetry order parameter $A(x)$, with time increasing upward and displaced vertically for clarity. (b) The interface pattern $U(x)$, at time intervals one tenth those in (a). Note how the number of cells in (b) has increased during the collision.

field, A playing the role of the electrochemical potential. At the core of a grain boundary and at the center of a collision, this coupling leads to periodic phase disturbances (related to the Eckhaus instability of the underlying symmetric component) analogous to phase slip centers[11] and phase slip oscillators[12] in one-dimensional superconductors.

We begin by recalling the essential symmetry considerations[8] underlying the form of amplitude equations[13] for A and ϕ at a parity-breaking transition. Referring to the decomposition in Eq. (1), in which U_S is an even function of its argument and U_A is odd, we find the dynamics of A and ϕ to be invariant under the joint transformations $x \to -x$, $\phi \to -\phi$ and $A \to -A$, $S \to S$, as well as to uniform shifts $\phi \to \phi + \text{const}$. Accordingly, among the leading terms in the normal form for the evolution of the phase are the contributions

$$\phi_t = \phi_{xx} + \omega A + \cdots , \qquad (2)$$

where ω is some coupling constant and subscripts indicate differentiation. As remarked earlier, (2) with (1) implies that a homogeneous broken-parity state ($A \neq 0$) is a traveling structure, with $\phi = \omega A t$.

The relevance of these phase dynamics for the pattern evolution near a grain boundary may be seen by noting that when the broken-parity state is dynamically the most stable, the order parameter may take on either of two values labeled $\pm A^*$. Far on either side of the defect, (2) leads to the phase evolution $\phi = \pm \omega A^* t$, that is, traveling waves with opposite propagation directions. Clearly, however, this differential forcing of the phase leads to an ever-increasing phase gradient at the core of the defect, the continual growth of which is physically untenable. It may be resolved within a description of the long-wavelength dynamics based on a complex amplitude, a formalism well known in the study of hydrodynamic instabilities,[13] within which phase gradients lead to the local vanishing of the amplitude of the periodic pattern. At such a point, the phase is undefined, allowing the total phase across the defect to change by 2π, corresponding to the creation or destruction of a cell. This process is reminiscent of the appearance of phase slips in a one-dimensional superconducting wire in the presence of a uniform electric field.[11] There, a sufficiently large current (phase gradient) destabilizes the superconducting order

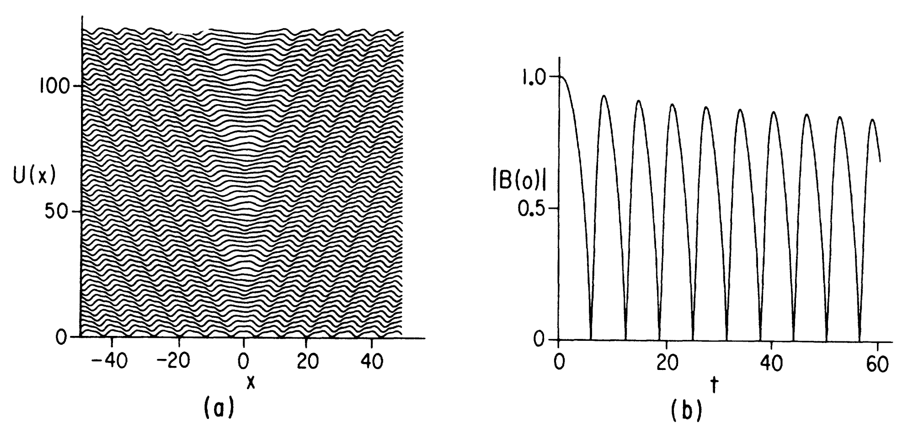

FIG. 2. (a) A spatiotemporal grain boundary, a source for traveling waves, in a system with broken parity. (b) The modulus of the symmetric amplitude at the defect core ($x = 0$) as a function of time, showing the periodic zero of $|B|$.

parameter.

We propose the following phenomenological model to address these issues for systems with broken parity.[14] Let $B(x,t)=Se^{i\phi}$ be the complex amplitude describing the symmetric component of the pattern as resolved in (1). A simple dynamics for B beyond the initial supercritical instability of the homogeneous state (e.g., the Mullins-Sekerka instability) is

$$B_t = B_{xx} + \nu B - |B|^2 B . \tag{3}$$

Here, ν is viewed as the fundamental control parameter of the problem, proportional to the deviation $r-r_c$ of some experimental control parameter r from its value at onset, r_c. The dynamics in Eq. (2) are embodied in a coupling term $i\omega AB$ in (3), and this is, in fact, perhaps the simplest one that respects the relevant symmetries. We may write the dynamics for B in the suggestive form

$$(\partial_t - i\omega A)B = B_{xx} + \nu B - |B|^2 B , \tag{4}$$

precisely the Ginzburg-Landau equation for a superconductor, with the term ωA playing the role of $-2\mu_e/\hbar$, where μ_e is the electrochemical potential.[15] Provided $|B| \neq 0$, it is meaningful to speak of the magnitude and phase of B and so to deduce the phase equation

$$\phi_t = \phi_{xx} + 2S^{-1}S_x\phi_x + \omega A , \tag{5}$$

the generalization of (2) to the case of a spatially varying symmetric amplitude. The associated amplitude equation

$$S_t = S_{xx} + (\nu - \phi_x^2)S - S^3 , \tag{6}$$

reveals the destabilizing effects of large phase gradients.

In generalizing the dynamics for the parity-breaking order parameter A to account for the complex nature of the symmetric amplitude, it is useful to separate the equation of motion of A into "variational" and nonvariational" parts. The former derives from the relation $A_t = -\delta\mathcal{L}/\delta A$, with the Lyapunov functional $\mathcal{L} = \frac{1}{2}A_x^2 + F(A)$, where the even polynomial $F(A)$ distinguishes between supercritical and subcritical bifurcations; for the latter (perhaps more relevant to experiments on directional solidification) a paradigmatic form is

$$F(A) = -\tfrac{1}{2}\mu A^2 - \tfrac{1}{4}\alpha A^4 + \tfrac{1}{6}A^6 , \tag{7}$$

with $\alpha > 0$. [For directional viscous fingering,[5] supercritical dynamics with $F(A) = \frac{1}{2}\mu A^4 + \frac{1}{4}A^4$ may be more appropriate.] By symmetry, the minima of F at $A = \pm A^*$ are of equal depth. It was suggested previously[8] that several of the observed parity-breaking transitions are well described by subcritical dynamics for A,

$$A_t = -\delta\mathcal{L}/\delta A + \epsilon A\phi_x + \gamma A A_X + \cdots , \tag{8}$$

the last two nonvariational terms being responsible for the motion of inclusions of the antisymmetric state and for various phenomena associated with wavelength relaxation.

To generalize (8), note that the phase gradient ϕ_x is proportional to the current $j \propto i(BB_x^* - B^*B_x)$, B^* being the complex conjugate of B. Making the additional plausible assumption that it is the growth in the amplitude of the symmetric component that drives the parity-breaking transition, we conclude that the linear stability of A should decrease as $|B|$ increases. We thus arrive at the model

$$A_t = A_{xx} + (\mu + |B|^2)A + \alpha A^3 - A^5 + i\frac{\epsilon}{2}(BB_x^* - B^*B_x)A + \gamma A A_x . \tag{9}$$

In the simplest interpretation, the parameters μ, α, ϵ, and γ are assumed fixed, with ν in (4) the relevant control parameter.

The dynamics in (4) and (9) reproduces all of the previously described[8] phenomena of wavelength selection and relaxation associated with the propagation of parity bubbles, and now provides for a coherent picture of the creation of new cells, as we now summarize.[16] For $\tilde{\mu} \equiv \mu + |B|^2 > \mu^* = -\frac{3}{16}\alpha^2$ (the Maxwell point at which the broken parity and symmetric states are of equal stability), the state with $A \neq 0$ becomes dynamically stable. Suppose then that a system with $\tilde{\mu} > \mu^*$ and $B = \nu^{1/2}$ is prepared with a kink-shaped amplitude $A(x)$. How does it evolve? Figures 2(a) and 2(b) show the results of numerical integration of (4) and (9) and a reconstruction[17] of the pattern U, with the dynamics of B obtained by solving for $u(x,t), v(x,t)$ in the decomposition $B = u + iv$. As the initially uniform state develops a phase gradient near $x = 0$, the modulus of B steadily decreases until both the real and imaginary parts smoothly cross through zero. This is reminiscent of the Eckhaus instability exhibited by B even in the absence of an inhomogeneous forcing, where the state with an imposed phase gradient, $\phi = Qx$, $S = (\nu - Q^2)^{1/2}$, becomes unstable for $|Q|$ sufficiently large. Note that the nonvariational forcing of A keeps the junction stationary. The vanishing of B at the core of the grain boundary, shown in Fig. 2(b), is found to be periodic in time, the frequency proportional to ωA^*, the rate at which the phase gradient grows. In this sense, the phase dynamics in (2) and (4) are seen as analogous to Josephson relations in superconductivity, and the periodic zero of B is essentially identical to those that occur at phase slip oscillators in superconductors.[12] A key experimental test of the validity of the above description of a spatiotemporal grain boundary would be a measurement of this behavior of the symmetric component of the pattern.

Returning to the collision in Fig. 1, we see that the junction between these two finite domains is essentially a transient grain boundary, the order parameter A locally having the shape of the kink connecting the two states $\pm A^*$. During the course of the collision the junction itself remains fixed in space, as a consequence of the equal and opposite variational and nonvariational forcing on its two halves, but the two outer edges continue traveling inward while a periodic phase instability (or several) occurs at the junction, yielding new cells. When viewed in terms of, say, the maxima of the pattern U in Fig. 1(b), these instabilities during a collision are spatiotemporal dislocations. As the far edge of the shorter domain reaches the defect core, the broken-parity order parameter collapses to zero, leaving the remainder of the longer domain to propagate in its original direction, slowly spreading as before. Were the domains of more equal length, the collision would have led to total annihilation. In general, the length subtraction rule is approximate up to deviations of a few correlation lengths of the order parameter [roughly the size of the critical nucleus associated with the free energy $F(A)$].

To summarize, we have shown, in qualitative accord with experiments, that certain defects in hydrodynamic systems exhibiting transitions to states of broken parity may be viewed as spatiotemporal grain boundaries. The cores of such defects act as sources or sinks of traveling waves by means of periodic phase instabilities. The dynamics of such structures appears to play an important role in the phenomena found during collisions of propagating inclusions of the broken-parity state.

Finally, we may expect that the formal connection between the dynamics of systems with broken parity and those of superconductors in applied electric fields may be extended. For example, superconductivity is, of course, intimately linked with the presence of a gauge field, the vector potential. Is there an analog of a gauge field[18] in the dynamics of periodic nonequilibrium patterns?

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