

Nonequilibrium Phase Diagram of Ising Model with Competing Dynamics

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We analyze the stationary nonequilibrium state of a spin system evolving under combined flips at temperature β^{-1} and exchanges at $\beta=0$. Computer simulations indicate that the phase transition changes, as the exchange rate Γ increases, from second to first order. We interpret this as a changeover from Ising behavior for small Γ to mean-field behavior for $\Gamma \rightarrow \infty$ where the magnetization is discontinuous in the "continuum limit."

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Consider an Ising spin system (equivalently a lattice gas) on a simple cubic lattice in d dimensions with configurations $\sigma = \{\sigma(x); x \in Z^d, \sigma(x) = \pm 1\}$. The system evolves by a combination of spin flips (Glauber)¹ and nearest-neighbor exchanges (Kawasaki).² The two processes occur independently in continuous time.

For a given σ , let $c(x; \sigma)$ be the Glauber flip rate at site x and $E(x, y; \sigma)$ the Kawasaki exchange rate for a pair of neighboring sites x and y . Choosing a suitable time unit, we let $E(x, y; \sigma) = \Gamma$ be independent of σ and make $c(x; \sigma)$ satisfy detailed balance,

$$c(x; \sigma)/c(x; \sigma^x) = \exp\{-\beta[U(\sigma^x) - U(\sigma)]\}. \quad (1)$$

Here σ^x represents the configuration obtained from σ by flipping the spin at site x and $U(\sigma)$ is an energy function which we take to be of nearest-neighbor type,

$$U(\sigma) = -J \sum_{\langle x, y \rangle} \sigma(x)\sigma(y). \quad (2)$$

A way of describing the dynamics is to say that the exchanges occur as if the system was in contact with a heat bath at infinite temperature, $\beta=0$, and the spin flips as if the bath temperature was β^{-1} .

Our interest here is in the nature of the stationary states, $\mu_{st}(\sigma)$, for some familiar rates $c(x; \sigma)$, i.e., the phase diagram of this nonequilibrium system as the parameters β and Γ are varied. This problem has also been studied by Dickman³ using a Bethe-type approximation. His results are in qualitative agreement with our findings (see below).

There are several remarks to be made: (i) For $\Gamma \equiv 0$ the stationary states do not depend on the details of c , as long as (1) holds. They are equilibrium states for $U(\sigma)$ whose nature is well known. In particular there is, for $d \geq 2$, a second-order phase transition at a critical $\beta = \beta_c$ such that there is a unique state for $\beta \leq \beta_c$ and spontaneous magnetization for $\beta > \beta_c$. (ii) For $c(x; \sigma) = 0$ the stationary states are of Bernoulli type, i.e., there is no

correlation between sites. There are an infinite number of such states, one for each magnetization $m \equiv \langle \sigma(x) \rangle$. This is a result of the fact that the magnetization is conserved by the exchanges. (iii) For the interesting case where Γ , c , and β are all positive, the stationary state, which will now depend on details of $c(x; \sigma)$, is not (as far as we know) an equilibrium state for any reasonable potential and its properties are not known. In particular, we do not even know if the stationary state is unique or not, i.e., if there is a phase transition (in the infinite-volume limit) in *any dimension, including $d=1$* .

Models of combined Glauber and Kawasaki dynamics have been investigated previously in the limit $\Gamma \rightarrow \infty$.⁴⁻⁶ More precisely, on rescaling of time by Γ and space by $\sqrt{\Gamma}$ it was shown in Ref. 5 that, in the limit $\Gamma \rightarrow \infty$, the macroscopic magnetization $m(\mathbf{r}, t)$ satisfies a diffusion-reaction equation of the form

$$\partial m(\mathbf{r}, t) / \partial t = \frac{1}{2} \nabla^2 m(\mathbf{r}, t) + F(m(\mathbf{r}, t)), \quad (3)$$

where $F(m)$ is a polynomial in m ,

$$F(m) = -2 \langle \sigma(x) c(x; \sigma) \rangle_m, \quad (4)$$

the average being taken in a Bernoulli state with uniform magnetization m . The basic idea of the proof in Refs. 4-6 is that, as $\Gamma \rightarrow \infty$, the fast exchanges bring the system to "local equilibrium" with magnetization $m(\mathbf{r}, t)$ at "infinite temperature," the temperature of the Kawasaki dynamics, where there are no correlations. The time evolution of the local magnetization is then governed by the macroscopic diffusion-reaction equation with coefficients evaluated in the local equilibrium ensemble.

We shall now present the form of $F(m)$ for several different $c(x; \sigma)$ and the corresponding time-independent spatially homogeneous solutions of (3), i.e., values of m for which $F(m) = 0$. This is relevant for understanding the nature of the phase diagram in the β, Γ plane which is our main concern here.

Case 1: The rates originally introduced by Glauber,¹

$$c(x;\sigma) = \frac{1}{2} \sum_{s=\pm 1} \prod_{i=1}^d \{1 + \frac{1}{2} s \gamma [\sigma(x+e_i) + \sigma(x-e_i)]\} [1 - s\sigma(x)], \quad (5)$$

where $\gamma = \tanh 2\beta J$. This yields

$$F_1(m) = -4[(1-m\gamma)^d(1+m) - (1+m\gamma)^d(1-m)] = mf_1(m^2), \quad f_1(\lambda) = -8[a_0 + a_1\lambda + \dots + a_k\lambda^k], \quad (6)$$

with $a_0 = 2(1-d\gamma)$, $a_1 = d(d-1)\gamma^2[1 - \frac{1}{3}(d-2)\gamma]$, and $2k = d$ for d even and $d-1$ for d odd.

Case 2: The familiar Metropolis rates⁷

$$c(x;\sigma) = \min\{1, \exp[-\beta\Delta U]\}. \quad (7)$$

The corresponding $F_2(m)$ can again be written as $mf_2(m^2)$ with f now a polynomial of order d . In particular for $d=1$ and 2 the Metropolis rates give

$$f_2(\lambda) = \frac{1}{2} [(3\bar{\gamma}-1) + (\bar{\gamma}-1)\lambda], \quad d=1, \quad (8)$$

$$f_2(\lambda) = \text{const}[(5\bar{\gamma}^2 + 12\bar{\gamma} - 1) + 2(\bar{\gamma}-1)(5\bar{\gamma}+1)\lambda + (\bar{\gamma}-1)(\bar{\gamma}-3)\lambda^2], \quad d=2, \quad (9)$$

where $\bar{\gamma} = \exp[-4\beta J]$.

Case 3: The form of $c(x;\sigma)$ used in Refs. 4-6 for studying a one-dimensional example,

$$c(x;\sigma) = 1 - \gamma\sigma(x)[\sigma(x-1) + \sigma(x+1)] + \gamma^2\sigma(x-1)\sigma(x+1). \quad (10)$$

This gives

$$F(m) = 2m[(1-2\gamma) + \gamma^2m^2], \quad d=1, \quad (11)$$

with $\gamma = \tanh\beta J$.

The time-independent uniform magnetization solutions of (3) correspond to real roots of the polynomial $F(m)$ with $m^2 \leq 1$. It can be checked that for the models considered here, where $F(m) = mf(m^2)$, there is only one such root, $m=0$, for small positive βJ . Other roots, corresponding to $f(m^2)=0$, with $m^2 \leq 1$, $m = \pm m^*$, will appear when β is larger than some $\bar{\beta}$ (with $J=1$). The solution of (3), $m(\mathbf{r},t)=0$, is stable for $\beta < \bar{\beta}$, and unstable for $\beta > \bar{\beta} \geq \bar{\beta}$ where the symmetry-breaking solutions $m(\mathbf{r},t) = \pm m^*$ are stable.⁴⁻⁶

The nature of the change at $\beta = \bar{\beta}$ will depend on how the admissible root of the polynomial $f(\lambda)$ appears at $\beta = \bar{\beta}$, i.e., on whether $\lambda(\bar{\beta})$ is equal to or greater than zero. In the case $\lambda(\bar{\beta})=0$, $\bar{\beta} = \bar{\beta}$, the "transition" is second order with $m^*(\beta) = (\beta - \bar{\beta})^{1/2}$ for $\beta \approx \bar{\beta}$ while in the other case there is a first-order transition with a jump in the spontaneous magnetization equal to $\sqrt{\lambda(\bar{\beta})}$. In terms of the mean-field-type free-energy function, which serves as the potential for the reaction term in (3),

$$\Psi(m^2) = - \int_0^{m^2} F(z) dz,$$

both types of behavior are well known: The first case is standard; in the second case, which occurs for four-body interactions, $\Psi(\lambda)$ develops a new local minimum at $\lambda(\bar{\beta})$ which becomes a global minimum at $\beta = \bar{\beta} > \bar{\beta}$ located at $\lambda(\bar{\beta})$. At a still larger β , the minimum at $\lambda=0$ may become unstable (other behavior is also possible).

For case 1, Eq. (6), $\bar{\beta} = \bar{\beta}$, $\lambda(\bar{\beta})=0$; $\bar{\beta}$ corresponds to the value of β for which $a_0=0$,

$$\bar{\gamma} = \tanh 2\bar{\beta}J = d^{-1}. \quad (12)$$

For Metropolis rates in $d=2$, Eq. (8), $\bar{\beta} \cong 0.515 \cong 1.17\beta_c$, and $\bar{\beta} \cong 0.474 \cong 1.08\beta_c$; β_c is the Onsager value of the critical β at $\Gamma=0$. The jump in the spontaneous magnetization at $\bar{\beta}$ is equal to 0.925.

In $d=1$, rates 1 and 2 give $\bar{\beta} = \infty$ while rate 3 gives $\tanh\bar{\beta} = \frac{1}{2}$ with $m^*(\bar{\beta})=0$. It is also easy to construct dynamics, e.g., Metropolis with next-nearest-neighbor interactions, which give $\bar{\beta} < \infty$, $m^*(\bar{\beta}) > 0$ in $d=1$. This shows the importance of the choice of $c(x;\sigma)$, at least in the $\Gamma \rightarrow \infty$ continuum limit.

The behavior for $\Gamma < \infty$ cannot be deduced from the above considerations. We expect that in all cases the one-dimensional system will not have a phase transition for $0 < \beta, \Gamma < \infty$. In more dimensions, however, where there is a transition even for $\Gamma=0$, we expect that

$$\bar{\beta} = \lim_{\Gamma \rightarrow \infty} \beta_0(\Gamma)$$

where $\beta_0(\Gamma)$ is the transition point at fixed Γ .

We have investigated salient features of the stationary state in $d=1$ and 2 at different values of β and Γ via computer simulations: A site x is chosen at random from a given (finite) lattice; then with probability p , $0 \leq p \leq 1$, the spin at x is exchanged with one of its $2d$ neighbors (picked at random) and with probability $(1-p)\min[1, \exp(-\beta\Delta U)]$ is flipped. Periodic boundary conditions are used. Our procedure corresponds, after normalization of time units (which are irrelevant for the stationary state), to case 2 with $\Gamma = p/d(1-p)$.

In $d=1$ we used chains of size 2500 and considered both nearest- and next-nearest-neighbor interactions

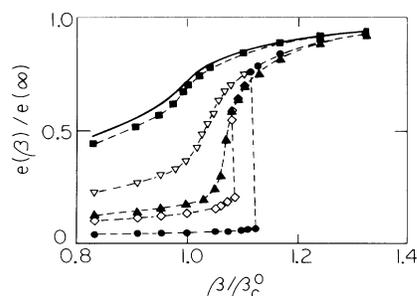


FIG. 1. The system energy, as a function of β (in units of the Onsager critical value $\beta_c^0 = 0.440J^{-1}$), for a two-dimensional system with ferromagnet Metropolis rates with different values of p . The solid line represents $p=0$, i.e., equilibrium for the infinite system. The symbols are for $p=0.10$ (squares), 0.60 (inverted triangles), 0.80 (triangles), 0.85 (lozenges), and 0.95 (circles); the dashed lines are guides to the eye.

—the latter (but not the former) giving a transition in the continuum $\Gamma \rightarrow \infty$ limit. As expected, the simulations carried out for $p \leq 0.96$ ($\Gamma=26$) gave no transition.

In $d=2$ we considered only nearest-neighbor interactions and carried out simulations on squares of different sizes, $N \leq 10^4$ sites. Figures 1 and 2 give the behavior of the energy (nearest-neighbor correlation) and of the magnetization as a function of β for several values of p . These figures show how increasing p from 0 (which corresponds to the familiar equilibrium state of the Ising model) modifies the transition; while $\beta_0(p)$ increases with p , the qualitative behavior remains the same as for the Onsager solution up to $p \approx 0.80$ or $\Gamma \approx 2$. In particular, the phase transition apparently remains second order for all $p < 0.80$, and the data near β_0 are “consistent” with the corresponding critical exponents being 0.125 and 1.75, independent of p . This is in agreement with renormalization-group calculations⁸ and is also consistent with our data for the “specific heat” C and “magnetic susceptibility” χ computed by measuring fluctuations. (The relation of these fluctuations to derivatives of the energy and magnetization is unknown for the non-equilibrium states considered here.)

The situation for $p > 0.85$ is qualitatively very different. We now observe the appearance of some well-defined metastable states during the system evolution and Figs. 1 and 2 suggest discontinuities at the transition temperature $\beta_0(p)$ —both facts indicating that the phase transition is first order for $p > 0.85$. This is also confirmed by the fluctuation data: The symmetry around β_0 which characterizes C for $p=0$ (and for $p < 0.80$ as well) is now absent, χ becomes even more asymmetric than before, and both $C(\beta)$ and $\chi(\beta)$ suggest a finite jump in the nearest-neighbor correlation and the magnetization at $\beta_0(p)$.

Figure 3 shows the phase diagram with a (nonequilibrium) tricritical point, whose location we estimate at

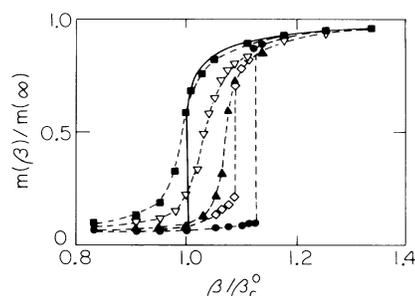


FIG. 2. The system magnetization as a function of β . Same system and symbols as in Fig. 1.

$p_t \approx 0.83$, corresponding to the changeover from second to first order. As $p \rightarrow p_t$, it becomes more difficult to estimate the values of the critical exponents.

Our machine computations may be compared with the Bethe-type approximations of Dickman³ for the same model. The results for the phase diagram agree qualitatively; $p_t \approx 0.72$ in Dickman’s approximation and the exponents are always mean field. In the limit $p \rightarrow 1$ Dickman’s approximation gives the correct result.

For a comparison between our machine computations and the continuum limit, we note that $\beta_0(p) \approx 0.47, 0.48$, and 0.49, respectively, for $p=0.80, 0.85$, and 0.95, while $\bar{\beta}$ computed following Eq. (12) is 0.515. This suggests that in fact

$$\lim_{\Gamma \rightarrow \infty} \beta_0(\Gamma) = \bar{\beta}.$$

Finally, we note that recent computations on a two-dimensional system using the flip rates given in (5) showed no changeover to a first-order transition lending support to our analysis.

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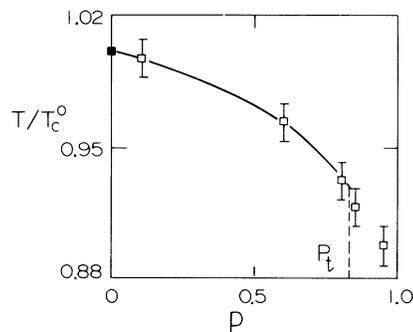


FIG. 3. The transition temperature $\beta_0(p)$ for the same system. The solid line represents a line of critical points for $p < p_t \approx 0.83$; the dotted line for $p > p_t$ corresponds to first-order phase transitions, $\beta_0(p_t) \approx 0.47J^{-1}$.

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