Critical relaxation in two-dimensional random-bond Potts models

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We present an extensive Monte Carlo study of the critical relaxation for the two-dimensional square lattice random-bond Potts model using Swendsen-Wang cluster flipping. The integrated autocorrelation time τ is calculated and the dynamic exponent z is estimated by analyzing the size dependence of τ. We find that $z \approx 0$ in agreement with estimates for the two-dimensional Ising model. We also present a study of the size dependence of the dynamic behavior of the pure eight-state Potts model which undergoes a first-order transition. The scaling is describable by the product of an exponential times a power law, a behavior which is quite different from that found in the random-bond case. [S1063-651X(96)05611-5]

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I. INTRODUCTION

Extensive research carried out over the last few decades has led to a quite good understanding of static behavior near the phase transition for many spin models. In two dimensions ferromagnetic q-state Potts models are known to exhibit first-order phase transitions if the number of states $q>4$. Recent work has shown, however, that if there are randomly distributed ferromagnetic bonds of two different strengths, the transition becomes second order [1–4] and the static behavior (at least for $q=8$) has exponents which are indistinguishable from those of the Ising model [3,4]. Time dependent properties of spin models in the vicinity of their transition points are generally less well known than their static counterparts, although substantial progress has been made in recent years. Nonetheless, there is no information available about any changes which might occur in the ''critical relaxation'' of q-state Potts models when random bonds are added, although the changes in the static behavior suggest that significant modification might occur in the time dependent properties as well.

For systems exhibiting second-order transitions, critical slowing down is described in terms of a dynamic critical exponent z, which describes the divergence of the characteristic relaxation time τ as the critical point T_c is approached,

$$\tau \propto t^{z\nu}, \tag{1}$$

where $t=|1-T/T_c|$. For local spin-flip dynamics with no conservation laws, $z \approx 2$ [5–9] for many spin systems. Thus single-spin-flip Monte Carlo investigations of phase transitions have been hampered by critical slowing down [10]. Recently developed cluster updating algorithms [11–13] can dramatically reduce critical slowing down and therefore are more efficient in studying phase transitions for many spin systems. For this reason we used a modified cluster-flipping algorithm in our previous study of static behavior in the random-bond Potts model. Theoretical predictions for the cluster dynamics critical exponent are sparse, although a rigorous bound on z for the Swendsen-Wang algorithm [11] for Potts models has been derived [14]. For the two-dimensional Ising model, simulations indicate that z is quite small: initial results suggested $z \approx \frac{1}{3}$ [11,15], further work [12] gave $z=\frac{1}{4}$, and it was later shown that the data were consistent with a logarithmic divergence, suggesting that $z \approx 0$ [13,16,17]. Quite limited numerical results with cluster dynamics have been published for the Potts model [17–19]. For first-order transitions the tunneling time between coexisting states also increases as the transition is approached, thus leading to long relaxation times. Unfortunately, the dynamic behavior for the pure eight-state Potts model as it undergoes a first-order phase transition is not exactly known. A pure exponential slowing down for a first-order phase transition was first suggested [20]; however, the product of an exponential times a power law was later found [18] for the $q=10$ Potts model.

The purpose of this study is to numerically determine, using the Swendsen-Wang algorithm, the dynamic behavior at the transition point for the two-dimensional (2D) random-bond Potts model as well as for the pure 2D Potts model so that the effects of bond randomness on the dynamic behavior can be determined by comparing the correlation times for both models. A comparison between the data for the random-bond Potts model and the 2D Ising model will also be made to determine if the dynamic and static universality classes agree. In the following sections, we first provide some theoretical background related to the dynamics of the Monte Carlo methods, followed by a brief description of the data analysis techniques. In Sec. IV we then present and discuss the simulation details and results. A summary of this study is given in the last section.

II. BACKGROUND

The ''dynamics'' of stochastic models [21] can be studied by determining the normalized autocorrelation function $\varphi_A(t)$ [22],

$$\varphi_A(t)=\frac{\langle A(0)A(t)\rangle-\langle A\rangle^2}{\langle A^2\rangle-\langle A\rangle^2}, \tag{2}$$

where the average is over Monte Carlo steps and the time t is measured in units of one sweep through the entire lattice for the cluster algorithm. $A(t)$ is some observable, usually chosen to be energy or magnetization. The time dependence of $\varphi_A(t)$ can be expressed [23], in general, as

$$\varphi_A(t)=\sum_i a_i e^{-t/\tau_i}. \tag{3}$$

It is believed that there is only one relevant time scale in critical dynamics just as there is only one length scale, the correlation length, in the statics. Therefore the long time behavior of any correlation function will be determined by the largest $\tau=\max[\tau_i]$. This defines the exponential autocorrelation time $\tau_{\rm exp}=\tau$. Another characteristic time, the integrated autocorrelation time $\tau_{\rm int}$, is defined as

$$\tau_{\rm int}=\sum_1^\infty \varphi(t). \tag{4}$$

If $\varphi(t)$ decays approximately as a pure exponential, then $\tau_{\rm exp}\approx\tau_{\rm inf}$; but in general $\tau_{\rm exp}$ may be much larger than $\tau_{\rm int}$. Note that $\tau_{\rm int}$ determines the statistical errors in Monte Carlo measurements of $\langle A\rangle$ once equilibrium has been attained. The total run length has to be much larger than $\tau_{\rm int}$ in order to produce reliable information about thermodynamic properties.

The autocorrelation time for an infinite d-dimensional system undergoing a second-order phase transition is expected to diverge as

$$\tau\sim\xi^z, \tag{5}$$

whereas for a finite system at the infinite volume transition point, dynamic finite-size scaling [24] predicts

$$\tau\propto L^z, \tag{6}$$

where the dynamic critical exponent z is ~ 2 for local algorithms without conservation laws. For a finite system undergoing a first-order phase transition it was suggested that the autocorrelation time grows as [18]

$$\tau\propto L^a e^{bL}. \tag{7}$$

We have performed Monte Carlo simulations for the $q=8$ random-bond Potts model on a two-dimensional square lattice with periodic boundary conditions

$$\mathcal{H}=-\sum K_{ij}\sigma_i\sigma_j, \tag{8}$$

where the ratio between the two bond strengths was $r=K_1/K_2=10$.

The simulations were carried out using the Swendsen-Wang algorithm on a cluster of IBM RS/6000 workstations. Data were obtained at the infinite-lattice transition coupling [25] ($K_1^C=0.312\,655\,667\ldots$) for lattices with linear size $L=16$–84. In each simulation, the initial 5×10^3 steps were discarded for equilibration. At each time step, i.e., a sweep for entire lattice, the energy E and the number of the sites in the maximum occupied state M are accumulated. The autocorrelation times, $\varphi_E(t)$ and $\varphi_M(t)$, were computed over samples of at least 10^6 Monte Carlo sweeps per lattice size. The configurational averages were performed for the autocorrelation times, such that

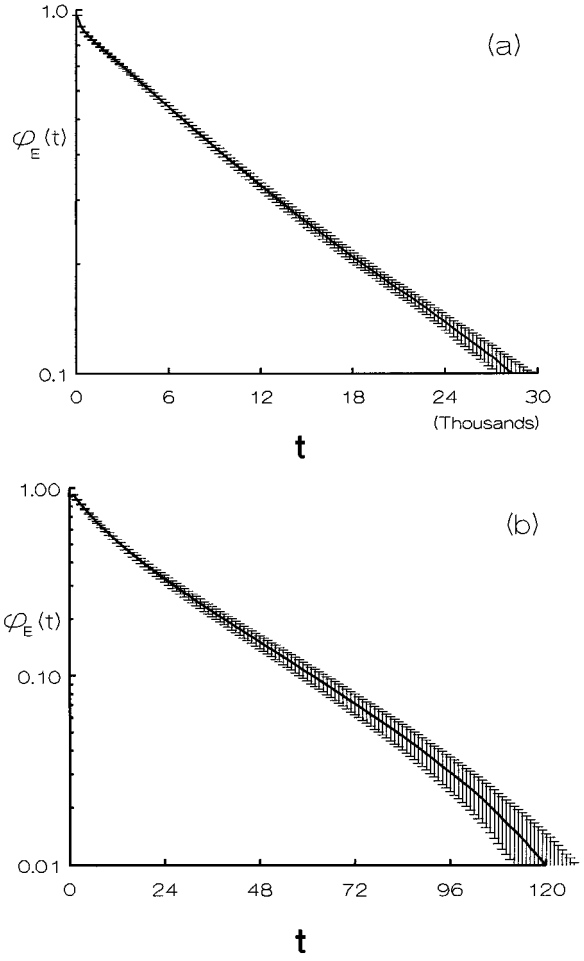

FIG. 1. Plots of typical time dependence of the autocorrelation functions. (a) $L=64$, random-bond Potts model, averaging over 30 bond configurations; (b) $L=64$ pure Potts model, averaging over five configurations. Time is measured in Monte Carlo steps per site.

$$\tau_L=\frac{1}{N}\sum_i^N \tau_i, \tag{9}$$

where N is the total number of bond configurations simulated for the size L. For each size, there were at least 30 bond distributions simulated and used in the configurational average over randomness to ensure that the bulk properties were correctly determined.

We have also carried out Swendsen-Wang simulations for the pure eight-state Potts model on an $L\times L$ square lattice with periodic boundary conditions for $12\leqslant L\leqslant 64$. Because we found much longer relaxation times than for the random-bond system, for these runs the first 10^5 steps in each simulation were discarded. For each size, we performed five independent simulations; each of them has a run length greater than 3×10^7 steps. The autocorrelation times, $\varphi_E(t)$ and $\varphi_M(t)$, were measured at the infinite-lattice critical point [25] [$K_C=\ln(1+\sqrt{q})=1.342\,454\ldots$].

Figure 1 is a log-log plot showing the general features of $\varphi_A(t)$. A smooth, linear regime extends from $t=t'$ to some $t=t_{\rm max}$, beyond which the data begin oscillating or varying abruptly, and meaningful information is difficult to extract from them. For the pure model, $\varphi(t)$ varies slightly for dif-

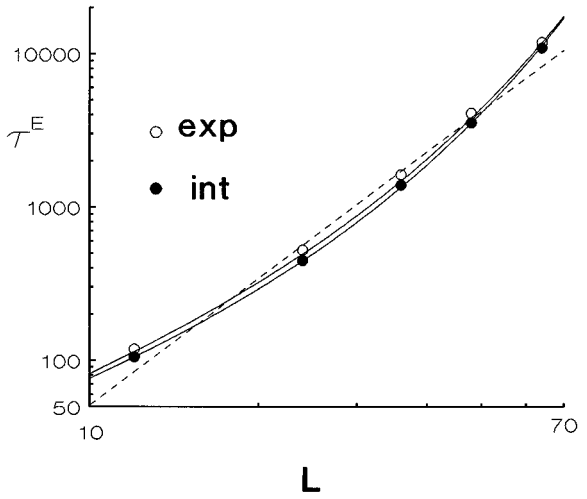

FIG. 2. Log-log plot of the energy autocorrelation time (measured in Monte Carlo steps per site) for the pure Potts model. Errors in the individual points are smaller than the symbol size. The solid curves are fits to Eq. (7) and the dashed line is a linear fit.

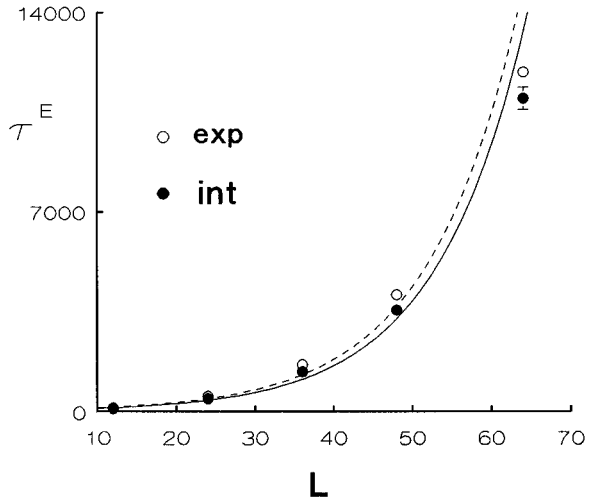

FIG. 3. The energy autocorrelation time (measured in Monte Carlo steps per site) for the pure Potts model fitted by a pure exponential.

ferent initial configurations with the same L and $t' \ll t_{\max}$, thus most $\varphi(t)$ can be well fitted by a single exponential term ($a_1 e^{-t/\tau_1}$); some $\varphi(t)$ can be fitted by two exponential terms ($a_1 e^{-t/\tau_1}$ and $a_2 e^{-t/\tau_2}$ with τ_1 being ten to 20 times as large as τ_2, and $a_2/a_1 < 0.05$). For the random-bond model, $\varphi(t)$ has larger fluctuations for different bond configurations. We fitted $\varphi(t)$ with two exponential terms, with the result that $\tau_1 > 4\tau_2$ and $a_2/a_1 < 0.1$. For $t \to \infty$, τ_1 governs the behavior of $\varphi(t)$, τ_1 is thus used as $\tau_{\exp}$ in later calculations for both pure and random systems.

The data for the integrated autocorrelation time were obtained by applying Eq. (4) in its original form and using the truncation approximation [16].

$$\tau_{\text{int}} = \sum_{t=1}^{t=t_{\max}-1} \varphi(t) + R(t_{\max}), \tag{10}$$

with

$$R(t_{\max}) = \varphi(t_{\max}) \frac{1}{1-k(t_{\max})}, \tag{11}$$

$$k(t_{\max}) = e^{-1/\tau_{\exp}}. \tag{12}$$

We used $\tau_{\exp}$ instead of $\varphi(t_{\max})/\varphi(t_{\max}-1)$ in calculating $k(t_{\max})$ to reduce the error due to fluctuations in the data.

III. RESULTS AND DISCUSSION

The results for the size dependence of the energy correlation times for the pure Potts model are shown in Fig. 2. The curvature of the best fit (compared with the linear fit shown by the dashed line) to the data on the log-log scale suggests that a simple power law does not provide a correct description of the size dependence of the relaxation of this system. The correlation time is compatible with the modified exponential (solid lines) of Eq. (7) with $a = 1.20$ and $b = 0.05$. A simple exponential fit of the L dependence of the correlation time is shown in Fig. 3; the substantial deviations of the data from the fitted curve for large sizes indicate that a pure exponential function is not suitable for describing the dynamics of this system either.

A theoretical computation along the lines of Ref. [20] suggests that b is twice the interface tension σ between the coexisting phases. For the $q = 10$ Potts model estimates are [18] $a \sim 1.5$ and $b \sim 0.09$ for Swendsen-Wang (SW) dynamics, and $a \sim 2.1$, $b \sim 0.09$ for the Metropolis method. The values of b agree with 2σ: for $q = 8$, 2σ is ~ 0.045 [26] and ~ 0.1 for $q = 10$ [26–28]. Therefore the size dependence of the autocorrelation time for the system undergoing a first-order transition might be written as

$$\tau \propto c L^a e^{2\sigma L^{d-1}}, \tag{13}$$

where d is the dimension of the lattice. The quantity $2\sigma L^{d-1}$ is just the free-energy barrier [29] between the maximum and minimum of the probability distribution of the energy. When the free-energy barrier is zero for all L, indicating a second-order phase transition, Eq. (13) reverts to a power-law function. The dynamic critical exponent z for local dynamics was estimated to be ≈ 2.17 for $q = 2,3,4$ Potts models [6]. A comparison of these results to a for $q = 10$ mentioned above suggests that a might have the same value as z for nonlocal dynamics, which implies that z has no q dependence [6,30]. The value of the power a clearly depends on the algorithm used in the simulations.

In Fig. 4(a) we show a semilog plot of the results for τ^E_{int} and $\tau^E_{\exp}$ as functions of L for the random-bond Potts model. The data can be well fitted by a straight line indicating that the correlation times for the random-bond Potts model can be described by the logarithmic behavior expected for the two-dimensional Ising model [16,17]. We also tried to fit the data on a log-log plot, shown in Fig. 4(b). The result gave the value of z as 0.25 ± 0.04 and 0.32 ± 0.04 from τ^E_{int} and $\tau^E_{\exp}$, respectively. For both logarithmic and power-law fits, the goodness of fits were ~ 0.8 and 0.2 for the τ^E_{int} and $\tau^E_{\exp}$, respectively. These values are also in agreement with the work of [12,17] for the two-dimensional Ising model.

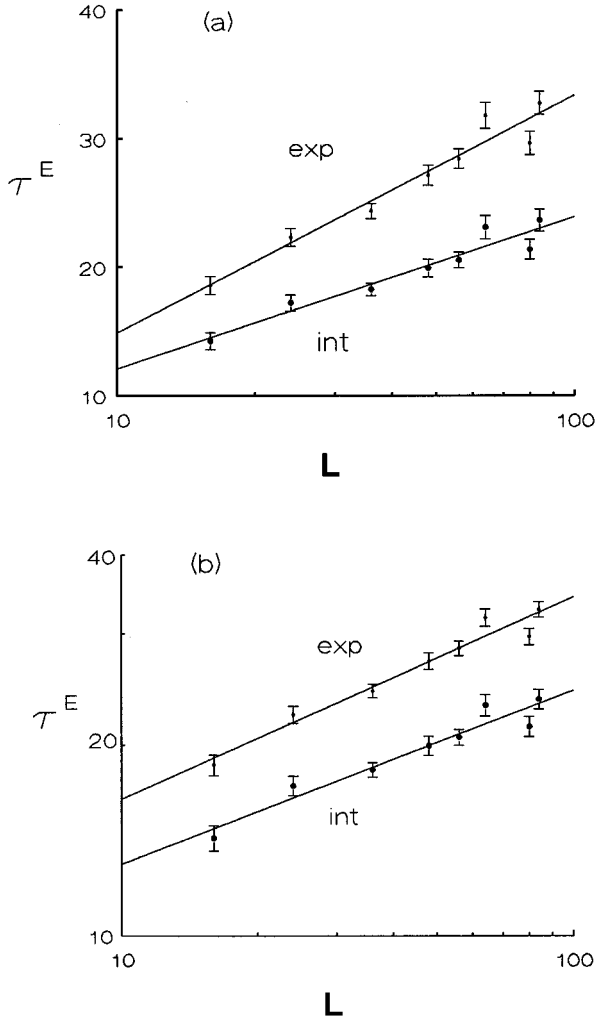

FIG. 4. (a) Semilog plot, and (b) log-log plot of the energy autocorrelation time (measured in Monte Carlo steps per site) for the $r=10$ random Potts model. Solid lines are linear fits.

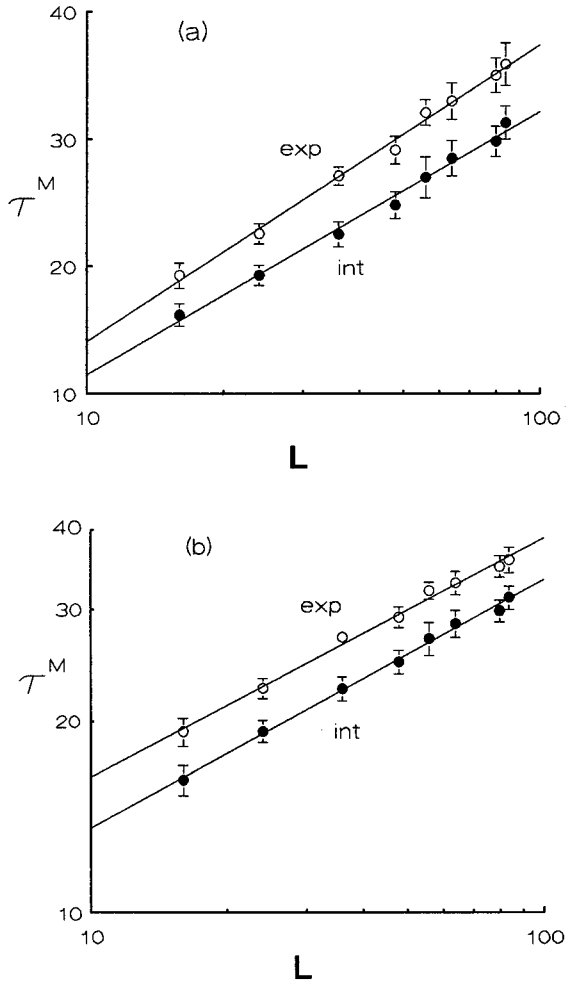

FIG. 5. (a) Semilog plot, and (b) log-log plot for the magnetization autocorrelation time (measured in Monte Carlo steps per site) for the random-bond Potts model. Solid lines are linear fits.

The difficulty in distinguishing between a logarithmic and a power law is substantial when the ''power'' is small. To see how this happens, consider the following Taylor series:

$$L^x = 1 + y\left(\frac{x}{1}\ln L + \frac{x^2}{2!}(\ln L)^2 + \cdots + \frac{x^n}{n!}(\ln L)^n + \cdots\right), \tag{14}$$

where $y=1/\ln e$. If $x \ll 1$, the higher-order term of x can be omitted, therefore

$$L^x = 1 + yx \ln L. \tag{15}$$

In principle, we can distinguish a power law from a logarithm by observing the trend of the data towards large L. If the slope of the successive points in the log-log plot decreases with L, we may conclude the function is logarithmic instead of a power law; however, the decrease may disappear at large L, resulting in a nonzero value of z. The autocorrelation time for the $q=2$ Potts model was investigated using the SW algorithm [17] with the result being that $z \approx 0.3$ for $\tau^E_{\rm int}$ if the fits were ''only'' performed for $L \leqslant 128$. The logarithmic behavior of the magnetization $\tau_{\rm int}$ was ''confirmed'' [16,17] for sizes up to 512. For simulations in a random system, where fluctuations of the thermodynamic properties over bond configurations are large, it is even more difficult to conclusively differentiate between a logarithm and a small value of $z<0.3$.

Figure 5 shows a semilog plot for the results of the $\tau^M_{\rm int}$ and $\tau^M_{\rm exp}$ for the random-bond Potts model. The behavior of τ^M is similar to that of τ^E: both can be described by a logarithmic law. However, when we fitted the data to a power law, we found $z \sim 0.40 \pm 0.04$ and $\sim 0.38 \pm 0.04$ for $\tau^M_{\rm int}$ and $\tau^M_{\rm exp}$, respectively. It seems that M, which is not a full symmetry magnetization, results in slower decorrelation and thus larger statistical errors in the data.

A comparison of integrated correlation times for the random-bond Potts model and the pure Potts model is shown in Fig. 6. The result from Ref. [17] for the Ising square lattice is also included for comparison. Clearly the randomness has a dramatic effect on the time dependent behavior. Upon the introduction of the bond randomness, the correlation times become much smaller and grow more slowly with increasing L. Although the autocorrelation times for the random Potts model are larger than those for the Ising model, they appear to have quite similar size dependence.

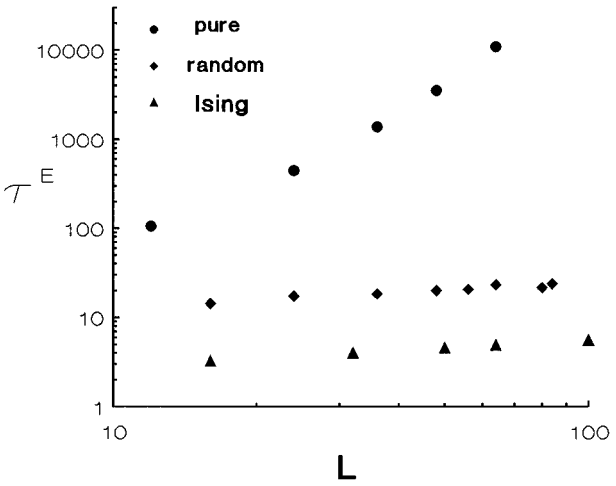

FIG. 6. Comparison of the autocorrelation times (measured in Monte Carlo steps per site) for the pure and random-bond Potts models, and the Ising model on a log-log scale.

IV. SUMMARY

Critical relaxation in the random-bond $q=8$ Potts model as well as the pure $q=8$ Potts model has been studied via extensive Monte Carlo simulations. Quite substantial differences are found: The autocorrelation times of the random-bond system obey power-law scaling, but with ($z\approx 0$) in contrast to the modified exponential behavior of a pure model. This difference fits nicely into the scenario obtained from the statics, i.e., the bond randomness induces a second-order transition in a system which would undergo a first-order transition without randomness. The dynamic critical behavior estimated for the random-bond Potts model is in agreement with that for the 2D Ising model. This could be expected from the dynamic scaling law [31] or the behavior of the cluster distribution [32,33], both of which lead to the relation between the dynamic critical exponent and the static exponents. Just as in the study [17] of critical relaxation in the two-dimensional pure Ising model, both a power law (with a small power) and a logarithm gave rather good fits. To unambiguously differentiate between a small power and a logarithm, we would need both to simulate more bond configurations for each size to reduce the fluctuation in the existing data and to consider much larger lattices to search for residual corrections to finite-size scaling. Since the CPU time already spent on the pure model was at least 1500 h, and more than 2000 h were needed for the random-bond Potts model, the task of improving the resolution noticeably will be formidable.

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