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Damage spreading during domain growth

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We study damage spreading in models of two-dimensional systems undergoing first order phase transitions. We consider several models from the same nonconserved order parameter universality class, and find unexpected differences between them. An exact solution of the Ohta-Jasnow-Kawasaki model [Phys. Rev. Lett. **49**, 1223 (1982)] yields the damage growth law $D \sim t^{\phi}$, where $\phi = d/4$ in d dimensions. In contrast, time-dependent Ginzburg-Landau simulations and Ising simulations with $d = 2$, using heat-bath dynamics, show a power-law growth, but with an exponent of approximately 0.36, independent of the system sizes studied. In marked contrast, Metropolis dynamics shows damage growing via $\phi \sim 1$, although the damage difference grows as $t^{0.4}$.

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The time dependence of fluctuations and correlations is a central aspect of the study of equilibrium and nonequilibrium phenomena. Fluctuations in the time evolution of a dynamical system have two different origins, arising either from the random assignment of the initial conditions or from random influences during the dynamics, i.e., the (thermal) noise. A particularly interesting method for isolating the influence of initial conditions on the subsequent evolution is *damage spreading* [1]. Consider a kinetic Ising model with site spins ± 1, evolving via Monte Carlo dynamics. We introduce damage as follows. Starting with two lattices with identical spin configurations we take one system, select at random a single site, and flip the spin. This introduces a microscopic fluctuation into the "damaged" system relative to the undamaged one. Both lattices, including the damaged site, are then evolved according to the same Monte Carlo dynamics, by using the same sequence of random numbers for both. Any subsequent difference between the two is due to the difference in the initial conditions, since without the initial damage the two systems are always identical.

One common measure of damage between two Ising systems is the Hamming distance between the configurations, given by

$$D(L,t) \equiv \frac{1}{2} \sum_i |S_i(t) - S_i^D(t)|, \qquad (1)$$

where S_i is the state of spin i in the undamaged lattice, S_i^D is the state of site i in the damaged lattice, and $N = L^d$ is the number of spins in a hypercubic lattice of size L. Another important measure is the damage difference, defined by

$$\Gamma(L,t) \equiv \frac{1}{4} \sum_i \left[S_o(0) - S_o^D(0)\right] \left[S_i(t) - S_i^D(t)\right]. \qquad (2)$$

This measures the difference between the amount of damage that is the same as that initially imposed at site o and time $t = 0$ and the amount that is of opposite orientation. The term $\left[S_o(0) - S_o^D(0)\right]$ defines the "parity" of the initial damage at site o and time $t = 0$. We say that damage is positive if it is the same as that initially imposed and negative otherwise. At equilibrium $\Gamma(t)$ can be related to thermodynamic quantities such as the susceptibility and correlation functions, provided the damaged site is frozen for all time in its $t = 0$ configuration [2,3]. There are no known relationships between damage and correlations when the damaged site is allowed to evolve, which is the method considered here. Lastly we remark that damage evolution in systems far from equilibrium has been little studied, and that the relationship between damage growth and traditional dynamical properties in these cases is unknown.

In this paper we examine this latter situation, namely, the evolution of damage in nonequilibrium systems, specifically during domain growth. Following a quench from a disordered state to a low-temperature state where phases coexist, a system dynamically evolves by the formation and subsequent growth of domains of ordered phase. The average size of those domains grows as $R \sim t^n$, for late times where n is the growth exponent, and the morphological evolution involves scale invariance, where all time dependence enters through the characteristic diverging length R. An important issue in this area is universality: what are the common features which characterize a universality class, like n, and how are universality classes determined? The most well established universality class in domain growth is model A [4], where the scalar order parameter is nonconserved, and [5] $n = 1/2$. Systems in this class include binary alloys undergoing order-disorder transitions, as well as the ferromagnetic spin-flip Ising model, and continuum models such as the time-dependent Ginzburg-Landau equation (TDGL) [5] and the Ohta, Jasnow, and Kawasaki (OJK) model [6]. Herein, we investigate damage evolution during domain growth in these latter three models. We find some similarities, but important differences, for the different models. Hence we suggest that universality in domain growth does not include damage evolution.

We first generalize the concept of damage to allow for nondiscrete variables. With this definition we are able to show that OJK dynamics leads to $D \sim t^{\phi}$, with a damage exponent $\phi = d/4$ in d dimensions. Two-dimensional simulation studies of the TDGL equations and of the Ising model using heat-bath dynamics both yield power-law growth for damage. However, $\phi \approx 0.36$, significantly smaller than the OJK model. More remarkably, Ising simulations using Metropolis dynamics in $d = 2$ show $\phi \sim 1$. It should be noted that in all the models studied damage disappears with high probability at long times. But for some realizations of the initial conditions and thermal noises, it attains macroscopic size. The power laws above apply to the damage averaged over samples of the full ensemble of realizations.

The OJK model [6] was introduced as an approximation to the Allen-Cahn equation describing interface motion during phase ordering with a nonconserved order parameter. It is considered an important model in its own right [7] as it readily yields analytic predictions for quantities such as the growth exponent and scaling functions.

Consider the evolution of a system described by an order parameter $\psi(\mathbf{x}, t)$ which takes the value ψ_{eq} in one of the phases and $-\psi_{\mathrm{eq}}$ in the other. In the OJK model the evolution of $\psi(\mathbf{x}, t)$ is given by

$$\psi(\mathbf{x}, t) = \psi_{\mathrm{eq}} \mathrm{sgn}[u(\mathbf{x}, t)] = \psi_{\mathrm{eq}} \frac{u(\mathbf{x}, t)}{|u(\mathbf{x}, t)|}\ , \tag{3}$$

where the auxiliary field $u(\mathbf{x}, t)$ satisfies the diffusion equation: $\dot{u}(\mathbf{x}, t) = \nabla^2 u(\mathbf{x}, t)$. Without loss of generality the values of ψ_{eq} and of the diffusion coefficient are taken here to be unity. The initial condition $u_0(\mathbf{x}) \equiv u(\mathbf{x}, t = 0)$ is usually taken as a random Gaussian field of zero average and short-range correlations. The exact solution of the diffusion equation is $u(\mathbf{x}, t) = \int d\mathbf{x} G(\mathbf{x} - \mathbf{x}', t) u_0(\mathbf{x}')$, where $G(\mathbf{x}, t)$ is a Green function. Substitution of this expression into Eq. (3) leads to an equation of evolution for $\psi(\mathbf{x}, t)$ representing the growth of domains of typical size $R(t) \sim t^{1/2}$ [6].

We need continuum definitions for the damage measure $D(L, t)$ and for the initial damage consistent with those used for the Ising model. We define the initial damage in terms of the initial unperturbed field $u_0(\mathbf{x})$. Several definitions of the "damaged" field u_0^D are possible: we found all to give essentially identical results. We present detailed results for the case in which $u_0^D(\mathbf{x}) \equiv -u_0(\mathbf{x})$ in a damaged region of volume V_D and $u_0^D(\mathbf{x}) \equiv u_0(\mathbf{x})$ outside. We define the damage measure by

$$D(L, t) \equiv \frac{1}{2} \int_{L^d} d\mathbf{x}\ |\psi(\mathbf{x}, t) - \psi^D(\mathbf{x}, t)| \tag{4}$$

$$= \frac{1}{2} \left(L^d - \int_{L^d} d\mathbf{x}\ \psi(\mathbf{x}, t) \psi^D(\mathbf{x}, t) \right) . \tag{5}$$

The calculation of the average damage (ensemble-averaged over different realizations of the random initial conditions) then reduces to the calculation of a correlation function and a subsequent integration. The detailed calculation will be presented elsewhere: here we quote the main results.

In the regime of long times and large L and with the initially damaged volume much smaller than system size

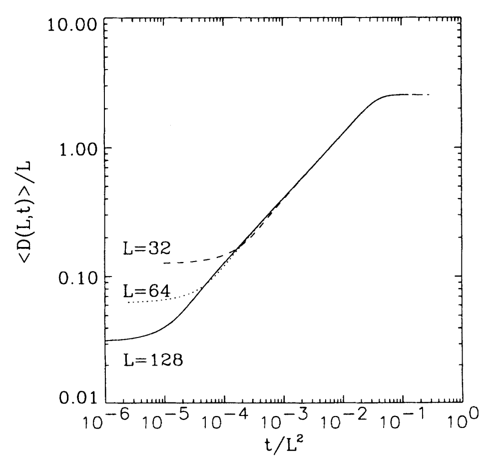

FIG. 1. The $d = 2$ OJK prediction for an initially damaged region of $V_D = 4$ and three different system sizes L. The scaling region and the damage growth via $t^{d/4}$ are evident, as are corrections to scaling at short times.

we find the following scaling result:

$$\langle D(L,t)\rangle = L^{\frac{d}{2}}F(t/L^2), \tag{6}$$

where the scaling function F is

$$F(\tau) = \frac{2\sqrt{V_D}}{\pi}\frac{1}{\sqrt{G(\mathbf{0},2\tau)}}\int_{I^d} d\mathbf{x}\ G(\mathbf{x},\tau). \tag{7}$$

I^d is the unit hypercube. The crucial and disputable element here is the $L^{d/2}$ factor. This arises from the assumption of Gaussian decoupling implicit in the OJK model. The scaling form in the limit $t \ll L^2$ is

$$\langle D(t \ll L^2)\rangle \sim t^{\frac{d}{4}}. \tag{8}$$

Plots of $\langle D(L,t)\rangle$ from Eqs. (6) and (7) for $d = 2$ are shown in scaled form in Fig. 1. The power-law regime is clearly seen, as are the corrections to scaling at short times.

We also numerically iterated the OJK equations on a lattice to visualize the evolution of the damage. We found that damage, when it exists, evolves along the interface between the two phases. Damage then either disappears as the interfaces disappear, or it grows to encompass the entire system. In addition, we confirmed that only one parity of damage dominates: in particular, if we damage only a single lattice site the propagated damage is always of the same parity as initially imposed. This result can be verified analytically. Therefore in OJK, with this damage prescription, the damage difference and Hamming distance are identical.

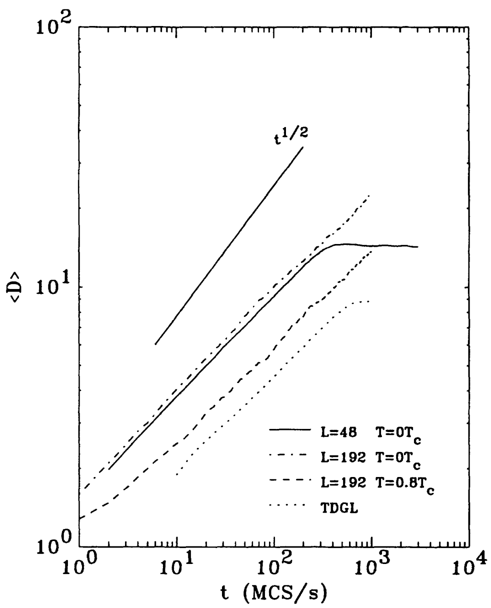

FIG. 2. Damage evolution for a $2d$ quenched Ising model using heat-bath dynamics, showing the effect of temperature and of system size. Time is in Monte Carlo steps per site (MCS/s). The growth of damage is evidently algebraic, even for the smaller systems ($L = 48$). The exponents are 0.36 ± 0.01 for $L = 48$, $T = 0.8T_c$ (24 576 runs averaged); 0.37 ± 0.03 for $L = 192$, $T = 0.0T_c$ (3072 runs averaged); and 0.36 ± 0.01 for $L = 192$, $T = 0.8T_c$ (3072 runs averaged). The dotted line shows the TDGL damage evolution averaged over 6400 realizations of the initial conditions, arbitrarily scaled to fit on the same scale as the Ising data. The system size is $L = 90.5$ and the initially damaged volume is $V_D = 0.5$. Note the discrepancy with the $t^{d/4} = t^{1/2}$ OJK prediction.

The OJK damage definition [Eq. (4)] also applies to the TDGL case. The initial damaged configuration in this case was chosen to be $\psi^D(\mathbf{x},t=0) = -\psi(\mathbf{x},t=0)$ inside a small damaged region and $\psi^D(\mathbf{x},t) = \psi(\mathbf{x},t=0)$ outside, where again $\psi(\mathbf{x},t=0)$ is a Gaussian random field with short-range correlations. Both ψ and ψ^D are evolved according to the TDGL equation:

$$\dot{\psi}(\mathbf{x},t) = \psi(\mathbf{x},t) + \nabla^2\psi(\mathbf{x},t) - [\psi(\mathbf{x},t)]^3. \tag{9}$$

Addition of a noise term does not significatively change the results. The average damage evolution is shown in Fig. 2. The power-law damage growth regime is clearly present and persists up until the system magnetization begins to saturate. We obtain $\phi = 0.36 \pm 0.02$, which is smaller than the OJK prediction of $d/4 = 1/2$. The errors are estimated by one standard deviation of the statistics of the data.

As with the OJK model, we found that the TDGL equations, solved on a discrete lattice, only propagate damage of the same parity as that initially imposed, provided we only damage a single lattice site. If we damage a larger domain there is a transient regime during which both parities of damage compete, but eventually one disappears and damage follows $\phi \approx 0.36$.

Ising simulations, using both heat-bath and Metropolis dynamics, were performed on two-dimensional square lattices, using a multispin coding algorithm described previously [8,9]. However, the block-spin coding trick [8] was avoided, as some kinds of parallel updating have been found to affect damage dynamics [10,11]. Spins to be evolved were chosen at random from among all spins, a single time step [in Monte Carlo steps per site (MCS/s)] being L^2 such attempts. The initial state was an infinite

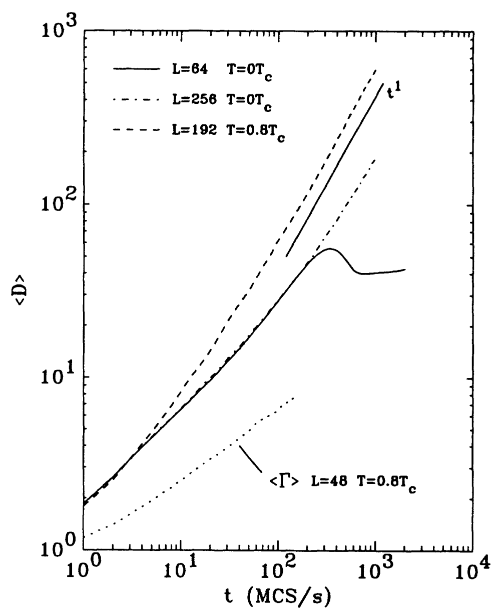

FIG. 3. Damage evolution for a $2d$ quenched Ising model using Metropolis dynamics, showing the effect of temperature and of system size. Time is in Monte Carlo steps per site (MCS/s). The regimes for damage are only evident for the larger system, and at late times. The solid line shows a damage evolution $\propto t$. The damage difference is also plotted, and the slow-growth behavior is evident. The late-time tangent to this growth gives an exponent of $\phi = 0.40 \pm 0.04$.

temperature equilibrium configuration.

Typical results for damage evolution via heat-bath dynamics are shown in Fig. 2, for two system sizes and for temperatures $T = 0.8T_c$ and $T = 0$. The early-time transient is very short, and is quickly followed by a slow power-law growth regime. The power-law exponents are 0.36 ± 0.02, identical with the TDGL results and smaller than the OJK prediction of 1/2. It also appears that the system size does not strongly affect this exponent: systems of size $L = 48$ have essentially the same slope as those four times as big. There is no evidence for faster growth at late times: the growth simply slows as finite-size effects are encountered, and then saturates. Temperature also does not appear to affect the exponent in the power-law regime. In general, increasing the temperature decreases the total damage. This is consistent with previous studies of damage in equilibrium systems using the heat-bath algorithm.

We cannot rule out the possibility that the 0.36 exponent is only an effective exponent, and that systematic errors preclude our observation of $d/4$. Our estimated errors are statistical, and comparable systematic errors are possible. However, we have made a careful study of systems of different sizes, and our numerical results for ϕ are not consistent with the exact result of the OJK model of $d/4$.

It was previously demonstrated that the heat-bath algorithm can only propagate damage of the same parity as that initially imposed [2]. Therefore as in the previous two cases the Hamming measure and the damage difference are identical.

We obtain remarkably different behavior using the Metropolis algorithm. Typical Metropolis dynamics results are shown in Fig. 3, where again we have plotted results demonstrating the effect of varying system size and temperature. The results are different from all results presented above. Even at earliest times the growth of damage is *faster* than $t^{1/2}$, with this exponent increasing with time. At intermediate times this damage saturates at $\phi \sim 1$, i.e., approximately twice as fast as seen by the other dynamics. Simulations to much later times indicate no deviation from this dependence until finite-size effects are encountered and growth stops.

Equivalence between the three numerical models can be recovered if we consider the damage difference, Eq. (2). A typical plot of the damage difference is shown in Fig. 3 for systems of size $L = 48$. Although quite noisy, these data clearly show a power-law growth slower than $t^{1/2}$. A best fit yields 0.40 ± 0.04, consistent with the TDGL and Ising heat-bath results. Of course we again cannot rule out the possibility that this exponent approaches 0.5 for larger systems, indicating strong finite-size effects. However, we see no evidence for such systematic errors in the range of sizes studied ($L = 48$ to $L = 192$).

The reason for the surprising differences between the Ising simulations lies, at the microscopic level, in the difference between the two dynamics. Metropolis dynamics allows both parities of damage to exist. By visualizing the damage evolution we find that Metropolis dynamics produces significant amounts of both damage. Individually averaging these two parities of damage shows that both are dominated by $\phi \sim 1$. Damage of the *same* parity as the initial damage shows a large initial transient related to the early-time growth of the damage difference, before crossing over to the faster growth, while the opposite-parity damage quickly assumes $\phi \sim 1$.

In conclusion, we have presented numerical evidence that nonequilibrium damage spreading lacks the universality of domain growth. In particular, we have shown that the TDGL model and the Ising models are equivalent, but only when the damage difference is used as the measure. More importantly our work suggests that the damage algorithm breaks the universality between the TDGL, Ising, and OJK models. More detailed comparisons between these models, including the consideration of finite-size effects, finite-size scaling, and the full derivation of the OJK analytical results will be presented in a future publication.

Note added. After we submitted this paper, Yeung [12] gave us an argument relating ϕ to the two-time correlation function exponent.

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[1] S.A. Kauffman, J. Theor. Biol. **22**, 437 (1969); B. Derrida and Y. Pomeau, Europhys. Lett. **1**, 45 (1986); B. Derrida, Philos. Mag. B **56**, 917 (1987); D. Stauffer, *ibid.* **56**, 901 (1987); B. Derrida and G. Weisbuch, Europhys. Lett. **4**, 657 (1987); H.E. Stanley, D. Stauffer, J. Kertész, and H.J. Herrmann, Phys. Rev. Lett. **59**, 2326 (1987).

[2] A. Coniglio *et al.*, Europhys. Lett. **8**, 315 (1989).

[3] H.J. Herrmann, in *Computer Simulation Studies in Condensed Matter Physics II*, edited by D.P. Landau, K.K. Mon, and H.-B, Schüttler, Springer Proceedings in Physics Vol. 45 (Springer-Verlag, Berlin, 1990); K. MacIsaac and N. Jan (unpublished); S.C. Glotzer, P.H. Poole, and N. Jan, J. Stat. Phys. **68**, 895 (1992); G. Batrouni and A. Hansen, J. Phys. A **25**, L1059 (1992).

[4] P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[5] J.D. Gunton, M. San Miguel, and P.S. Sahni, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, London, 1983), Vol. 8.

[6] T. Ohta, D. Jasnow, and K. Kawasaki, Phys. Rev. Lett. **49**, 1223 (1982).

[7] C. Yeung and D. Jasnow, Phys. Rev. B **42**, 10523 (1990).

[8] G. Bhanot, D. Duke, and R. Salvador, J. Stat. Phys. **44**, 985 (1986); C. Roland and M. Grant, Phys. Rev. B **39**, 11 971 (1989).

[9] I.S. Graham and M. Grant, J. Phys. A **25**, L1195 (1992).

[10] E.T. Gawlinski, M. Grant, J.D. Gunton, and K. Kaski, Phys. Rev. A **31**, 281 (1985); F.D. Nobre, A.M. Mariz, and E.S. Sousa, Phys. Rev. Lett. **69**, 13 (1992).

[11] We found that the vectorized (block-spin coding) and nonvectorized computer codes gave slightly different asymptotic damage values, in keeping with the notion that this quantity is nonuniversal and can depend on the implementation of the dynamics. Other quantities, such as the scaling exponents, were unaffected.

[12] C. Yeung (private communication).