Noise and Dynamical Pattern Selection

Douglas A. Kurtze*

Department of Physics, North Dakota State University, SU Station, Box 5566, Fargo, North Dakota 58105-5566 (Received 13 November 1995)

In pattern-forming systems, such as Rayleigh-Bénard convection or directional solidification, a large number of linearly stable, patterned steady states exist when the basic, simple steady state is unstable. Which of these steady states will be realized in a given experiment appears to depend on unobservable details of the system's initial conditions. We show, however, that weak, Gaussian white noise drives such a system toward a *preferred wave number* which depends only on the system parameters and is independent of initial conditions. We give a prescription for calculating this wave number, analytically near the onset of instability and numerically otherwise. [S0031-9007(96)00562-5]

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The classic problem of pattern selection is that of predicting which of a large number of available steady states a system will ultimately reach under given experimental conditions. In a typical example, that of directional solidification, there is a simple steady state of the system in which the solidification front is planar and advances into the melt at a constant speed. By varying a control parameter, one reaches a regime in which this state is linearly unstable against all perturbations with wave numbers in a given interval. In this regime the front settles into a spatially periodic, cellular shape. Ample evidence exists that there is one such patterned steady state with each wave number q in the interval of instability. Moreover, there is a finite subrange of wave numbers for which the cellular steady states are themselves linearly stable. The pattern selection question is then this: Into which of these patterned states will the system restabilize in a given experiment?

The answer to this question appears to be that the final wave number depends not only on the system parameters, but also on the details of the initial conditions from which the system evolves. Since these details cannot be observed in practice, the final wave number is not reproducible. We will argue in this Letter, however, that among the possible steady-state wave numbers there is one which is *preferred*, in the sense that subjecting the system to weak, Gaussian white noise drives it toward that wave number, and in the long-time limit that wave number is overwhelmingly more probable than any other. We will show how this preferred wave number can be calculated for one-dimensional systems.

Noise effects on pattern-forming systems have been studied by many authors, although few have considered the role of noise in readjusting the wave number of an established, periodic pattern. Deterministic evolution from random *initial conditions* has been studied in amplitude equations [1-3], and noise effects on the initial stages of pattern formation have been investigated in Bénard convection [4], dendritic growth [5,6], and cellular [7] and dendritic [8] arrays in directional solidification. Several numerical studies of the Swift-Hohenberg equation (which

is relaxational) have all shown [9-13] that noise selects the wave number which minimizes the underlying free energy, as expected. In a series of papers which are particularly relevant to our work, Kerszberg carried out numerical simulations of directional solidification with and without Gaussian white noise [14,15]. This is a system which has no underlying free energy. With noise added, the system restabilized into a cellular state with a unique, reproducible wave number independent of initial conditions, while without noise the final wave number depended on initial conditions.

The relaxational, or "gradient," case is quite helpful for motivating our calculations. Suppose we have a finite, one-dimensional system whose state is specified by giving a set of amplitudes x_k of Fourier modes of wave number k, chosen so that the simple steady state of the system is $x_k \equiv 0$, and that the control parameter has been set so that this state is linearly unstable. (We will also take the x_k to be real, so that the pattern is left-right symmetric.) The amplitudes evolve according to

$$\frac{dx_k}{dt} \propto -\frac{\partial \Phi(x)}{\partial x_k},\tag{1}$$

where $\Phi(x)$ is the free energy. This evolution always makes Φ decrease with time. A patterned steady state with wave number q will have x_k nonzero only when k is an integer multiple of q; let the value of the free energy of this state be $\Phi_{\rm ss}(q)$. If we add noise of strength ϵ to (1), it will produce occasional large fluctuations which take the system far enough out of the local free energy minimum at the state of wave number q that it then relaxes to a different local minimum, with wave number q'. The relative probability of a transition from q to q' versus a transition from q' back to q is proportional to $\exp\{2[\Phi_{ss}(q) - \Phi_{ss}(q')]/\epsilon\}$. That is, fluctuations are more likely to take the system from a state of higher free energy to one of lower free energy than vice versa. In pattern-forming systems, the steady states near the edges of the band of stable wave numbers, which are almost unstable, have higher free energies than states in the interior of the band, so noise drives the system away from those states and toward the absolute minimum of the free energy.

We argue here that the same thing happens in nongradient systems, i.e., ones in which the time evolution is given by

$$\frac{dx_k}{dt} = F_k(x),\tag{2}$$

but the F_k cannot be put into the form (1). To see this, we first add noise to the dynamics to obtain the Langevin equation

$$\frac{dx_k}{dt} = F_k(x) + \sqrt{\epsilon} \,\xi_k(t),\tag{3}$$

where the ξ_k are independent Gaussian random variables with mean zero and unit variance,

$$\langle \xi_k(t) \, \xi_{k'}(t') \rangle = \delta_{kk'} \, \delta(t - t'). \tag{4}$$

The x_k are then random variables, and a standard argument [16] leads to the Fokker-Planck equation for the time evolution of their probability distribution. If (3) is a mixing process [16], then this converges in the long-time limit to a steady-state distribution $\mathcal{P}_{ss}(x)$, which satisfies

$$-\frac{\partial}{\partial x_k} \left[F_k(x) \mathcal{P}_{\rm ss}(x) - \frac{\epsilon}{2} \frac{\partial \mathcal{P}_{\rm ss}}{\partial x_k} \right] = 0.$$
 (5)

Here and below, repeated indices are to be summed. Since the noise terms in (3) are independent of x, there is no difference here between the Itô and Stratonovich interpretations.

In the weak-noise limit $\epsilon \to 0$, we can solve (5) using a WKB method [17]. Since probability distributions must be positive, we may write

$$\mathcal{P}_{\rm ss}(x) \equiv \exp[-S(x)/\epsilon]$$
 (6)

so that *S* plays a role similar to that of the free energy in the gradient case; in fact, the exact solution of (5) is $S = 2\Phi$ in that case. Keeping only the zerothorder approximation to *S* does not give an asymptotic approximation to the function \mathcal{P}_{ss} —it neglects factors of order unity in (6)—but it does give the controlling factor in the leading behavior of \mathcal{P}_{ss} as $\epsilon \to 0$. Although we will need to be careful if *S* has singular points, this should suffice for our purposes. From (5) we find that, to leading order in ϵ , *S* satisfies

$$\frac{\partial S}{\partial x_k} \left[\frac{1}{2} \frac{\partial S}{\partial x_k} + F_k(x) \right] = 0.$$
 (7)

From this we see that any steady state of the deterministic dynamics (2), i.e., a point where all F_k vanish, is a stationary point of *S*. We will see below that a linearly stable steady state of (2) is in fact a local minimum of *S*.

We can also see that the function S(x) plays the role of Φ in a different sense. The deterministic evolution (2) never makes S(x(t)) increase, since

$$\frac{dS}{dt} = \frac{\partial S}{\partial x_k} \frac{dx_k}{dt} = \frac{\partial S}{\partial x_k} F_k(x) = -\frac{1}{2} \frac{\partial S}{\partial x_k} \frac{\partial S}{\partial x_k} \le 0.$$
(8)

Thus even a nongradient system can be considered relaxational, since there is a function S(x) which is nonincreasing. In gradient systems, however, that function is just the free energy, which is generally easier to compute.

Equation (7) can be solved by the method of characteristics, or equivalently by recognizing it as the Hamilton-Jacobi equation, with energy 0, for the Hamiltonian

$$\mathcal{H}(p,x) \equiv -\frac{1}{2} p_k p_k - p_k F_k(x).$$
(9)

The characteristic curves are given by

$$\dot{x}_k = -p_k - F_k(x), \qquad \dot{p}_k = p_{k'} \frac{\partial F_{k'}}{\partial x_k}, \qquad (10)$$

where overdots represent derivatives with respect to some parameter τ . Along a characteristic, *S* is given by

$$\dot{S} = p_k \dot{x}_k = -p_k (p_k + F_k).$$
 (11)

Since we have $\mathcal{H} = 0$, this becomes $\dot{S} = -(p_k p_k)/2$, so *S* always *decreases* along a characteristic.

To find the preferred wave number, we need only calculate S(x) at each stable steady state of (2). The wave number of the state with the lowest value of S is the preferred wave number: by (6), if the wave numbers are discrete, then all others are exponentially less probable. We do this by finding characteristics running from the (unstable) simple steady state $x_k \equiv 0$ to each stable steady state. That this is possible comes from a counting argument. Fixed points of (10) occur where $p_k \equiv 0$ and $F_k(x) \equiv 0$; linearizing about any fixed point gives

$$\dot{\delta x} = -\delta p - M\delta x, \qquad \dot{\delta p} = M^T \delta p, \qquad (12)$$

where M is the matrix which gives the linear stability of the deterministic dynamics (2),

$$M_{kk'} = \left. \frac{\partial F_k}{\partial x_{k'}} \right|_{\rm ss.}$$
(13)

If there are *N* amplitudes x_k , then the phase space (x, p) is 2*N* dimensional; from (12) we see that there are *N* (possibly generalized) eigenvectors at each fixed point with eigenvalues which are the same as the stability eigenvalues of the corresponding deterministic steady state, and another *N* eigenvectors with the negatives of those eigenvalues—and all *p* components equal to 0. From (10), we see that the $p \equiv 0$ subspace of phase space is invariant, and (11) shows that following a trajectory in this subspace would leave *S* unchanged. Thus we want characteristics *not* to be in this subspace. However, the only eigenvectors coming out (i.e., having positive

eigenvalues) from a fixed point which corresponds to a linearly stable steady state are those which lie in the p = 0 subspace. Thus we cannot have a characteristic leaving such a fixed point; all nearby characteristics must be directed towards it. Since S always decreases along characteristics, a linearly stable steady state of the deterministic dynamics must then be a local minimum of S. However, the steady state at x = 0 is not stable; it has (at least) one linearly unstable direction for each fundamental wave number q against which it is unstable. Correspondingly, for each such q there is (at least) one steady state which bifurcated from the x = 0 state as the control parameter was increased to its present value. It is then natural to expect that there will be one characteristic running from (x, p) = (0, 0) to each fixed point corresponding to a linearly stable steady state.

To do the calculation numerically, it is useful to have the expression for the Lagrangian corresponding to the Hamiltonian (9):

$$\mathcal{L}(x, \dot{x}) = -\frac{1}{2} [\dot{x}_k + F_k(x)] [\dot{x}_k + F_k(x)].$$
(14)

From (10), we see that on the characteristics this is equal to $-(p_k p_k)/2$, which in turn is equal to S. Thus we can set up the calculation of S at the steady state as a minimization problem, using Hamilton's principle: we wish to find the trajectory which approaches (x, p) =(0,0) as $\tau \to -\infty$, approaches the steady state x (and p = 0) as $\tau \to \infty$, and minimizes $\int \mathcal{L} d\tau$. The resulting minimum value is the value of S for that particular steady state. Minimizing this result in turn over the possible fundamental wave numbers q gives the preferred wave number. This procedure is made much easier by the fact that the structure of the deterministic equations (2) is usually such that the multiples of any fundamental wave number q form an invariant subspace. This property is inherited by the equations (10) for the characteristics, and so only a relatively small number of modes must be kept for each q.

When the control parameter is only slightly beyond the onset of instability of the simple steady state, it is possible to calculate the preferred wave number analytically. Consider, for example, the nongradient equation

$$\partial \psi / \partial t = [\gamma - (\nabla^2 + 1)^2]\psi - \psi^3 - |\nabla \psi|^2 \psi, \quad (15)$$

which is a model for the order parameter ψ in Rayleigh-Bénard convection [18]. For $\gamma > 0$ the steady state $\psi \equiv 0$ is linearly unstable against perturbations with wave numbers within $\gamma^{1/2}$ of 1. For small positive γ , we may write $\psi = x_1 \cos(qx) + x_3 \cos(3qx) + \cdots$, and we generally expect that x_1 will be of order $\gamma^{1/2}$ and x_3 of order $\gamma^{3/2}$. Inserting this ansatz into (15) gives

$$F_{1} = \sigma_{q}x_{1} - a_{11}x_{1}^{3} - a_{12}x_{1}^{2}x_{3} - a_{13}x_{1}x_{3}^{2} - \cdots,$$

$$F_{3} = -|\sigma_{3q}|x_{q} - a_{31}x_{1}^{3} - a_{32}x_{1}^{2}x_{3} - \cdots,$$
 (16)

with $\sigma_k = \gamma - (k^2 - 1)^2$, and all the a_{ij} being linear in q^2 . Note that σ_q is of order γ for q in the unstable

range of wave numbers. To calculate S, we write the equations (10) with the rescalings

$$x_1 = \gamma^{1/2} x, \qquad p_1 = \gamma^{3/2} p,$$

 $x_3 = \gamma^{3/2} y, \qquad p_3 = \gamma^{5/2} r.$ (17)

This reveals that \dot{x} and \dot{p} are of order γ , while \dot{y} and \dot{r} are of order unity. Thus y and r follow the current values of x and p:

$$y = -a_{31}x^3/|\sigma_{3q}| + O(\gamma),$$

$$r = -a_{12}x^2p/|\sigma_{3q}| + O(\gamma).$$
 (18)

We insert this into the Hamiltonian (9), and solve $\mathcal{H} = 0$ for p in terms of x. We can then integrate $p_1 dx_1 + p_3 dx_3$ from (0,0) to the steady state of (16) to get S. The result is

$$S = -\frac{\sigma_q^2}{2a_{11}} - \frac{a_{12}a_{31}\sigma_q^3}{3|\sigma_{3q}|a_{11}^3} - O(\sigma_q^4).$$
(19)

(The σ_q^4 term can be calculated, but is too lengthy to reproduce here.) Inserting the explicit expressions for the coefficients and minimizing over q yields the preferred wave number,

$$q = 1 - \frac{\gamma}{32} - \frac{37\gamma^2}{24576} - \frac{511\gamma^3}{3145728} - O(\gamma^4).$$
(20)

We could get higher order terms by including higher order terms in (16); we would need to keep an $x_5 \cos(5qx)$ term in ψ to do this consistently.

We have carried out the analogous calculations for the Greenside-Cross equation [19] for Bénard convection,

$$\partial \psi / \partial t = [\gamma - (\nabla^2 + 1)^2] \psi + 3 |\nabla \psi|^2 \nabla^2 \psi.$$
 (21)

For small γ we find that the preferred wave number is given by

$$q = 1 - \frac{\gamma}{4} - \frac{101\gamma^2}{1024} - \frac{981\gamma^3}{16384} - O(\gamma^4).$$
(22)

In one spatial dimension, the Greenside-Cross equation is a gradient system, and this result agrees with the expansion obtained by minimizing the free energy. Cross and Meiron [13], in numerical simulations of deterministic, two-dimensional evolution with random initial conditions, find that the system reaches a wave number $q \approx 0.78$ for long times for $\gamma = 1/2$. For this value of γ , the Eckhaus instability sets in at $q \approx 0.65$. For $\gamma = 1/2$, Eq. (22) gives q = 0.843 (the first three terms give 0.850). These results cannot be compared directly, since the numerical simulation does not include noise. However, the large two-dimensional system should have the freedom to get closer to its preferred wave number than a onedimensional system would without noise. It is encouraging that both approaches give wave numbers significantly below the maximum q = 1 of the linear growth rate, and within 10% of each other.

In this Letter we have argued that pattern-forming systems have a naturally preferred wave number, namely, that which the system would approach if it were subjected to weak, additive, Markovian, Gaussian white noise. This is not to say that the noise actually experienced by such a system has any of these five properties; but Gaussian white noise is appropriate because it does not bias the system's preference for a wave number, as colored noise, for example, would do. The argument does suggest, however, that the role of noise is not limited to providing the initial fluctuation which takes the system out of its simple steady state and starts it evolving toward one of its possible restabilized states, as is usually taken (implicitly) to be the case. Rather it has a continuing role in readjusting the wave number of the patterned state, generally through occasional large fluctuations which either create or destroy a cell, as was seen in Kerszberg's simulations [15].

An obvious question which needs to be addressed in the future is that of the rate at which the steady-state probability distribution \mathcal{P}_{ss} is established. It should be possible to use the same classical-mechanics techniques to study this question as we have used above, since substituting the time-dependent generalization of ansatz (6) into the Fokker-Planck equation leads directly to the timedependent Hamilton-Jacobi equation for the Hamiltonian (9). Further work on this point is under way.

Other important issues arise when we model the noise to which a system is actually subjected, which may not be additive, white, Gaussian, Markovian, or weak. For instance, the relevant fluctuations might be in the value of the control parameter. If any of the first four properties are lacking, then the appropriate Fokker-Planck equation will not have the simple form (5). Even if the relevant noise source is thermal, evolution equations of the form (2) often arise only after considerable manipulation of some more complex model which is written down from first principles. The ϵ in (3) may then be replaced by something which depends on q and even x. In all such cases the subsequent calculations need to be modified appropriately.

When the noise strength is finite, several important effects arise. One is that we may need the next higher order correction to the leading-order S(x) which we have calculated. A second, related point is that the relevant probabilities to compare are not just the heights of the peaks in \mathcal{P}_{ss} , but the areas under the peaks—including not just the exact steady states, but also perturbations of those states. These effects have been seen by Kerszberg [20], who found that even in a gradient system the observed wave number was not equal to the wave number which minimized the free energy when noise was included in his calculations. Finally, in an infinite system the possible band of wave numbers is continuous, so that it is not

true that one wave number has a probability which is exponentially larger than all others. Rather the probability $\exp[-S(q)/\epsilon]$ is appreciable for all wave numbers within a range of order $\epsilon^{1/2}$ around the "preferred" wave number. Thus if the noise variance is larger than something of the order of the inverse square of the size of the system, then there is still a range of possible wave numbers that one might observe even in the long time limit, albeit a very narrow range for finite but weak noise.

Finally, it would of course be far more satisfying to have a direct physical interpretation of the criterion for the preferred wave number, rather than just a prescription for calculating it.

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*Electronic address: kurtze@plains.NoDak.edu

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