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Finite-size calculations for the kinetic Ising model

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Using a Hamiltonian formulation of the master equation, we carry out finite-size calculations for the dynamical critical exponent z of the kinetic Ising model in one and two dimensions. In one dimension, different appropriately normalized transition probabilities give different values for z; this result is based on both exact and finite-size calculations. We show that this "nonuniversal" behavior is due to the fact that the critical temperature for the one-dimensional Ising model is zero. In two dimensions we combine our finite-size calculations with finite-size scaling theory to calculate z. Even in this case we find that z depends on the form of the transition probability—a result that contradicts the universality hypothesis for dynamical critical behavior. We discuss the possible reasons for this contradiction.

In this paper we study the critical dynamics of the d-dimensional ($d=1,2$) Ising model (IM) (a chain or a square lattice with periodic boundary conditions). This problem has been studied by many authors. Here we wish to show the following: (1) For $d=1$, universality does not hold in the usual sense,[1,2] because of certain pathological behavior associated with the zero critical temperature of the IM (we shall make this precise later); and (2) for $d=2$, finite-size Hamiltonian methods, which have given excellent results for static critical exponents,[3,4] do not lead to conclusive results for dynamical critical exponents.

The Hamiltonian for the IM is

$$\frac{-\mathcal{H}}{T}=K\sum_{\langle ij\rangle}\sigma_i\sigma_j,\ \sigma_i=\pm 1 \quad , \tag{1}$$

where K is the exchange coupling (divided by the temperature, T) between spins, σ_i, on nearest-neighbor lattice sites $\langle ij\rangle$. We take the Boltzmann constant to be one. The dynamics of the IM is described by the master equation,[5,6]

$$\frac{\partial P}{\partial t}(\sigma_1,\ldots,\sigma_N;t)=-\sum_i(1-f_i)w_i(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_N)P(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_N;t) \quad , \tag{2}$$

where $P(\sigma_1,\ldots,\sigma_N;t)$ is the probability that the system has the spin configuration $(\sigma_1,\ldots,\sigma_N)$ at time t, and $w_i(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_N)$ is the transition probability per unit time for the spin flip $\sigma_i\rightarrow-\sigma_i$; f_i is an operator defined by $f_i g(\sigma_i)=g(-\sigma_i)$ for an arbitrary function, g, of σ_i. We only consider w_i's that do not conserve the magnetization or any other thermodynamic quantity, and depend only on σ_i and its nearest neighbors. The w_i's must satisfy the condition of detailed balance, but this does not specify their form completely.[5,6]

At the critical temperature, T_c, of the IM, the longest relaxation time, τ, diverges. According to the dynamical scaling hypothesis,[2,7] $\tau\sim\xi^z$ as $T\rightarrow T_c$; z is the dynamical critical exponent, and ξ is the correlation length for the IM. For $d=1$, $\xi\sim e^{2K}$ as $T\rightarrow T_c=0$;[8] for $d>1$, $\xi\sim|T-T_c|^{-\nu}$ as $T\rightarrow T_c$,[8] where ν is the usual static critical exponent. According to the dynamical universality hypothesis, as long as there are no special conserved quantities, z should not depend on the form of the w_i's.

For $d=1$, the most general form of w_i which satisfies the condition of detailed balance, and depends only on σ_i and its nearest neighbors may be written as

$$w_i=\frac{\eta}{2}\left[1-\frac{\gamma}{2}\sigma_i(\sigma_{i+l}+\sigma_{i-l})\right](1+\delta\sigma_{i+1}\sigma_{i-l}) \quad , \tag{3}$$

where $\gamma=\tanh(2\,K)$. η and δ are, for the time being, unspecified functions of γ. From (2) it follows that η sets the time scale.

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For the w_i's given by (3), z has been calculated exactly in the following cases: (1) $\eta=1, \delta=0 (z=2)$; (Glauber; Ref. 5); (2) $\eta=1, \delta=\gamma/(2-\gamma); (z=4)$ (Ref. 9); (3) $\eta=e^{2K}\cosh(2K)+1, \delta=\gamma/(2-\gamma)$; $(z=2)$ (Ref. 10). The third choice of η leads to a singular time scale as $T\to 0$. In cases (1) and (2), however, the time scale remains finite for all T. It is easy to see that the difference between cases (2) and (3) stems from the singular behavior of η [for case (3)] at $T=0$. This difference can be eliminated trivially by normalizing η (i.e., w_i) so that as $T\to 0$, $\eta\to$ const. When we normalize η, we get $z=4$ even for case (3). We see, then, that it is possible to obtain at least two different values of z, namely, 2 and 4, analytically. In what follows we use η's that are appropriately normalized (in the above sense). We show that it is possible to get any value of $z(\geq 2)$ for $d=1$. This result is based on numerical calculations which we now describe.

The master equation (1) can be cast into a Hamiltonian form.[11] The gap (the difference between the two lowest eigenvalues), G, of the resulting Hamiltonian, H, is proportional to $(1/\tau)$, which implies that $G\sim\xi^{-z}\to 0$ as $T\to T_c$. The condition of detailed balance implies that the lowest eigenvalue of H is zero for all T.[10]

We calculate G for IM's of finite sizes—chains of N spins for $d=1$ and $N\times N$ squares for $d=2$. Since N is finite, H is a finite dimensional matrix ($2^N\times 2^N$ for $d=1$). We find its low-lying eigenvalues, and hence G, by using the Lanczos method.[3]

For a finite system there is no phase transition and ξ remains finite at all temperatures. This implies that G_N, the gap for a system of linear size N, does not vanish at any temperature. Both z and ν can be determined, however, by using finite-size scaling.[3,12,13] We use this tactic for $d=2$.

It turns out that we cannot use finite-size scaling for $d=1$ because $G_N=0$ at $T=0$ for all values of N. This can be shown analytically for the Galuber[5] and the "exponential"[14] form of w_i. For other forms of w_i we find $G_N\to 0$ (to machine accuracy) as $T\to 0$. In particular, $G_N\sim(e^{2K})^{-z_N}\to 0$ as $T\to 0$ with z_N *independent* of N.

Our results for $d=1$, based on calculations for $N=7$, are summarized in Table I. Our transition probabilities are appropriately normalized (in the sense discussed above) and therefore the value of η

TABLE I. The dynamical critical exponent, z, for various transition probabilities, w_i, for the $d=1$ kinetic Ising model. We do not display the complete form of w_i but only the $T\to 0$ form of $(1-\delta)$ [see Eq. (3)].

Transition probability: $(1-\delta)$ for $T\to 0$	z
1 [Glauber (Ref. 5)]	2
$\frac{6}{5}$	2
$4e^{-2K}$ [Exponential (Ref. 14)]	3
$6e^{-2K}$	3
$4(e^{-2K})^2=4e^{-4K}$	4
$8(e^{-2K})^{2.5}=8e^{-5K}$	4.5
$4(e^{-2K})^3=4e^{-6K}$	5

TABLE II. The critical coupling, K_c^f, determined from our finite-size calculations, the static exponent, ν, and the dynamical critical exponents z and Δ for different transition probabilities for the $d=2$ kinetic Ising model. For comparison, the exact values of K_c and ν are 0.441 and 1, respectively (Ref. 8). The currently accepted value for z is 2.13 ± 0.1 (Refs. 16–18). $\sigma_{i,j}$ denotes a spin on the lattice site i,j.

Transition probability	K_c^f	ν	z	Δ
$w_{ij}=\dfrac{\exp[-K\sigma_{i,j}(\sigma_{i+1,j}+\sigma_{i-1,j}+\sigma_{i,j+1}+\sigma_{i,j-1})]}{\cosh K(\sigma_{i+1,j}+\sigma_{i-1,j}+\sigma_{i,j+1}+\sigma_{i,j-1})}$ [$d=2$ Glauber (Ref. 18)]	0.43	0.95	2.09	1.99
$w_{ij}=\dfrac{\exp[-K\sigma_{i,j}(\sigma_{i+1,j}+\sigma_{i-1,j}+\sigma_{i,j+1}+\sigma_{i,j-1})]}{\cosh K(\sigma_{i+1,j}+\sigma_{i-1,j})\cosh K(\sigma_{i,j+1}+\sigma_{i,j-1})}$ (Ref. 19)	0.41	1.1	1.63	1.79
$w_{ij}=\exp[-K\sigma_{i,j}(\sigma_{i+1,j}+\sigma_{i-1,j}+\sigma i,j+1+\sigma_{i,j-1})]$ [$d=2$, exponential (Ref. 14)]	0.48	0.65	3.17	2.16

(which does not affect the value of z) is not given in Table I. The first column of Table I gives the value of $(1-\delta)$ as $T \rightarrow 0$ and the second column gives the calculated value of z. The factor $(1-\delta)$ appears in w_i for $\sigma_{i-1} = -\sigma_{i+1}$ [see Eq. (3)]. This means that any state made up of clusters of two or more parallel spins relaxes infinitely slowly at $T=0$. If $(1-\delta) \neq 0$ at $T=0$ (e.g., Glauber's case) only the ferromagnetic ground state gets frozen. Comparing the two columns we see that the value of $(1-\delta)$ as $T \rightarrow 0$ is related to z. If δ is chosen such that $(1-\delta) \sim (e^{-2K})^p \sim \xi^{-p}$ as $T \rightarrow 0$ (note that $\xi \sim e^{2K}$ holds only for $d=1$ as $T \rightarrow 0$, the critical temperature for $d=1$), then our results indicate that $z = 2+p$, where p is real and positive.[15] It is clear that this nonuniversality is a consequence of the pathology of the $d=1$ IM, namely that $T_c = 0$. We do not expect nonuniversal z's for $d > 1$ where $T_c > 0$.

Our results, based on calculations performed on lattices of sizes 2×2, 3×3, and 4×4, are summarized in Table II; in the first column we give the transition probability, in the second column we give the calculated value of the critical coupling, K_c^f, and in the third and fourth columns we give the values of ν and z, respectively, which we obtained by using finite-size scaling. In the fifth column we give the value of $\Delta = \nu z$. The results for the Glauber transition probability are in excellent agreement with the currently accepted value of z[16–18] and the exact result, $\nu = 1$.[8] For the Glauber transition probability, Yalabik and Gunton[19] have obtained similar results from finite-size calculations for $d=2$. Our results for the second transition probability[20] are not very good. For the exponential transition probability[14] the results are quite bad. Recently, Nightingale and Blöte have reported preliminary results for z (1.92 to 1.99) using finite-size calculations and yet another transition probability.[21] It is interesting to note, that $\Delta = 2.0 \pm 0.2$ for all three transition probabilities, which is the result obtained by most other methods.[6] On the basis of universality we expect both Δ and z to be the same for all the three cases studied. We do fairly well in this regard for Δ, but not for z. As we do not expect nonuniversal z's for $d > 1$, we are forced to conclude that finite-size scaling sets in at different linear sizes for different transition probabilities. Any good results that might be obtained from finite-size calculations on lattices of small sizes (such as our results for the Glauber transition probability, or the results obtained in Ref. 21) are, therefore, quite fortuitous.

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[15] After this work had been completed we learned about a recently published paper by Haake and Thol (Ref. 22) who constructed analytically upper and lower bounds for z. Our result $z = 2+p$ suggests that the upper bound found by these authors is actually an exact result for z for any positive value of p.

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