Breakdown of Scaling in the Nonequilibrium Critical Dynamics of the Two-Dimensional *XY* Model

A. J. Bray, A. J. Briant, and D. K. Jervis

Department of Physics and Astronomy, The University, Manchester, M13 9PL, United Kingdom

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The approach to equilibrium, from a nonequilibrium initial state, in a system at its critical point is usually described by a scaling theory with a single growing length scale, $\xi(t) \sim t^{1/z}$, where z is the dynamic exponent that governs the *equilibrium* dynamics. We show that, for the 2D *XY* model, the rate of approach to equilibrium depends on the initial condition. In particular, $\xi(t) \sim t^{1/2}$ if no free vortices are present in the initial state, while $\xi(t) \sim (t/\ln t)^{1/2}$ if free vortices are present.

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While the theory of equilibrium critical phenomena has been a mature subject for more than 20 years, nonequilibrium critical phenomena still pose some interesting challenges. The simplest scenario consists of a system evolving at its critical point from a nonequilibrium initial state in which the system was prepared at time $t = 0$. Since the characteristic relaxation time is infinite at criticality, an infinite system will never reach equilibrium. Instead, the system evolves towards equilibrium through a nonequilibrium scaling state. Consider, for example, the equal-time pair correlation function, $C(r,t) = \langle \phi(\mathbf{x},t)\phi(\mathbf{x}+\mathbf{r},t)\rangle$, where ϕ is the order-parameter field. In the nonequilibrium scaling state it has the form

$$C(r,t) = \frac{c}{r^{d-2+\eta}} f\left(\frac{r}{\xi(t)}\right), \tag{1}$$

where d is dimension of space, η is the usual critical exponent, and c is a constant. The scaling form (1) holds in the limit $r \gg a$, $\xi(t) \gg a$, with $r/\xi(t)$ arbitrary, where a is a microscopic cutoff, e.g., a lattice spacing. The first factor in (1) is the equilibrium correlation function: Requiring that this be recovered for $t = \infty$ forces $f(0) = 1$.

The physical interpretation of $\xi(t)$ is the length scale up to which critical correlations have been established at time t: $C(r,t) \sim c r^{-(d-2+\eta)}$, the equilibrium result holds, for $a \ll r \ll \xi(t)$. Dynamical scaling suggests

$$\xi(t) \sim t^{1/z} \tag{2}$$

for large t, where z is the usual dynamic exponent characterizing temporal correlations *in equilibrium*. This result has been demonstrated in an expansion in $\epsilon = 4 - d$ using standard field-theoretic renormalization group methods [1]. The importance of this result is that it shows that relaxation *to* equilibrium is governed by the same exponent as correlations *in* equilibrium. A second important result of Ref. [1] is that the relation $\xi(t) \sim t^{1/z}$ holds independently of the nonequilibrium initial state, which can affect the scaling function, $f(x)$, in (1) but not the exponent z (since this is a property of the equilibrium renormalization group fixed point).

Two special cases illustrate the dependence of $f(x)$ on the initial conditions. For a disordered initial condition, the system will remain disordered on scales $r \gg \xi(t)$, so $f(x)$ will fall off rapidly for $x \gg 1$. For an initial condition with long-range order (i.e., nonzero initial magnetization), dynamical scaling predicts that the magnetization $M(t)$ will decay asymptotically as $t^{-\beta/\nu z} \sim \xi(t)^{-\beta/\nu}$. In this case $C(r,t)$ approaches $C(\infty,t) = M^2(t) \sim t^{-2\beta/\nu z} = t^{-(d-2+\eta)/z}$ using standard scaling laws. So in this case $f(x) \sim x^{d-2+\eta}$ for $x \to \infty$.

The purpose of this Letter is to challenge this simple picture for the *XY* model in $d = 2$, with nonconserved order parameter, at (and below) the Kosterlitz-Thouless (KT) transition [2]. Specifically we argue that the growing length scale $\xi(t)$ satisfies (2), with $z = 2$, if the initial state contains no free vortices, whereas $\xi(t) \sim (t/\ln t)^{1/2}$ if free vortices are present. Earlier workers [3,4] have demonstrated a growing length scale $(t/\ln t)^{1/2}$ for the zero-temperature coarsening dynamics of a system with free vortices (e.g., one quenched to $T = 0$ from high temperatures). Here we argue that this form holds for all temperatures $T \le T_{\mathrm{KT}}$ whenever free vortices (and antivortices) are present in the initial state.

We first present numerical simulation results supporting this scenario and then provide the theoretical interpretation. The two types of initial states we shall consider are (a) completely ordered (no free vortices) and (b) completely random (free vortices present).

The *XY* model consists of planar spins $\{\vec{S}_i\}$ at the sites of a square lattice of linear size L, with Hamiltonian $H = -\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$, where the sum is over lattice links and we have taken the exchange interaction to have strength unity. We adopt conventional "heat-bath" dynamics in which a spin is moved to a trial configuration chosen at random on the unit circle, and the move accepted with probability $[1 + \exp(\Delta E/T)]^{-1}$, where ΔE is the energy change associated with the move and T is the temperature. The lattice is divided into two sublattices, and the sublattices

are updated alternately. One unit of time corresponds to an attempted move of every spin.

A convenient quantity to study is the "time-dependent Binder cumulant" [5,6], $g_L(t)$, defined by

$$g_L(t) = 2 - \frac{\langle(\vec{M}^2)^2\rangle}{\langle\vec{M}^2\rangle^2}, \tag{3}$$

where $\vec{M}(t) = \sum_i \vec{S}_i(t)$ is the total magnetization at time t, and $\langle\cdots\rangle$ indicates an average over independent Monte Carlo runs (10^4 runs were used in practice). Because the powers of $\vec{M}$ in the numerator and the denominator are the same, $g_L(t)$ depends (at a critical point, and if dynamical scaling holds) only on the ratio $\xi(t)/L$, where L is the (linear) size of the lattice:

$$g_L(t) = G\left(\frac{\xi(t)}{L}\right), \tag{4}$$

provided, as always, that both $\xi(t)$ and L are sufficiently large. This result provides the basis for a determination of $\xi(t)$ using finite-size scaling. If conventional dynamical scaling holds, the scaling *function* $G(x)$ may depend on the initial state, but the scaling *variable*, $\xi(t)/L = t^{1/z}/L$, will not. For an ordered initial state (all spins parallel) $G(0) = 1$, while for a random initial condition (each spin chosen independently from a unit circle) $G(0) = 0$ follows from the Gaussian distribution (central limit theorem) of $\vec{M}(0)$. For $t \to \infty$, $G(x)$ approaches, in both cases, the universal value $G(\infty)$ characteristic of the critical point. For the KT phase there is actually a line of such fixed points, $T \leq T_{\mathrm{KT}}$ [and a corresponding set of values $G_T(\infty)$], but we will focus primarily on the KT point, T_{KT}, using the accepted value $T_{\mathrm{KT}} = 0.90$ [7].

Data for the ordered initial state are presented in Fig. 1, for system sizes $L = 12$, 16, 24, 32, and 48. The abscissa, t/L^2, corresponds to a scaling variable t/L^z with $z = 2$. This choice of z is dictated by the spin-wave theory (i.e., no free vortices) that describes the large-scale properties of the KT phase everywhere along the fixed line $T \leq T_{\mathrm{KT}}$. The best collapse using all the data favors a slightly lower value, but the value $z = 2$ clearly gives a good scaling collapse for larger L, i.e., $L \geq 24$ (note the expanded scale compared to Figs. 2 and 3). Collapsing the data for pairs of L gives effective exponents $z(L_1, L_2)$ given by $z(12, 16) = 1.75(5)$, $z(16, 24) = 1.83(3)$, $z(24, 32) = 1.96(2)$, $z(32, 48) = 2.00(2)$, consistent with a convergence to $z = 2$ for $L \to \infty$. Recent simulations by Luo *et al.* [8] give similar results: $z = 1.96(4)$ for $T = 0.90$ and an ordered initial state.

The data for a random initial condition are presented in Figs. 2 and 3. In Fig. 2, we attempt to collapse the data with a scaling variable t/L^z. The scaling collapse is very good, but a much higher value of the dynamical exponent, $z \simeq 2.35$, is required than for an ordered initial state. For a random initial condition Luo *et al.* found, by direct measurement of the time dependence for a large lattice ($L = 512$), the slightly smaller result $z = 2.29(1)$ [8].

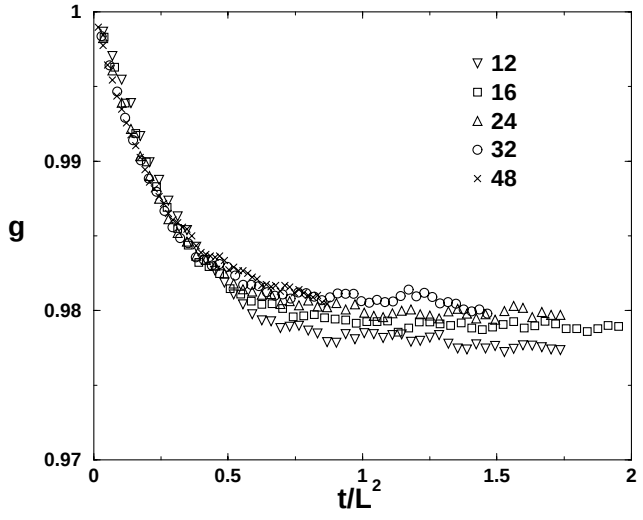

FIG. 1. Scaling plot, with $z = 2$, for the time-dependent Binder parameter, starting from an ordered initial condition, for system sizes $L = 12$, 16, 24, 32, and 48.

At first sight, these results seem remarkable: Different values of z are required to fit the approach to equilibrium from ordered (or "low-temperature") and disordered (or "high-temperature") initial states, whereas dynamical scaling predicts a unique value of z, namely, that which describes equilibrium correlations (in this case $z = 2$). What is going on here? It is worth noting that for Ising systems the two different initial conditions give compatible results [9]. The data for the *XY* model in $d = 2$ seem to point clearly to a breakdown of dynamical scaling. This is indeed our conclusion, but the breakdown is weaker than the naive fit shown in Fig. 2 suggests. We will argue that, for a disordered initial condition, the characteristic length scale $\xi(t)$ grows as $(t/\ln t)^{1/2}$ rather than $t^{1/z}$. Before presenting the arguments, we test this prediction in Fig. 3, where

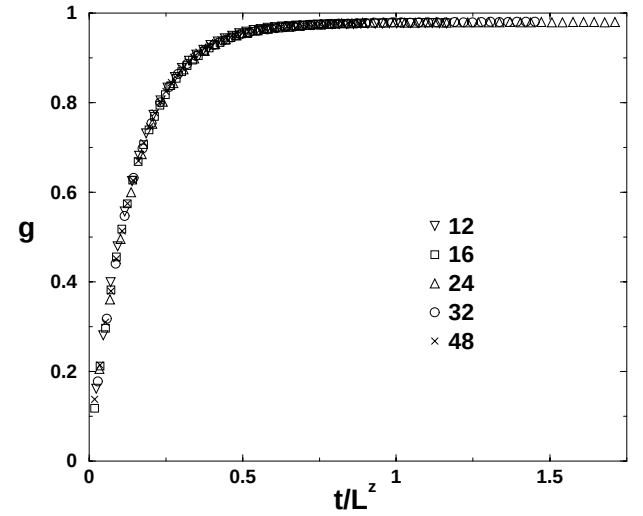

FIG. 2. Scaling plot, with $z = 2.35$, for the time-dependent Binder parameter, starting from a disordered initial condition, for system sizes $L = 12$, 16, 24, 32, and 48.

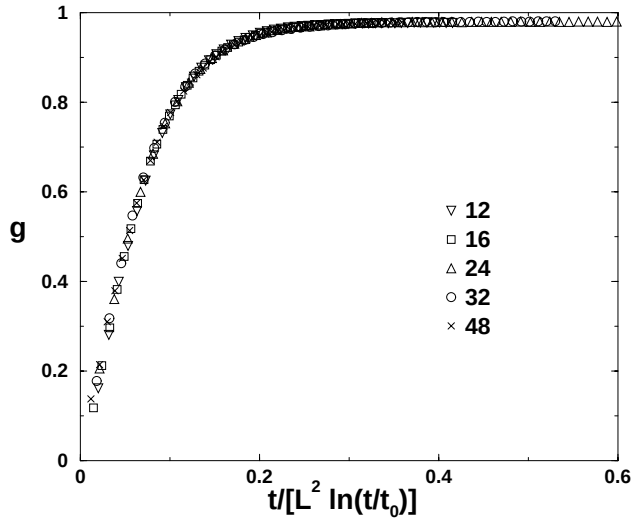

FIG. 3. Same as Fig. 2, but for scaling variable $t/[L^2 \ln(t/t_0)]$, with $t_0 = 0.5$.

$t/L^2 \ln(t/t_0)$ is used as abscissa. The fit is excellent. The value $t_0 = 0.5$ was used for the short-time cutoff, but the fit is not too sensitive to this value.

The quality of the scaling collapses in Figs. 2 and 3 are comparable [10], but the fit used in Fig. 3 has a theoretical underpinning. First, however, we note that the scaling form (1), with $z = 2$, follows from the spin-wave theory for an ordered initial state: No free vortices are present at $t = 0$, and none gets generated by thermal noise for any $T \leq T_{\mathrm{KT}}$. The calculation of $C(r, t)$ is straightforward [11] and gives precisely the scaling form (1) with $\xi(t) = t^{1/2}$ and $f(x) = \exp[-\eta J(x)/2]$, where $J(x) = \int_0^{x^2/8} (dy/y)[1 - \exp(-y)]$ and $\eta = 1/4$ for $T = T_{\mathrm{KT}}$.

For a disordered initial condition, very different considerations are involved. The initial state contains many free vortices and antivortices. The approach to the equilibrium critical state proceeds through the annihilation of vortex-antivortex pairs, which is a slower process than the equilibration of spin waves. For pedagogical purposes, we consider first the case where the system evolves at $T = 0$, instead of T_{KT}. The evolution of the system via vortex-antivortex annihilation is an example of phase-ordering dynamics [12]. It is convenient to adopt a continuum approach based on the nonlinear sigma model Hamiltonian $H = (\rho_s/2) \int d^2 r (\nabla \vec{\phi})^2$ (where ρ_s is the spin-wave stiffness), with local constraint $\vec{\phi}^2 = 1$. A field configuration describing a single free vortex, $\vec{\phi} = \vec{r}/|\vec{r}|$, has an energy $E_v = \pi \rho_s \ln(L/a)$, where L and a are the system size and microscopic cutoff as before. A vortex-antivortex pair, separated by distance R, screen each other's far fields at scales larger than R, leading to a pair energy $E_p \simeq 2\pi \rho_s \ln(R/a)$, and an attractive force $F = -dE_p/dR = -2\pi \rho_s/R$ between the vortex and the antivortex.

To discuss pair annihilation, some dynamics has to be imposed. The Monte Carlo dynamics used here is in the "nonconserved" universality class (i.e., the magnetization is not conserved) described (at $T = 0$) by the continuum model $\partial \vec{\phi}/\partial t = -\Gamma \delta H/\delta \vec{\phi}$. This equation can be used [3] to compute an effective friction constant $\gamma(R)$ associated with the motion of the vortex and antivortex under the force F. An isolated vortex moving at speed v in the x direction has field configuration $\vec{\phi}(x, y, t) = \vec{\phi}_v(x - vt, y)$. Energy is dissipated at a rate $dE/dt = \int d^2 r (\delta H/\delta \vec{\phi}) \cdot (\partial \vec{\phi}/\partial t) = -(1/\Gamma) \int d^2 r (\partial \vec{\phi}/\partial t)^2 = -(v^2/\Gamma) \int d^2 r (\partial \vec{\phi}_v/\partial x)^2 = -\gamma_v v^2$. Inserting the equilibrium vortex configuration, which is isotropic, gives the limiting zero-velocity friction constant as $\gamma_0 = E_v/\rho_s \Gamma$, i.e., γ_0, like the vortex energy E_v, diverges logarithmically with the system size, L. For a vortex-antivortex pair, this translates into a logarithmic dependence on the separation [3], $\gamma(R) = (\pi/\Gamma) \ln(R/a)$.

In the many-vortex situation envisaged for the nonequilibrium critical dynamics, the usual scaling arguments [3,4,12] can be invoked, in which the pair separation, R, is replaced by the typical spacing, $\xi(t)$, between vortices and antivortices. The typical force on a vortex (or antivortex) is then $F \sim \rho_s/\xi$, while the typical friction constant is $\gamma \sim (1/\Gamma) \ln(\xi/a)$. So the typical speed of a vortex is $d\xi/dt \sim F/\gamma \sim \rho_s \Gamma/[\xi \ln(\xi/a)]$, giving $\xi(t) \sim [\rho_s \Gamma t/\ln(t/t_0)]^{1/2}$, with $t_0 \sim a^2/\rho_s \Gamma$. An alternative approach leading to the same result is given in [4].

For all T in the range $0 \leq T \leq T_{\mathrm{KT}}$, the large-scale properties in equilibrium are controlled by a fixed point with zero vortex fugacity, i.e., by the spin-wave theory, where the role of bound vortex-antivortex pairs is to renormalize the spin-wave stiffness and kinetic coefficient to temperature-dependent functions $\rho_s(T)$ and $\Gamma(T)$. In the nonequilibrium case where free vortices and antivortices are present, due to a disordered initial condition, the dynamics on scales less than $\xi(t)$ should therefore be described, in the limit of large $\xi(t)$, by renormalized spin-wave theory, and the asymptotic result $\xi(t) \sim [t/\ln(t/t_0)]^{1/2}$ should apply to *all* temperatures $T \leq T_{\mathrm{KT}}$, including T_{KT} itself. This is our interpretation of the data in Fig. 3. It accounts for the good data collapse using the appropriate scaling variable.

The treatment of the case $T > 0$ via functions $\rho_s(T)$ and $\Gamma(T)$ is, however, only part of the story. A complete treatment of thermal fluctuations should also incorporate vortex diffusion. Consider once more a free vortex-antivortex pair, but now at $T > 0$. The scale-dependent friction constant suggests the following Langevin equation for the relative position $\mathbf{r}$ of the vortex and antivortex, valid at large separation [13]:

$$\gamma(r) \frac{d\mathbf{r}}{dt} = -\frac{4\pi \rho_s}{r} \hat{\mathbf{r}} + \sqrt{\gamma(r)}\, \boldsymbol{\xi}(t), \qquad (5)$$

where $\gamma(r) \sim \ln(r/a)$ and each component of $\boldsymbol{\xi}(t)$ is an independent Gaussian white noise with strength $4T$. This

equation can be recast as a one-dimensional Langevin equation for a new coordinate $x \simeq r\sqrt{\gamma(r)}$:

$$dx/dt = (2T - 4\pi\rho_s)/x + \xi(t). \quad (6)$$

Thus thermal fluctuations induce a repulsive potential for this coordinate, which competes against the usual attraction. Simple power counting shows that, as expected, T is an exactly marginal variable in the renormalization group sense. However, one can show that, for any $\rho_s > 0$, vortex-antivortex annihilation (x reaching zero) will still occur with probability one, with a characteristic time which scales as x_0^2 (where x_0 is the initial value of x), i.e., as $r^2 \ln(r/a)$. Thus thermal fluctuations change the deterministic annihilation into a stochastic annihilation (with the probability distribution of the time-to-annihilation depending on T) but do not change the dependence of the characteristic time scale on the initial separation [13]. Full details of this calculation will be given elsewhere.

Clearly our result, $\xi(t) \sim (t/\ln t)^{1/2}$ for a disordered initial condition, is asymptotically equivalent to an exponent $z = 2$ (though the logarithmic correction still represents a scaling violation). So as L and t are increased we would expect the effective exponent, obtained by forcing a fit with a scaling variable t/L^z, to decrease towards 2. Collapsing data for pairs of L gives effective exponents $z(L_1, L_2)$ given by $z(12, 16) = 2.47(3)$, $z(16, 24) = 2.37(3)$, $z(24, 32) = 2.29(3)$, and $z(32, 48) = 2.34(3)$. The quoted errors are subjective. They are estimated from the quality of the data collapse, but make no allowance for statistical errors in the data. They therefore represent lower bounds on the true errors [14]. With this caveat the overall decreasing trend of the effective z with increasing L is clear and accords with our expectations.

Although the data presented here are restricted to the Kosterlitz-Thouless transition temperature, T_{KT}, the theoretical interpretation we have outlined holds for all $T \leq T_{\mathrm{KT}}$. In Ref. [8], data were obtained for a range of temperatures at and below T_{KT}: $T = 0.90, 0.86, 0.80$, and 0.70. For a uniform initial state, the corresponding values of z are $1.96(4), 1.98(4), 1.94(2)$, and $1.98(4)$, consistent with the result $z = 2$, for all $T \leq T_{\mathrm{KT}}$, expected from spin-wave theory. The equivalent effective exponents obtained with a disordered initial state are consistently larger: $z = 2.29(1), 2.31(2), 2.33(1)$, and $2.38(2)$. We have argued that the correct interpretation of these anomalously large z values is a logarithmically modified growth, $\xi(t) \sim [t/\ln(t/t_0)]^{1/2}$, of the characteristic length scale. The slow increase of the effective exponent with decreasing T can be accounted for by a weak temperature dependence of the time scale t_0 inside the logarithm.

For the ordered initial condition, the scaling function $G(x)$ in Eq. (4) can, in principle, be calculated exactly using the spin-wave theory. This is technically more difficult, however, than the calculation [11] of the pair correlation function, because the evaluation of $\langle(\vec{M}^2)^2\rangle$ involves four-point correlation functions. We hope to present a detailed theory for $G(x)$ in future work.

To summarize, we have argued that the rate of approach to equilibrium at (and below) the Kosterlitz-Thouless transition temperature depends on whether or not the initial state contains unbound vortices. Thus for a disordered initial state, where free vortices are present, the relaxation to equilibrium is slower, by logarithmic factors, than for an ordered initial state where no free vortices are present. It is possible that this result is peculiar to systems with defect-driven phase transitions. It goes against the expectation [1] that the scale length $\xi(t)$ controlling the relaxation to equilibrium, e.g., in (1) and (4), should be independent of the initial conditions (although the corresponding scaling *functions* may not be). This expectation is based on a perturbative renormalization group treatment in $4 - \epsilon$ dimensions. Such an approach is not sensitive to the effects of topological defects (vortices, in this case), which are the source of the scaling violations reported here.

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