First-Order Transition in a Three-Dimensional Disordered System

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We present the first detailed numerical study in three dimensions of a first-order phase transition that remains first order in the presence of quenched disorder (specifically, the ferromagnetic-paramagnetic transition of the site-diluted four states Potts model). A tricritical point, which lies surprisingly near the pure-system limit and is studied by means of finite-size scaling, separates the first-order and second-order parts of the critical line. This investigation has been made possible by a new definition of the disorder average that avoids the diverging-variance probability distributions that plague the standard approach. Entropy, rather than free energy, is the basic object in this approach that exploits a recently introduced microcanonical Monte Carlo method.

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The combination of phase coexistence and chemical disorder plays a major role, for instance, in colossal magnetoresistance oxides [1]. In these situations one faces a fairly general question: which are the effects of quenched disorder [2] on systems that undergo a first-order phase transition in the ideal limit of a pure sample? For $D = 3$ systems, D being the space dimension, we only know that disorder somehow smooths the transition. More is known in $D = 2$, where the effects of disorder are so strong that the slightest concentration of impurities switches the transition from first order to second order [3–5].

A useful physical picture in $D = 3$ is provided by the Cardy-Jacobsen conjecture [4]. Consider a ferromagnetic system undergoing a first-order phase transition for a pure sample. Let T be the temperature while p is the concentration of magnetic sites. A transition line, $T_c(p)$ separates the ferromagnetic and the paramagnetic phases in the (T, p) plane. In $D = 3$ a critical concentration is expected to exist, $1 > p_t > 0$, such that the phase transition is of the first order for $p > p_t$ and of the second order for $p < p_t$ (at p_t one has a tricritical point). When p approaches p_t from above, the latent heat and the surface tension vanish while the correlation length $\xi(T_c(p))$ diverges. The universality class is expected to be related with that of the random field Ising model (RFIM). However, the Cardy-Jacobsen conjecture relies on a mapping between two still unsolved models (in $D = 3$), the (large Q) disordered Potts model [6], and the RFIM.

Numerical simulation is an important tool for theoretical investigations in $D = 3$. In this way, large portions of the transition line $T_c(p)$ were found to be second order [7–9]. However, the study of the tricritical point as well as that of the first-order part of the transition line seemed hopeless. The problem comes from the long-tailed probability distribution functions (PDF) encountered at $T_c(p)$, when comparing the specific heat or the magnetic susceptibility of different samples [8]. Long-tailed PDFs follow from the standard definition of the quenched free energy at temperature T as the average of the samples' free energy *at the same* T [2], which is dominated by rare events [10]. Furthermore, the simulation of a sample of linear size L with previous methods is intrinsically hard even for a pure system (see [13]). In fact, previous work [7,8] was limited to $L \leq 25$.

Here, we study for the first time the tricritical point separating the first- and the second-order pieces of the transition line. Furthermore, we characterize a first-order transition that remains so in the presence of quenched disorder. This has been made possible by two alternative methods of performing the sample average that avoid long-tailed PDFs, reproduce the correct thermodynamic limit, and provide complementary information. Essential for this study has been the capability of studying directly the entropy, using a recently proposed microcanonical Monte Carlo method [14] combined with a cluster algorithm [15]. We studied systems of size up to $L = 128$, which allowed a neat finite-size scaling investigation of the elusive tricritical point.

Specifically, we consider the site-diluted $Q = 4$ Potts model with periodic boundary conditions. The spins $\sigma_i = 1, \ldots, Q$ occupy the nodes of a cubic lattice with probability p. We consider nearest neighbor interaction:

$$\mathcal{H}^{\text{spin}} = -\sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \delta_{\sigma_i \sigma_j}. \tag{1}$$

The ϵ_i are quenched occupation variables ($\epsilon_i = 0$ or 1 with probability $1 - p$ and p, respectively) [16]. The pure system, $p = 1$, undergoes a first-order phase transition [8,14], which is generally regarded as very strong.

We introduce a real-valued conjugated momentum per occupied site, π_i [14]. The total Hamiltonian is $\mathcal{H} = \mathcal{H}^{\text{spin}} + \sum_i \epsilon_i \pi_i^2/2$ (the internal energy density will be $e = \mathcal{H}/N$ [18]). In the canonical ensemble, $\langle e \rangle_T = 1/(2T) + \langle \mathcal{H}^{\text{spin}}/N \rangle_T$. We consider instead the microca-

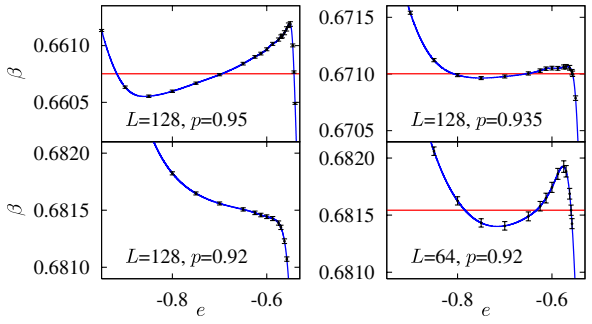

FIG. 1 (color online). Sample-averaged e derivative of the entropy, $\beta(e)$, for several lattice sizes, L, and spins concentrations, p. Metastability requires a nondecreasing $\beta(e)$. The horizontal line marks the critical (inverse) temperature $1/T_c$, obtained through Maxwell's construction. At fixed L the surface tension increases for growing p. Note that, for fixed dilution, a seemingly first-order transition ($L = 64$, bottom right), may actually be of the second order if studied on larger lattices ($L = 128$, bottom left).

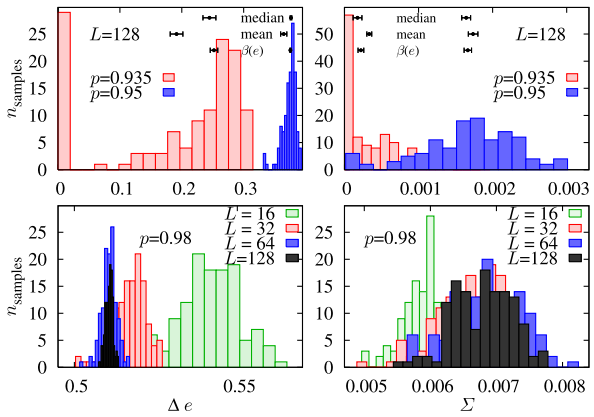

FIG. 2 (color online). Histograms for the sample-dependent latent-heat $\Delta_{\{\epsilon\}}e = e_d - e_o$ (left) and surface-tension (right). In the top panels we show results in the largest lattice, where two very close spin concentrations behave very differently. The three types of drawn horizontal lines (indicating central value and statistical error) correspond, from top to bottom, to the median, the mean, and the value obtained from $\beta(e)$. In the lower panels we show the histograms for $p = 0.98$ and several L (mind the difference in the horizontal scales with the upper part). The latent heat is self-averaging while the surface tension is not.

nonical ensemble for the extended model $\{\sigma_i, \pi_i\}$ at fixed e, and integrate out the $\{\pi_i\}$ to obtain a fluctuation-dissipation formalism. The basic quantity is a function of e and the spins, $\hat{\beta} = (N-2)/(Ne - \mathcal{H}^{\text{spin}})$. Its microcanonical mean value $\beta_{\{\epsilon\}}(e) = \langle\hat{\beta}\rangle_e$ is the e derivative of the entropy per spin, $s(e)$, for that particular sample $\{\epsilon\}$.

Connection with the canonical formalism is made by solving the equation $\beta_{\{\epsilon\}}(e) - 1/T = 0$ that yields the internal energy as a function of temperature. Thermodynamic stability requires $\beta_{\{\epsilon\}}(e)$ to be a decreasing function of e. Yet, at phase coexistence and for finite N, it is not (see Fig. 1 and Ref. [14]): the equation $\beta_{\{\epsilon\}}(e) - 1/T = 0$ has several roots. For $T = T_c$, we name, respectively, e_d and e_o the rightmost and leftmost solutions, which correspond to the energy densities of the coexisting disordered and ordered phases. The critical temperature is fixed by Maxwell construction: the e integral of $\beta_{\{\epsilon\}}(e) - 1/T_c$ from e_d to e_o vanishes [19]. The surface tension Σ is $L^{D-1}/2$ times the integral of the positive part of $\beta_{\{\epsilon\}}(e) - 1/T_c$ for $e_o < e < e_d$.

For a disordered system, one analyzes the set of functions $\beta_{\{\epsilon\}}(e)$ corresponding to a large enough number of samples. There are two natural possibilities. On one hand, one can use the Maxwell construction for each sample, extracting T_c, e_d, e_o, and Σ and considering afterwards their sample average or even their PDF, Fig. 2. The second alternative is to compute the sample average $\beta(e) = \overline{\beta_{\{\epsilon\}}(e)}$, and then perform on it the Maxwell construction [i.e., take the sample average of $s(e)$, rather than the average of the free energy at fixed T].

We have empirically found that the two sample averages are equivalent in the first-order piece of the critical line. This is hardly surprising, because the internal energy as a function of T is a self-averaging quantity for all temperatures but the critical one. Therefore, also e_d, e_o, and T_c are self-averaging properties in the first-order piece of the critical line. The first method offers more information, but it is computationally more demanding (it requires high accuracy for each sample). The method featuring $\beta(e)$ can be used as well in the second-order part of the critical line; nevertheless, its merit in that region is yet to be researched.

We have investigated the phase transition for several p values in the range $0.75 \leq p \leq 1$. As a rule, we found that at fixed p the latent heat is a monotonically decreasing function of L; see Fig. 3. For each p value, we simulated $L = 16, 32, 64$, and 128 (for a given p, we did not consider larger lattices once the latent heat vanished). For all pairs (L, p) we simulated 128 samples. Besides, some intermediate L values were added for the finite-size scaling study below (see Fig. 4), and we have raised to 512 the number of samples for ($L = 16$, 32, $p = 0.86$, 0.875).

We used a Swendsen-Wang (SW) version of the microcanonical cluster method [14]. For disordered systems, SW updates properly loosely connected regions [20] and does not require painful parameter tunings. For each sample, we simulated at least 20 e values in the range $-1.2 < e < -0.5$. The values of e were decreased sequentially to make use of the thermalization effort at the previous energy density. The microcanonical cluster method, which is not rejection-free, depends on a tunable parameter κ. In order to maximize the acceptance of the SW attempt (SWA), κ should be chosen as close as possible to $\beta_{\{\epsilon\}}(e)$. After every e change, we performed cycles consisting of 10^3 Metropolis steps, κ refreshing, then 10^3 SWA, and a new κ refreshing. The cycling was stopped, and κ fixed, when

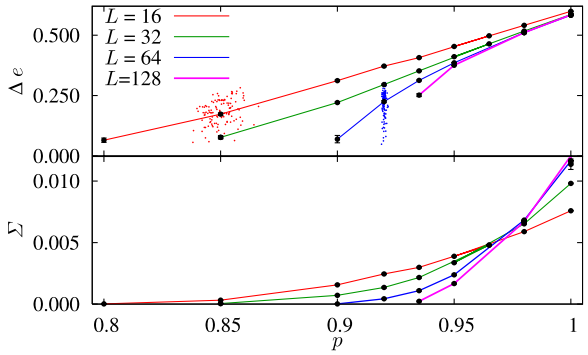

FIG. 3 (color online). Top: Latent heat as obtained from $\beta(e)$ vs spin concentration for several lattice sizes (lines are linear interpolations). Data for $p = 1$ and $L = 128$ were taken from Ref. [14]. To illustrate the sample dispersion, we plot as well the scatterplot of $(N/L^D, \Delta_{\{\epsilon\}}e)$ for the 128 samples at $L = 16$, $p = 0.85$ and $L = 64$, $p = 0.92$. Bottom: as top part, for the surface tension.

the SWA acceptance exceeded 60%. Afterwards we performed (2–4) $\times 10^5$ SWA, taking measurements every 2 SWA. In addition, we performed thermalization checks that included comparisons of hot and cold starts or even mixed configurations (bands [14]).

Our results for the latent heat, $\Delta e = e_d - e_o$, and the surface tension are in Fig. 3. The apparent location of the tricritical point (i.e., the p where both Δe and Σ vanish) shifts to upper p for growing L rather fast. For lattice sizes comparable with those of previous work, $L = 16$, we obtain $p_t^{L=16} \approx 0.75$, at a sizable distance from $p = 1$, but the estimate of p_t increases very fast with L.

The PDFs for Δe and Σ, Fig. 2, display an interesting L evolution. When the $\beta(e)$ changes behavior from nonmonotonic ($L = 64$, Fig. 1, bottom right) to monotonic ($L = 128$, Fig. 1, bottom left), the two PDFs becomes enormously wide [21]; see top panels in Fig. 2. This arises because for many $L = 128$ samples, the curve $\beta_{\{\epsilon\}}(e)$ is becoming flat, or even monotonically decreasing (i.e., $\Delta e = \Sigma = 0$), while no such behavior was seen for $L = 64$. Only for $p = 0.98$, the width of the PDFs for Δe scales as $L^{-D/2}$, as expected for a self-averaging quantity (Fig. 2, bottom left). The surface tension is *not* self-averaging (Fig. 2, bottom right).

From Figs. 1–3 one cannot rule out that $p_t = 1$: a disordered first-order transition would not exist. Fortunately, we can solve this dilemma by considering the correlation length, obtained from the sample-averaged correlation function,

$$C(r) = L^{-D}\overline{\sum_x \epsilon_x \epsilon_{x+r} \langle \delta_{\sigma_x,\sigma_{x+r}} - Q^{-1}\rangle_e}, \qquad (2)$$

as $\xi^2(e) = [-1 + \hat{C}(0,0,0)/\hat{C}(2\pi/L,0,0)]/[2\sin\pi/L]$, where $\hat{C}$ is the Fourier transform of $C(r)$ [22,23].

We take the correlation length in units of the lattice size at e_d, e_o as obtained from $\beta(e)$ (a jackknife method [23] takes care of the statistical correlations). For all $p < p_t$, one expects that both $\xi(e_d)/L$ and $\xi(e_o)/L$ tend to nonvanishing and different limits for large L [24]. On the other hand, for $p > p_t$, $\xi(e_d)/L$ is of order $1/L$, while $\xi(e_o)/L \sim L^{D/2}$. For a fixed L, upon increasing p, the behavior goes from second-order-like to first order (see Fig. 1). Hence, a finite-size scaling approach [23] is needed.

Consider the curves of $\xi(e_d)/L$ versus p, for different L, Fig. 4 (top left). There is a unique concentration, $p^{L,2L}$, where the correlation length in units of the lattice size coincides for lattices L and $2L$. One has [25]

$$p^{L,2L} \approx p_t + A_d L^{-x}. \qquad (3)$$

An analogous result holds for $\xi(e_o)/L$. Since A_d and A_o are rather different (see Fig. 4, right), a joint fit of all data yields an accurate estimate for the location of the tricritical point:

$$p_t = 0.954(3), \qquad x = 1.23(9), \qquad \frac{\chi^2}{\text{dof}} = \frac{4.23}{3}, \qquad (4)$$

Of course, due to higher-order scaling corrections, Eq. (3) should be used only for lattices larger than some $L^{\min}$ [26]. The fit χ^2 was acceptable taking $L_o^{\min} = 16$ and $L_d^{\min} = 12$ (for the sake of clarity we do not display data for $L = 12$ in the figures). We thus conclude that $p = 0.98$ is definitively in the first-order part of the critical line.

We now look at ξ/L at $p^{L,2L}$; see Fig. 4. Consider $\xi(e_d)/L$ [$\xi(e_o)/L$] as a function of (L, p), in the region $p < p_t$. The salient features are (i) for fixed L, $\xi(e_d)/L$ is a decreasing function of p [$\xi(e_o)/L$ is increasing], (ii) for fixed p, $\xi(e_d)/L$ has a minimum [$\xi(e_o)/L$ has a maximum], at a crossover length scale, $L_{\text{co}}(p)$, that separates

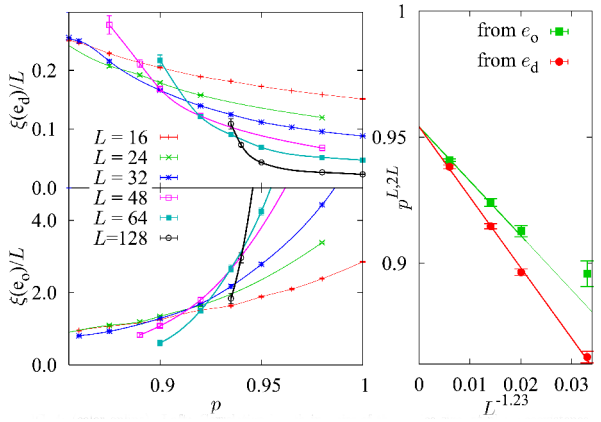

FIG. 4 (color online). Left: Correlation length in units of the lattice size, at phase coexistence for the paramagnetic (top) and ordered (bottom) phases, as a function of spin concentration for several L (lines are cubic spline interpolations for data at fixed L). Right: Spin concentration where ξ/L (data from left panel) coincide for lattices L and $2L$ versus $1/L^x$; see Eqs. (3) and (4). Lines are a joint fit for x, p_t, A_d, and A_o.

the first-order-like behavior from the second-order one, (iii) at the crossing point $p^{L,2L}$ we have $L < L_{\rm co}(p^{L,2L}) < 2L$, and (iv) at least within the range of our simulations, $L_{\rm co}(p)$ is a growing function of p. A standard scaling argument, combined with (i)–(iv), yields that $\xi(e_d)/L$ at $p^{L,2L}$ is of order $1/L_{\rm co}$ [$\xi(e_o)/L \sim L_{\rm co}^{D/2}$]. If $L_{\rm co}(p)$ diverges at p_t, $\xi(e_d)/L$ at $p^{L,2L}$ should tend to zero for large L, which is indeed consistent with our data.

In this work, we have performed for the first time a detailed study of a disordered first-order transition in $D = 3$, by site diluting the $Q = 4$ Potts model, a system suffering a prototypically strong first-order transition. A fairly small degree of dilution smooths the transition to the point of becoming second order, at a tricritical point, p_t. A delicate finite-size scaling analysis is needed to firmly conclude that $p_t < 1$. We thus claim that (quenched) disordered first-order transitions do exist in $D = 3$, although quenched disorder is astonishingly effective in smoothing the transition (we speculate that the percolative mechanism for colossal magnetoresistance proposed in [1] could be fairly common in $D = 3$). We also observe that, for a given $p < p_t$, a crossover length scale $L_{\rm co}(p)$ exists such that for $L < L_{\rm co}(p)$ the behavior is first-order-like. The asymptotic second-order behavior appears only for $L > L_{\rm co}(p)$. Our data are consistent with a divergence of $L_{\rm co}(p)$ at p_t. The successful location of the tricritical point has been made possible by new definitions of the quenched average that avoids long-tailed PDF [8]. It was crucial in this approach, a recently introduced microcanonical Monte Carlo method that features the entropy density rather than the free energy [14].

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