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Defect Formation in a Dynamic Transition

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When a system that undergoes a continuous phase transition is swept through its critical point the initial symmetry is broken and domains are formed. Because of critical slowing down it is not possible to sweep adiabatically; the number of domains therefore depends on the rate of increase of the critical parameter. We give a summary of recent theoretical results for the number of defects produced as a function of how rapidly the transition point is passed. They are obtained from a simplified model, using a stochastic partial differential equation that is also solved numerically.

We start with a simple system: an overdamped particle in a potential that is slowly changed from single-welled to double-welled (Fig. 1). The particle does not slide down into one of the minima until well after the central position becomes unstable. The lingering at the top of the hill, known as the delay of bifurcation, has a characteristic time given by $\mu^{-1}\hat{g}$, where $\hat{g} = \sqrt{2\mu|\log\epsilon|}$, μ is the rate of increase of g and ϵ the magnitude of additive fluctuations (Jansons and Lythe, 1998; Lythe and Proctor, 1993; Stocks *et al.*, 1989; Swift *et al.*, 1991; Torrent and San Miguel, 1988; van den Broeck and Mandel, 1987).

The same delay is found in spatially extended systems. In addition, there is a characteristic length for the spatial structure after the "quench" (Laguna and Zurek, 1997; Lythe, 1994, 1996, 1997; Moro and Lythe, 1999). The spatial structure formed during the sweep through the critical point from the symmetric to broken-symmetry regime is frozen in by the nonlinearity when, sufficiently far into the symmetry-broken regime, the system attains a metastable state. Analytical progress is possible because the critical region is well described by an equation which, although stochastic and nonautonomous, is linear (Lythe, 1996; Moro and Lythe, 1999). We describe the calculation for the overdamped Ginzburg–Landau equation. Similar results have been found for the Swift–Hohenberg equation (Lythe, 1996) and for the the Ginzburg–Landau equation with arbitrary damping (Moro and Lythe, 1999).

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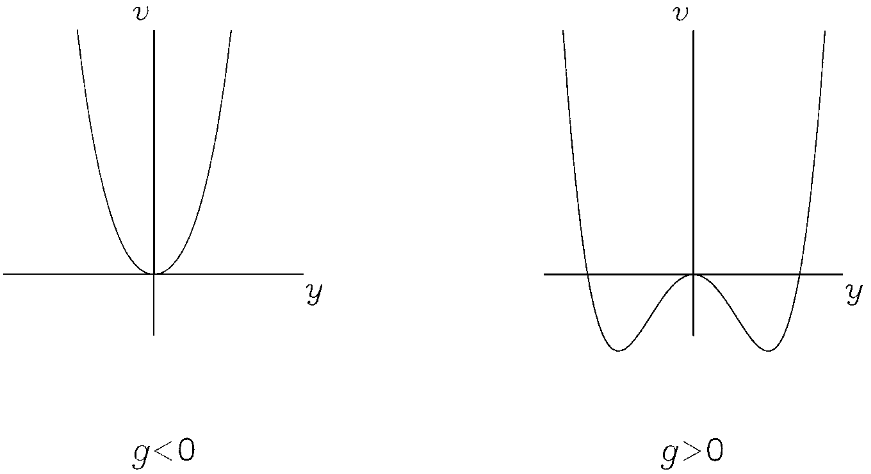

Fig. 1. The potential $v = -(1/2)gy^2 = y^4$. The parameter g is explicitly time-dependent.

A new scenario for the formation of structures in the early universe and a proposal for its test in laboratory experiments, using liquid Helium, resulted from an early understanding of this nonequilibrium effect (Zurek, 1985, 1993, 1996). Experimental results to date tend to support the proposed scenario, but precise comparison has not yet been possible (Bäuerle *et al.*, 1996; Dodd *et al.*, 1998; Ducci *et al.*, 1999; Gill and Kibble, 1996; Hendry *et al.*, 1994; Karra and Rivers, 1998; Kavoussanaki *et al.*, 2000).

1. THE GINZBURG–LANDAU SPDE

The equation describing the dynamics is written in the following dimensionless form:

$$\mathrm{d}\mathbf{Y}_t(x) = (g(t)\mathbf{Y}_t(x) - \mathbf{Y}_t(x)^3 + \mathcal{L}\mathbf{Y}_t(x))\,\mathrm{d}t + \epsilon\,\mathrm{d}\mathbf{W}_t(x). \tag{1}$$

Here $\mathbf{Y} : [0, L]^m \times [-1/\mu, 1/\mu] \times \Omega \to \mathcal{R}$, Ω is a probability space and $\mathbf{W}_t(x)$ is the Brownian sheet. The equations are solved as initial value problems, with

$$g(t) = \mu t \tag{2}$$

slowly increased from -1 to 1. Periodic boundaries in x are used so that no spatial structure is a boundary effect. The constants μ, ϵ, and $1/L$ are all $\ll 1$. The spatial operator $\mathcal{L} = \Delta$, where $\Delta = \sum_{i=1}^{m} \partial^2/\partial x_i^2$, the Laplacian in $\mathcal{R}^m$.

An alternative scaling of (1) is sometimes illuminating: if x is rescaled so that $[0, L] \to [0, 1]$, (1) becomes

$$\mathrm{d}\mathbf{Y}_t(x) = (g(t)\mathbf{Y}_t(x) - \mathbf{Y}_t(x)^3 + D\Delta\,\mathbf{Y}_t(x))\,\mathrm{d}t + D^{\frac{m}{4}}\epsilon\,\mathrm{d}\mathbf{W}_t(x), \qquad (3)$$

where $D = L^2$.

The Wiener process can be thought of as assigning to each successive interval of the time axis a Gaussian random variable with variance proportional to the length of the interval. The Brownian sheet assigns to each volume element in $\mathbb{R}_+ \times \mathbb{R}^m$ a Gaussian random variable whose variance is proportional to the volume of the element (Walsh, 1986). More precisely, it is possible to define a map $\mathcal{A}$ from $\mathcal{B}(\mathbb{R}_+ \times \mathbb{R}^m)$ to a probability space such that for each $h \in \mathcal{B}(\mathbb{R}_+ \times \mathbb{R}^m)$, $\mathcal{A}(h)$ is a Gaussian random variable with mean zero and $\langle \mathcal{A}(h_1)\mathcal{A}(h_2)\rangle = l(h_1 \cap h_2)$, where l is the Lebesgue measure (Walsh, 1986). The Brownian sheet, so called because its realizations in $m = 1$ look like a ruffled bedsheet tucked in on two adjacent sides, is defined as $\mathbf{W}_t(x) = \mathcal{A}([0, t] \times [0, x])$, where $[0, x]$ is the element (interval, square, cube, ...) with opposite corners at the origin and at $x \in \mathbb{R}^m$. Thus $\mathrm{W} : \Omega \times \mathbb{R}_+ \times \mathbb{R}^m \to \mathbb{R}$. The set Ω is the set of labels for realizations; averages over realizations are denoted by angle brackets. Each $\mathbf{W}_t(x)$ is a real-valued Gaussian random variable with mean zero and variance $\langle \mathbf{W}_t^2(x)\rangle = tx^m$.

2. DYNAMICS FOR FIXED g

For $g < 0$, the linearized SPDE is known as the infinite-dimensional Ornstein–Uhlenbeck process (Da Prato and Zabczyk, 1992; Doering, 1987; Funaki, 1983; Gyöngy and Pardoux, 1993; Walsh, 1986). Its spatial correlation function is exponential, with characteristic length proportional to $g^{-1/2}$. For $g > 0$ fixed, one sees a pattern of regions in which $\mathbf{Y}_t(x)$ is positive and regions in which $\mathbf{Y}_t(x)$ is negative (domains), separated by narrow transition layers (kinks). Although the equation is fully nonlinear, the correlation function can be exactly calculated using the transfer integral. The method applies to arbitrarily nonlinear SPDEs in one space dimension, provided they have a stationary density (Currie *et al.*, 1980; Krumhansl and Schrieffer, 1975; Lythe and Habib, in press; Scalapino *et al.*, 1972). At late times there is a dynamic balance between nucleation and annihilation of kink–antikink pairs (Habib and Lythe, 2000).

3. NUMERICAL SOLUTION

The finite difference method for a parabolic SPDE consists of replacing the infinite-dimensional system (1) by N^m ordinary SDEs on a grid of equally spaced points in $[0, L]^m$ separated by Δx. The SDE at position x is

$$d\Upsilon_t(x) = -g\Upsilon_t(x)\,\mathrm{d}t + \rho\tilde{\Delta}\Upsilon_t(x)\,\mathrm{d}t + \Delta x^{-\frac{m}{2}}\epsilon\,\mathrm{d}\mathbf{W}_t(x), \qquad (4)$$

where $\langle d\mathbf{W}_t(x)\, d\mathbf{W}_t(x')\rangle = \delta_{x-x'}\, dt$,

$$\tilde{\Delta}\Upsilon_t(x) = \sum_{x'} \Upsilon_t(x') - 2m\Upsilon_t(x), \tag{5}$$

with the sum over the $2m$ nearest neighbours of x.

The transfer integral can be used to calculate the dependence of thermodynamic quantities such as the correlation function on the grid spacing. The lowest order corrections to the continuum in one space dimension are proportional to Δx^2 and equivalent to a corrected on-site potential (Bettencourt *et al.*, 1999; Trullinger and Sasaki, 1987). An algorithm has been devised, with the potential augmented by a term proportional to Δx^2, which gives improved convergence to the continuum (Bettencourt *et al.*, 1999; Lythe and Habib, in press).

4. LINEARIZATION

The first hypothesis that facilitates analytical solution is that everywhere $\mathbf{Y}_t(x)$ remains small for $g < g_c$, where

$$g_c = \sqrt{2\mu |\log \epsilon|}. \tag{6}$$

Thereafter the emerging pattern of domains can be studied without the cubic term. The solution of the linearized version of (1) is

$$\mathbf{Y}_t(x) = \int_{[0,L]^m} G(t, t_0, x, v) f(v)\, dv + \epsilon \int_{t_0}^{t} \int_{[0,L]^m} G(t, s, x, v)\, dv\, d\mathbf{W}_s(v), \tag{7}$$

where

$$G(t, s, x, v) = (4\pi(t-s))^{\frac{-m}{2}} \exp(-\mu(t^2 - s^2)) \times \sum_{j=-\infty}^{\infty} \exp\left(-\frac{(x - v - jL)^2}{4(t-s)} \right). \tag{8}$$

The first term in (7), dependent on the initial data $f(x)$, decays exponentially. After an initial transient, the correlation function is therefore obtained from the second, stochastic, integral in (7). Performing the integration over space, assuming $L \gg \mu^{-1/2}$ gives

$$c(x) = \langle \mathbf{Y}_t(x')\mathbf{Y}_t(x'+x)\rangle = \epsilon^2 \int_{t_0}^{t} \frac{e^{\mu(t^2-s^2)}\, e^{-\frac{x^2}{8(t-s)}}}{(8\pi(t-s))^{\frac{m}{2}}}\, ds. \tag{9}$$

Since $\mathbf{Y}_t(x)$ satisfies a nonautonomous SPDE, the correlation function is explicitly a function of time. In the early part of the evolution, however, the deviation from that obtained from the corresponding static ($g =$ constant) equation is small. We consider this quasistatic period by making the change of variables $u = t - s$ in (9). Then

$$\exp(\mu(t^2 - s^2)) = \exp(2\mu tu - \mu u^2) = \exp(2\mu tu)\,(1 - \mu u^2 + \cdots) \tag{10}$$

and

$$c(x) = \frac{\epsilon^2}{(8\pi)^{\frac{m}{2}}} \left(\int_0^\infty \frac{e^{-2|g|u}}{u^{\frac{m}{2}}}\, e^{-\frac{x^2}{8u}}\, du - \mu \int_0^\infty \frac{e^{-2|g|u}}{u^{\frac{m}{2}-2}}\, e^{-\frac{x^2}{8u}}\, du + \cdots \right). \tag{11}$$

Thus

$$c(x) = \frac{\epsilon^2}{2} \frac{|g|^{\frac{m}{4}-\frac{1}{2}}}{(2\pi)^{\frac{m}{2}}} x^{1-\frac{m}{2}} \left(K_{\frac{m}{2}-1}\big(x\sqrt{|g|}\big) + \frac{\mu}{g^2}\frac{x^2}{16}|g| K_{\frac{m}{2}-3}\big(x\sqrt{|g|}\big) + \cdots \right). \tag{12}$$

where K_m is the modified Bessel function of order m. For example, when $m = 1$,

$$c(x - x') = \frac{\epsilon^2}{4\sqrt{|g|}}\, e^{-|x-x'|\sqrt{|g|}} \left(1 - \frac{3}{16}\frac{\mu}{g^2}\left(1 + x\sqrt{|g|} + \frac{1}{3}x^2|g|\right) + \cdots \right). \tag{13}$$

The first term in (12) is the (long-time) correlation function for the SPDE obtained by fixing $g < 0$ (Knight, 1981). Clearly the expansion in μ/g^2 is no longer useful for $g > -\sqrt{\mu}$. The correlation function itself, however, remains well behaved as g passes through 0; the divergences associated with critical slowing down are not present.

In one space dimension, the solution of the SPDE (1) is a stochastic process, with values in a space of continuous functions (Da Prato and Zabczyk, 1992; Doering, 1987; Funaki, 1983; Gyöngy and Pardoux, 1993; Walsh, 1986). That is, for fixed $\omega \in \Omega$ and $t \in [-1/\mu, 1/\mu]$, one obtains a configuration $\mathbf{Y}_t(x)$ that is a continuous function of x. This can be pictured as the shape of a string, at time t, that is constantly subject to small random impulses all along its length. In more than one space dimension, however, the $\mathbf{Y}_t(x)$ are not continuous functions but only distributions (Walsh, 1986), and the correlation function $c(x)$ diverges at $x = 0$. In the nonautonomous equations studied here, however, the divergent part does not grow exponentially for $g > 0$ and, after the quench, it is only apparent on extremely small scales, beyond the resolution of any feasible finite difference algorithm.

We now examine the evolution for $g > \sqrt{\mu}$, where we can approximate (9) using Laplace's formula:

$$c(x) \simeq \frac{\epsilon^2}{\sqrt{\mu}} \frac{e^{\mu t^2}}{(8t)^{\frac{m}{2}}}\, e^{-\frac{x^2}{8t}}. \tag{14}$$

Thus typical values of $\mathbf{Y}_t(x)$ increase exponentially fast and the correlation length at time t is $\sqrt{8t}$. Once $c(0) > \mathcal{O}(\epsilon)$, the noise no longer greatly influences the evolution; its effect can be thought of as wiping out the memory of the initial condition at $g < 0$ and replacing it with an effective random initial condition. From (14), we see that, at $g = \sqrt{2\mu|\log\epsilon|}$, $c(0) = \mathcal{O}(1)$ and the cubic nonlinearity can no longer be ignored.

5. FREEZING IN

The second hypothesis that enables the characteristic domain size to be estimated is that the effect of the cubic nonlinearity, when it finally makes itself felt, is to freeze in the spatial structure. This is indeed the case in numerical simulations: no perceptible changes occur between $g = g_c$ and $g = 1$ (Lythe, 1994, 1996). Thus the correlation length at $g = g_c$,

$$\lambda = \sqrt{\frac{8g_c}{\mu}} = 2^{\frac{7}{4}}\left(\frac{|\log\epsilon|}{\mu}\right)^{\frac{1}{4}}, \tag{15}$$

becomes the characteristic length for the spatial structure after $g = g_c$.

6. DENSITY OF UPCROSSINGS

Consider a homogeneous Gaussian random field $\mathbf{Y}_t(x)$ in one space dimension with correlation function $c(x)$. Then $\mathbf{Y}_t(x + \Delta x) - \mathbf{Y}_t(x)$ is a Gaussian random variable with mean zero and variance

$$\langle(\mathbf{Y}_t(x+\Delta x) - \mathbf{Y}_t(x))^2\rangle = b(\Delta x),$$

where

$$b(\Delta x) = 2(c(0) - c(\Delta x)) = -2c'(0)\Delta x - c''(0)\Delta x^2 + \cdots. \tag{16}$$

The probability that $\mathbf{Y}_t(x)$ has an upcrossing of 0 between x and $x + \Delta x$ is given by

$$\begin{aligned}
&\mathcal{P}[(\text{upcrossing} \in (x, x+\Delta x))]\\
&= \int_{-\infty}^{0} \mathcal{P}[\mathbf{Y}_t(x) = u]\mathcal{P}[\mathbf{Y}_t(x+\Delta x) - \mathbf{Y}_t(x) > u]\,\mathrm{d}u\\
&= (2\pi)^{-1}(b(\Delta x)c(0))^{-\frac{1}{2}} \int_0^\infty \mathrm{e}^{\frac{-u^2}{2c(0)}} \int_u^\infty \mathrm{e}^{\frac{-v^2}{2b(\Delta x)}}\,\mathrm{d}v\,\mathrm{d}u\\
&= \frac{1}{2}\left(\frac{b(\Delta x)}{\pi c(0)}\right)^{\frac{1}{2}} \int_0^\infty \exp\left(-w^2\frac{b(\Delta x)}{c(0)}\right)(1 - \mathrm{erf}(w))\,\mathrm{d}w\\
&= \frac{1}{2\pi}\arctan\left(\left(\frac{b(\Delta x)}{c(0)}\right)^{\frac{1}{2}}\right).
\end{aligned} \tag{17}$$

Now consider a grid of total length L made up of N sites separated by Δx. Let $\Delta x \to 0$ with L fixed, i.e. let $N \to \infty$. We find the density of upcrossings by a Taylor expansion of (17) as $\Delta x \to 0$:

$$\mathcal{P}[(\text{upcrossing} \in (x, x + \Delta x))] \to \frac{1}{2\pi}\left(\frac{b(\Delta x)}{c(0)}\right)^{\frac{1}{2}} \quad \text{as} \quad \Delta x \to 0. \tag{18}$$

- It $c'(0) \neq 0$, the probability of an upcrossing in a given interval is proportional to $\Delta x^{\frac{1}{2}}$. The *density* of zero crossings is thus proportional to $\Delta x^{-\frac{1}{2}}$ for $\Delta x \to 0$, and is infinite in the continuum limit. This is true of many stochastic processes.
- If $c'(0) = 0$ and $c''(0) < 0$, the mean number of zero crossings per unit length r/L approaches a finite number as $\Delta x \to 0$, given by (Adler, 1981; Ito, 1964):

$$\frac{r}{L} = \frac{1}{2\pi}\sqrt{\frac{-c''(0)}{c(0)}}. \tag{19}$$

This is the case for the correlation function after a quench in one space dimension (14).

7. DISCUSSION

There are three successive regimes in the evolution, as the critical parameter is increased.

- In the earliest regime, sufficiently far from the critical point, the evolution is quasiadiabatic: a small perturbation of that found for constant parameters.
- In the second region, close to the critical point, the system can no longer react quickly enough to the time dependence of the critical parameter.
- In the final region, the spatial structure consists of narrow kinks separating long regions where the field is close to one of the minima of the potential. The spatial structure is frozen in in the sense that the motion, merging and occasional nucleation of kink-antikink pairs, happens on a slower timescale than the process that formed them.

For the purposes of calculating the number of kinks formed, the end of the second, nonequilibrium region is the key.

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