

Bicritical Point and Crossover in a Two-Temperature, Diffusive Kinetic Ising Model

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The phase diagram of a two-temperature kinetic Ising model which evolves by Kawasaki dynamics is studied using Monte Carlo simulations in dimension $d = 2$ and solving a mean-spherical approximation in general d . We show that the equal-temperature (equilibrium) Ising critical point is a *bicritical point* where two *nonequilibrium* critical lines meet a first-order line separating two distinct ordered phases. The shape of the nonequilibrium critical lines is described by a crossover exponent, φ , which we find to be equal to the susceptibility exponent, γ , of the Ising model.

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Phase transitions in nonequilibrium systems have been much investigated in the last decade. The main thrust of this research is to find some generic features of nonequilibrium steady states by trying to answer the following question: What happens to the universality of critical phenomena when equilibrium systems are dynamically perturbed so that phase transitions are forced to occur in nonequilibrium steady states? The answer does not appear to be simple. There are numerous examples where the equilibrium critical behavior is not affected by the perturbations [1,2]. There also exist examples where the universality class changes under the perturbation but the new class is a known equilibrium class [3–5]. Finally, in a few cases, new, nonequilibrium (non-Hamiltonian) classes [6] emerge.

Since the emphasis in these studies is on general properties, not much attention has been paid to the details of phase diagrams. Taking equilibrium theories as a guide, however, we should note that phase diagrams may also display universal features [7]. At a bicritical point, e.g., two critical lines meet a critical point at the end of a first order line, and the shape of the critical lines is universal, characterized by a crossover exponent φ . Whether this universality remains valid for a *nonequilibrium* phase diagram near a bicritical point is an open question and, below, this problem will be investigated by studying a two-temperature, diffusive kinetic Ising model [8]. We find that this system displays a relatively simple bicritical phase structure since the bicritical point turns out to be an Ising critical point. A further simplifying feature is that the nonequilibrium phase transition across one of the critical lines is expected to belong to the universality class of uniaxial ferromagnets with dipolar interactions [5]. Thus, provided universality extends to the nonequilibrium case, we have a prediction for φ since the Ising-to-uniaxial-dipole crossover is described [9] by the susceptibility exponent of the Ising model ($\varphi = \gamma$). We confirm this prediction first by using Monte Carlo (MC) simulations to determine the phase diagram in $d = 2$ and, second, by exactly solv-

ing the spherical limit of a coarse-grained version of the model.

The two-temperature, diffusive kinetic Ising model [8] is a generalization of Kawasaki's model [10]. Ising spins $\sigma_i = \pm 1$ at sites \mathbf{i} of a d -dimensional hypercubic lattice interact by nearest-neighbor ferromagnetic interactions of strength J , and the dynamics consist of exchanges of nearest-neighbor spins. Exchanges along one of the axes of the lattice (called "parallel" direction) satisfy detailed balance at an inverse temperature $\beta_{\parallel} = J/T_{\parallel}$ while exchanges in the remaining $d - 1$ "perpendicular" directions are produced by a heat bath of inverse temperature $\beta_{\perp} = J/T_{\perp}$ [11].

For $\beta_{\perp} = \beta_{\parallel} = \beta$ (diagonal in Fig. 1), this is the Kawasaki model [10] which relaxes to the equilibrium Ising model at β and, consequently, it displays a continuous transition at $\beta_{\perp} = \beta_{\parallel} = \beta_c \approx 0.4407$. Since the dynamics conserves the total magnetization, the ordering for $\beta_{\perp} = \beta_{\parallel} > \beta_c$ appears as a phase separation.

For $\beta_{\perp} \neq \beta_{\parallel}$, on the other hand, there is a flow of energy between the \parallel and \perp heat baths, and the system relaxes to a nonequilibrium steady state. This steady state has previously been studied by MC simulations [8,12] in $d = 2$, along the axes ($\beta_{\perp} = 0, \beta_{\parallel}$) and ($\beta_{\perp}, \beta_{\parallel} = 0$) of the ($\beta_{\perp}, \beta_{\parallel}$) plane. Critical points along these lines, ($\beta_{\perp} = 0, \beta_{\parallel c}$) and ($\beta_{\perp c}, \beta_{\parallel} = 0$), were found with phase separation occurring in the ordered states. Because of the dynamical anisotropy, however, these phase separations are distinct from those occurring in equilibrium: The interfaces between the domains of up and down spins align with normals along the directions of lower temperatures, i.e., their normals point in the \parallel direction for ($\beta_{\perp} = 0, \beta_{\parallel} > \beta_{\parallel c}$) (we call this parallel order) while they can point in any of the $d - 1$ \perp directions for ($\beta_{\perp} > \beta_{\perp c}, \beta_{\parallel} = 0$) (perpendicular order). Thus the symmetries of the \parallel and \perp orders are different from the symmetry of the equilibrium order where interfaces with normals along any of the d axes of the lattice coexist (isotropic ordering). As a consequence, the universality classes of the \parallel and \perp orderings are distinct from the Ising class [8,12,13].

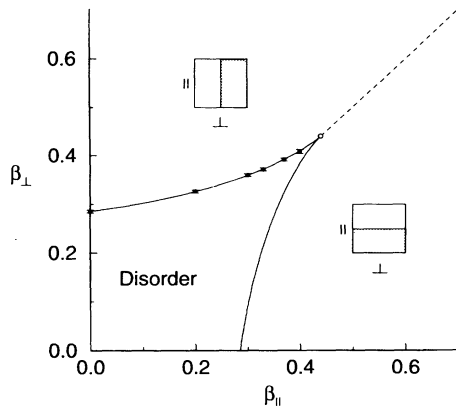


FIG. 1. Phase diagram in $d = 2$. Dimensionless inverse temperatures are denoted by $\beta_{\perp} = J/T_{\perp}$ and $\beta_{\parallel} = J/T_{\parallel}$. The open circle marks the Ising critical point where two nonequilibrium critical lines (solid curves) meet a first-order line (dashed line). The critical lines are drawn as guides to the eye reflecting the MC results (solid circles). Insets show schematic drawings of domains of up and down spins in the ordered state.

Furthermore, renormalization group calculations [13] indicate that if there are critical lines connecting the Ising critical point to the nonequilibrium critical points ($\beta_{\perp} = 0, \beta_{\parallel c}$) and ($\beta_{\perp c}, \beta_{\parallel} = 0$), then the critical behavior along these lines falls into the universality class of the corresponding \parallel or \perp orderings. In particular, the universality class of the \parallel ordering is expected to coincide with that of a uniaxial ferromagnet with dipolar interactions [5].

In our MC simulations of the $d = 2$ system, we aimed at showing that (i) the ($\beta_{\perp} = 0, \beta_{\parallel c}$) and ($\beta_{\perp c}, \beta_{\parallel} = 0$) points are connected to the Ising critical point (β_c, β_c) by critical lines; (ii) the shape of the critical lines near (β_c, β_c) is described by the Ising-to-uniaxial-dipole crossover exponent; and (iii) the coexistence line of the equilibrium system ($\beta_{\perp} = \beta_{\parallel} > \beta_c$) is a first-order line.

In order to accomplish (i) and (ii), MC simulations were performed at various values of β_{\perp} with β_{\parallel} fixed at 0.0, 0.2, 0.3, 0.33, 0.37, or 0.4. Note that the phase diagram in $d = 2$ is symmetric with respect to reflection through the $\beta_{\perp} = \beta_{\parallel}$ diagonal since $\beta_{\perp} \leftrightarrow \beta_{\parallel}$ just corresponds to renaming the axes of the lattice. Thus it is sufficient to consider the $\beta_{\perp} \geq \beta_{\parallel}$ region. A difficulty in simulating the system is that the anisotropy introduced by the dynamics requires anisotropic finite size scaling, i.e., one has to compare systems whose shapes scale as $(L_{\perp}, L_{\parallel}^{1+\theta})$ where θ is an anisotropy exponent [14]. Since both renormalization group calculations [13] and simulations [12] indicate that $\theta \approx 0.9 - 1.0$, we chose system sizes of 8×4 , 12×9 , 16×16 , 24×36 , and 32×64 , which are related by the naive scaling $L_{\perp} \times L_{\parallel}^2$. In anticipation of the expected ordering, the order parameter Ψ was defined as the following long-wavelength limit of the structure factor

$$\Psi = C(2\pi/L_{\perp}, 0), \quad (1)$$

where $C(q_{\perp}, q_{\parallel})$ is the Fourier transform of the spin configuration with $(q_{\parallel}, q_{\perp})$ being the components of the wave vector \mathbf{q} in the \parallel and \perp directions, respectively. We measured the time evolution of Ψ and, after producing a rough estimate of its relaxation time, determined the time averages $\langle \Psi \rangle$ and $\langle \Psi^2 \rangle$ in the steady state. The location of the critical point ($\beta_{\perp c}, \beta_{\parallel}$) at fixed β_{\parallel} was first estimated from the finite-size scaling of the cumulants of Ψ [15], and then a more accurate estimate was produced from the scaling plots of $L_{\perp}^{2-\theta} \langle \Psi \rangle$ versus $L_{\perp}^{1/\nu} (\beta_{\perp} - \beta_{\perp c}) / \beta_{\perp c}$. The values of $\nu = 0.6$ and $\theta \approx 0.9 - 1.0$ were taken from [12], assuming that the universality class of the transition is that of the nonequilibrium ordering at ($\beta_{\perp c}, \beta_{\parallel} = 0$). Then the fitting parameter $\beta_{\perp c}$ was determined by observing collapse of data. Conservative error bars on $\beta_{\perp c}$ were obtained from noting unambiguous declines in the quality of the scaling plots as $\beta_{\perp c}$ was changed. We observed good collapse of data in a narrow range of $\beta_{\perp c}$ and, we believe, this can be taken as an indication that (a) the ordering occurs through critical phase transition, and (b) the assumption about the universality class of this transition is correct.

The details of the MC simulations will be published elsewhere; here we summarize the results in Figs. 1 and 2. Figure 1 displays the phase diagram in the $(\beta_{\perp}, \beta_{\parallel})$ plane with insets showing the alignment of surfaces in the ordered states. The locations of transition points parametrized as $\varepsilon = (2\beta_c - \beta_{\perp c} - \beta_{\parallel c}) / \sqrt{2}$ and $\Delta = (\beta_{\perp c} - \beta_{\parallel c}) / \sqrt{2}$ are shown on the log-log plot in Fig. 2. A straight line on this plot would imply $\Delta \sim \varepsilon^{\varphi}$, and thus the slope of the line would determine the crossover exponent φ . One can see that the MC points do not quite lie on a straight line indicating that there are corrections to scaling in the ε range studied. Comparing with the

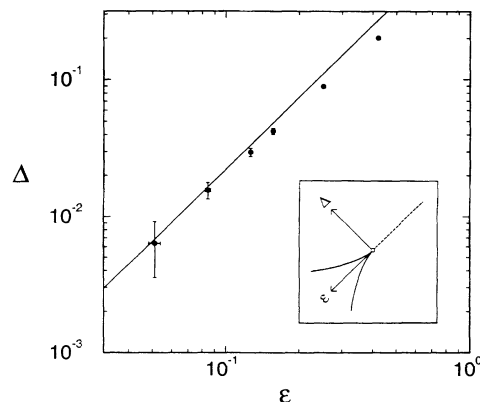


FIG. 2. MC results for the location of the critical points in coordinates (ε, Δ) measured from the bicritical point as shown in the inset. Error bars are not shown where they are smaller than the symbol size. The solid line has a slope equal to the susceptibility exponent of the equilibrium Ising model ($\gamma = 1.75$).

solid line which has a slope equal to the susceptibility exponent ($\gamma = 1.75$), however, one can also observe a trend: The slope of the MC curve which is about 1.6 for large ε slowly increases, and it approaches 1.75 as ε is decreased. Thus, we believe that Fig. 2 strongly suggests that asymptotically $\varphi = \gamma = 1.75$.

MC simulations were also used to study metastability near the coexistence line (dotted line in Fig. 1). Square samples (16×16 and 32×32) were brought to steady state in the region of \perp order ($\beta_{\perp} = \beta + \delta, \beta_{\parallel} = \beta$ with $\beta < \beta_c$ and $\delta \approx 0.01 - 0.1$), and then the inverse temperatures were switched to the other side of the coexistence line ($\beta_{\perp} = \beta, \beta_{\parallel} = \beta + \delta$). Measuring the time evolution of the difference of the \perp and \parallel order parameters, $\delta\Psi = C(2\pi/L_{\perp}, 0) - C(0, 2\pi/L_{\parallel})$, we could observe characteristic features of metastability: (a) After switching the temperatures, $\delta\Psi$ did not change significantly from its initial value $\delta\Psi_0$ for times, τ_{\pm} , which were 2–3 orders of magnitude larger than the steady-state relaxation time τ_s . (b) The scatter in the values of τ_{\pm} was large. (c) Once the change of order started, $\delta\Psi$ changed to $-\delta\Psi_0$, in a time of order τ_s . (d) τ_{\pm} diverged as the coexistence line was approached. We believe the above points provide evidence that the coexistence line is indeed a line of first-order transitions.

In order to investigate problems (i) and (ii) from an analytic point of view, we turn now to a coarse-grained version of the two-temperature, diffusive Ising model. In the classification scheme of critical dynamics [16], it is a generalization of model B: The order parameter is the density of particles and, to make the spherical approximation used later more transparent, the order-parameter field is assumed to have n components, $S^i(\mathbf{x}, t)$ ($i = 1, \dots, n$). The Ising case corresponds to $n = 1$, but it will be clear from the results that the two-temperature vector models ($n \geq 2$) may also be an interesting new class of nonequilibrium models. The order parameter evolves by diffusion which satisfies detailed balance at temperature T_{\parallel} in one direction and at temperature T_{\perp} in the remaining $d - 1$ dimensions. The Hamiltonian in the detailed balance condition is the Landau-Ginzburg free energy, so the equation of motion for the Fourier transform of the field, $S_{\mathbf{q}}^i(t)$, is given by the following Langevin equation

$$\dot{S}_{\mathbf{q}}^i(t) = \mathcal{L}_{\parallel}(q)S_{\mathbf{q}}^i + \eta_{\parallel}^i(\mathbf{q}, t) + \mathcal{L}_{\perp}(q)S_{\mathbf{q}}^i + \eta_{\perp}^i(\mathbf{q}, t). \quad (2)$$

Here the diffusion in the $\alpha = \parallel$ and $\alpha = \perp$ directions are described by the corresponding \mathcal{L}_{α} terms:

$$\mathcal{L}_{\alpha}S_{\mathbf{q}}^i = -D_{\alpha}q_{\alpha}^2 \left[(r_0^{\alpha} + q^2)S_{\mathbf{q}}^i + u \sum_{j=1}^n \int_{\mathbf{q}'} \int_{\mathbf{q}''} S_{\mathbf{q}'}^j S_{\mathbf{q}''}^j S_{\mathbf{q}-\mathbf{q}'-\mathbf{q}''}^i \right], \quad (3)$$

and the noise terms represent Gaussian-Markovian random forces with correlations of the form

$$\langle \eta_{\alpha}^i(\mathbf{q}, t) \eta_{\alpha'}^j(\mathbf{q}', t') \rangle = 2D_{\alpha}q_{\alpha}^2 \delta_{\alpha\alpha'} \delta_{ij} \delta(\mathbf{q} + \mathbf{q}') \delta(t - t').$$

The parameters D_{α} and u are constants with the relevant temperature dependence contained in $r_0^{\alpha} = T_{\alpha} - T_0$ where T_0 is another constant. For $r_0^{\parallel} = r_0^{\perp}$, we have model B with anisotropic diffusion, thus the steady state is an equilibrium state at $T_{\parallel} = T_{\perp} = T$. For $r_0^{\parallel} \neq r_0^{\perp}$, on the other hand, there is a competition between the diffusion dynamics in the \parallel and \perp directions, each trying to bring the system to equilibrium at temperatures T_{\parallel} and T_{\perp} , respectively. The resulting nonequilibrium steady state displays nonequilibrium phase transitions which will be studied below using the spherical approximation where one assumes that $n \rightarrow \infty$ and $u \sim 1/n$.

Before proceeding with the calculation, we note that coarse graining should lead, in principle, to a Langevin equation in which the constants u and T_0 are different in \mathcal{L}_{\parallel} and \mathcal{L}_{\perp} and, furthermore, the D_{α} in \mathcal{L} and in the corresponding noise correlations could also be distinct. By neglecting all these differences, we introduce a minimal model which displays all the symmetries, conservation laws, anisotropies, and dynamical competitions present in the microscopic process.

The spherical limit is a self-consistent approximation for arbitrary n . It becomes exact for $n \rightarrow \infty$ since the fluctuations in $u \sum S_{\mathbf{q}}^j(t) S_{\mathbf{q}'}^j(t)$ may be neglected in this limit, and one can write

$$u \sum_{j=1}^n \langle S_{\mathbf{q}}^j(t) S_{\mathbf{q}'}^j(t) \rangle = unC(\mathbf{q}, t) \delta(\mathbf{q} + \mathbf{q}'). \quad (4)$$

Here the brackets $\langle \rangle$ denote averaging over both the initial conditions and the noise η_{\parallel} and η_{\perp} . Note that the dynamic structure factor $C(\mathbf{q}, t) = \langle S_{\mathbf{q}}^i(t) S_{-\mathbf{q}}^i(t) \rangle$ is assumed to be independent of j , i.e., we restrict our studies to the high-temperature phase and to the phase-transition point.

Using (4), the equation of motion (2) becomes linear, and its solution yields the following self-consistency equations for the steady-state structure factor $C(\mathbf{q}) = C(\mathbf{q}, t \rightarrow \infty)$:

$$C(\mathbf{q}) = \frac{q^2 + aq_{\perp}^2}{q_{\parallel}^2(r_0^{\parallel} + q^2 + S) + aq_{\perp}^2(r_0^{\perp} + q^2 + S)}, \quad (5)$$

where $a = D_{\perp}/D_{\parallel}$ and

$$S = un \int d\mathbf{q} C(\mathbf{q}). \quad (6)$$

The phase boundaries where the high-temperature phase becomes unstable are found by locating the divergences of the parallel and perpendicular susceptibilities [17] $\chi_{\parallel} \sim C(q_{\parallel} \rightarrow 0, q_{\perp} = 0)$ and $\chi_{\perp} \sim C(q_{\parallel} = 0, q_{\perp} \rightarrow 0)$. Accordingly, two types of instabilities are obtained, and one finds that two nonequilibrium critical lines meet at the equilibrium critical point $r_{0c}^{\parallel} = r_{0c}^{\perp} = r_{0c}$.

Consider first the case of $T_{\parallel} > T_{\perp}$ with T_{\perp} being decreased. Then χ_{\perp} diverges first, and the perpendicular

phase boundary is obtained. Denoting the critical values of r_0^α by r_{0c}^α , the self-consistency conditions (5) and (6) yield the equation defining the phase boundary:

$$r_{0c}^\perp = -un \int d\mathbf{q} \frac{q_\parallel^2 + aq_\perp^2}{q_\parallel^2(r_{0c}^\parallel - r_{0c}^\perp) + q^2(q_\parallel^2 + aq_\perp^2)}. \quad (7)$$

The crossover exponent is now found from the shape of the phase boundary near the equilibrium critical point where one writes

$$\varepsilon = (r_{0c}^\parallel + r_{0c}^\perp - 2r_{0c})/\sqrt{2}, \quad \Delta_\varepsilon = (r_{0c}^\parallel - r_{0c}^\perp)/\sqrt{2}, \quad (8)$$

and $\Delta_\varepsilon \sim \varepsilon^\varphi$ gives the crossover exponent in the $\varepsilon \rightarrow 0$ limit. Substituting (8) into (7) and using the known equilibrium result $r_{0c} = -un \int d\mathbf{q} q^{-2}$, we obtain

$$\Delta_\varepsilon = W_\perp \varepsilon^{2/(d-2)}, \quad \varphi = \frac{2}{d-2}, \quad (9)$$

where W_\perp is proportional to un and otherwise depends on d and a only. Since the susceptibility exponent of the equilibrium spherical model is $\gamma = 2/(d-2)$, we find $\varphi = \gamma$ in agreement with the MC results. The case of $T_\perp > T_\parallel$ with T_\parallel being decreased is treated along the same line and the equation for the parallel phase boundary again yields $\varphi = \gamma$.

As can be seen from (9), φ diverges in $d = 2$. This is a consequence of the fact that there is no phase transition in the equilibrium system in $d = 2$, and thus $r_{0c} \rightarrow -\infty$ as $d \rightarrow 2$. It does not mean, however, that the nonequilibrium transitions also disappear from the model. Indeed, Eq. (7) yields finite r_{0c}^\perp and r_{0c}^\parallel in $d = 2$. The lower critical dimension d_l^\perp where the perpendicular phase boundary disappears can be investigated by finding the dimension where r_{0c}^\perp diverges for fixed r_{0c}^\parallel (e.g., at $r_{0c}^\parallel = 0$). The divergence stems from the long-wavelength singularity of the structure factor, and it occurs only at $d_l^\perp = 1$ where the perpendicular direction disappears entirely. Similar considerations about the disappearance of the parallel phase boundary yields the lower critical dimension $d_l^\parallel = 3/2$ for the parallel phase transition.

Since there are nonequilibrium phase transitions in the ($d = 2, n = 1$) case and we have found transitions in the ($d = 2, n \rightarrow \infty$) limit as well, we arrive at a rather interesting conclusion. Namely, our results indicate the presence of nonequilibrium phase transitions in two-temperature diffusive models for $d = 2$ and arbitrary n . It is an intriguing question: What is the nature of this transition in the XY and Heisenberg models?

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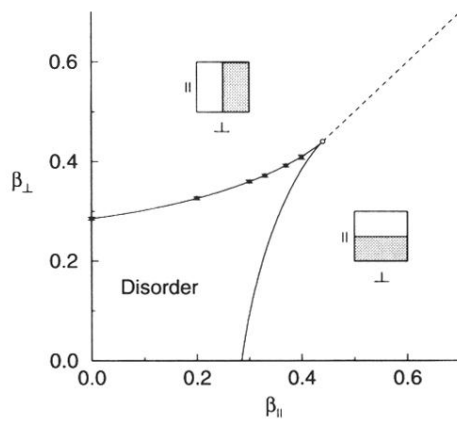


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