First Order Phase Transition in a 3D disordered system

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Abstract.
We present a detailed numerical study on the effects of adding quenched impurities to a three dimensional system which in the pure case undergoes a strong first order phase transition (specifically, the ferromagnetic/paramagnetic transition of the site-diluted four states Potts model). We can state that the transition remains first-order in the presence of quenched disorder (a small amount of it) but it turns out to be second order as more impurities are added. A tricritical point, which is studied by means of Finite-Size Scaling, separates the first-order and second-order parts of the critical line. The results were made possible by a new definition of the disorder average that avoids the diverging-variance probability distributions that arise using the standard methodology. We also made use of a recently proposed microcanonical Monte Carlo method in which entropy, instead of free energy, is the basic quantity.

Keywords: Phase transitions, quenched disorder, Potts model, microcanonical Montecarlo, tricritical point.
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INTRODUCTION

At first order phase transitions, system properties such as energy, pressure or magnetisation change abruptly when a control parameter (temperature, presssure, magnetic field, etc.) cross a critical value. Although first order transitions are fairly common in Nature, not much is known about the consequences of adding quenched impurities to such systems. Studies on this question are compulsory given that most of natural systems contains impurities. It is useful to classify the encountered disorder in one of two types [1]: quenched or annealed. In the annealed case, there is not an orders of magnitude mismatch for the characteristic times of the impurities and of the pure system (think of the movement of molecules in a solution), so that the impurities may reach thermal equilibrium with the degrees of freedom of the pure system. On the other hand, in the quenched case, the dynamics of the impurities is exceedingly slower (consider vacancy diffusion in a magnetic crystal lattice). In the so called quenched approximation, impurities do not evolve and are completely unaffected by the dynamics of the pure system's degrees of freedom.

The question we ask, and partly answer, in this work (see also [2]) is: what happens to a system undergoing a first-order phase transition on a perfectly pure sample if one

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increasingly deteriorates the quality of the sample by introducing quenched impurities? This is still an open problem in Statistical Mechanics but also one with implications in technical fields such as highly correlated electron systems (as high temperature superconductors or colossal magnetoresistance oxides) where phase coexistence and chemical disorder play crucial roles [3]).

The question has been solved in two-dimensions [4]: even the most insignificant amount of impurities is enough to switch the phase transition from first-order to second-order (for the Universality Classes see [5]). In $D=3$ the most useful physical picture is provided by the Cardy-Jacobsen conjecture [5]: considering a ferromagnetic system undergoing a first order phase transition for a pure sample, $T_c(p)$ separates the ferromagnetic and the paramagnetic phases in the (T,p) plane (T is the temperature and p the concentration of magnetic sites). 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 must vanish with the critical exponent of the magnetisation in the Random Field Ising Model (RFIM). Also the surface tension, Σ, vanishes at p_t, while the correlation-length $\xi(T_c(p))$ diverges, with RFIM related critical exponents. The main objection to this argument is that the Cardy-Jacobsen conjecture relies on a mapping from the (large Q) disordered Potts model [6] onto the RFIM (two unsolved models in $D=3$). As a result, if the $D=3$ RFIM phase transition turned out to be of the first order [7], the conjecture would not be valid.

The $D=3$ problem has already been numerically studied in the past [8, 9, 10]. Large regions of the critical line $T_c(p)$ were found to be second order. Unfortunately, the study of the tricritical point as well as that of the first-order part of the critical line seemed beyond hope, mainly due to two factors. Firstly, an important difficulty comes from the long-tailed probability distribution functions (PDF) encountered when comparing the specific-heat or the magnetic susceptibility of different samples at $T_c(p)$ [10]. Note that diverging-variance PDF arises from the common practice of defining the quenched free-energy at temperature T as the average of the samples free-energy at T [1], which, in the case of phase-coexistence, is dominated by rare events. Secondly, the other difficulty is that the simulation of a sample of linear size L with previous methods is intrinsically hard: the required simulation time grows exponentially with L^{D-1} [11] due to the so called Exponential Critical Slowing Down. These two factors have limited previous works [9, 10] to $L \leq 25$.

To overcome these difficulties, on the one hand, we propose two alternative methods of performing the sample average, both reproducing the correct thermodynamic limit, avoiding diverging-variance PDF, and providing complementary information. On the other hand, we exploit a novel microcanonic Monte Carlo method [12] which allows to study directly the system entropy. This method, combined with a slightly modification of a standard cluster algorithm [13], has permitted us to study systems of size up to $L=128$, also making possible to perform a Finite-Size Scaling to study the *elusive* tricritical point as well as the associated critical behaviour.

THE MODEL

We consider a prototypical three-dimensional model undergoing a first order phase transition on the pure case: the site diluted $Q=4$ Potts model [6]. We take periodic boundary conditions. The spins $\sigma_i = 1,\ldots,Q$ occupy the nodes of a cubic lattice with probability p. We only consider nearest neighbour interaction. The Hamiltonian for this model is:

$$\mathscr{H}^{\text{spin}} = -\sum_{<i,j>} \varepsilon_i \varepsilon_j \delta_{\sigma_i \sigma_j}\,, \tag{1}$$

where ε_i are quenched occupation variables ($\varepsilon_i = 0$ or 1 with probability $1-p$ and p respectively). In the following, $V = L^3$ will be the system volume, and L its linear size. Each one of the specific disorder realizations is called a *sample*. The number of spins actually present in a sample is named N. Note that $N \approx pV$ with fluctuations of order $\sim 1/\sqrt{V}$. [1]. The pure system is recovered for $p=1$. It undergoes a first order phase transition [10, 12] generally regarded as *very strong*.

MEASURED QUANTITIES

A valid order parameter for the model described in the previous section is the magnetisation density (a Q-dimensional vector), defined as

$$M_q = \frac{1}{V}\sum_i \varepsilon_i \left[\frac{Q\delta_{\sigma_i,q}-1}{\sqrt{Q(Q-1)}}\right]. \tag{2}$$

We define the magnetic susceptibility as,

$$\chi = V|M|^2 \tag{3}$$

In addition, we consider the correlation length obtained from the correlation function [15]:

$$\xi \equiv \left(\frac{\overline{\chi}/\overline{F}-1}{4\sin^2(\pi/L)}\right)^{\frac{1}{2}}, \tag{4}$$

where

$$\overline{F} \equiv \frac{V}{3}\overline{\langle |F(2\pi/L,0,0)|^2 + |F(0,2\pi/L,0)|^2 + |F(0,0,2\pi/L)|^2\rangle}\,, \tag{5}$$

with

$$F(k) \equiv \frac{1}{V}\sum_r e^{ik\cdot r}\varepsilon_r\sigma_r. \tag{6}$$

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[1] To reduce statistical fluctuations, we kept only the spins in the percolating cluster [14] which control the critical behaviour. However, in the most interesting region ($p \approx 0.96$) this correction is extremely small.

NUMERICAL METHODOLOGY

The Extended Microcanonical approach

In the microcanonical Monte Carlo method proposed in [12] a real-valued conjugated momentum, π_i, is introduced in each occupied node of the lattice. The total Hamiltonian is

$$\mathscr{H} = \mathscr{H}^{\text{spin}} + \sum_i \varepsilon_i \pi_i^2/2, \tag{7}$$

the internal energy density will be $e = \mathscr{H}/N$. In the canonical ensemble,

$$\langle e \rangle_T = 1/(2T) + \langle \mathscr{H}^{\text{spin}}/N \rangle_T . \tag{8}$$

On the contrary, we can consider the *microcanonical 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 of the new formalism is simply a function of e and the spins:

$$\hat{\beta} = \frac{N-2}{Ne - \mathscr{H}^{\text{spin}}} . \tag{9}$$

Its microcanonical mean value $\beta_{\{\varepsilon\}}(e) = \langle \hat{\beta} \rangle_e$ is the e-derivative of the entropy per spin, $s(e)$, for that particular sample.

Thermodynamic stability requires that $\beta_{\{\varepsilon\}}(e)$ be a decreasing function of e. Nevertheless, at the phase coexistence region and for finite N, it is not (see Fig. 1 and Ref. [12]). As the equation $\beta_{\{\varepsilon\}}(e) - 1/T = 0$ has several roots which, for e_{d} and e_{o}, respectively the rightmost and leftmost solutions, are the energy densities of the coexisting disordered and ordered phases. The critical temperature is fixed by Maxwell construction: the e-integral of $\beta_{\{\varepsilon\}}(e) - 1/T_{\text{c}}$ from e_{d} to e_{o} must vanish. This fact enforces the relation,

$$s_{\text{d}} - s_{\text{o}} = (e_{\text{d}} - e_{\text{o}})/T_{\text{c}} . \tag{10}$$

The latent heat is directly defined as

$$\Delta e = e_{\text{d}} - e_{\text{o}}, \tag{11}$$

while the surface-tension, Σ, is $L^{D-1}/2$ times the integral of the positive part of $\beta_{\{\varepsilon\}}(e) - 1/T_{\text{c}}$.

Sample Averaging Methods

For a disordered system, one has to analyse a set of functions $\beta_{\{\varepsilon\}}(e)$ corresponding to a large enough number of samples. There are two natural possibilities. The first one is to 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. This is the most straightforward solution to the long-tailed pdf.

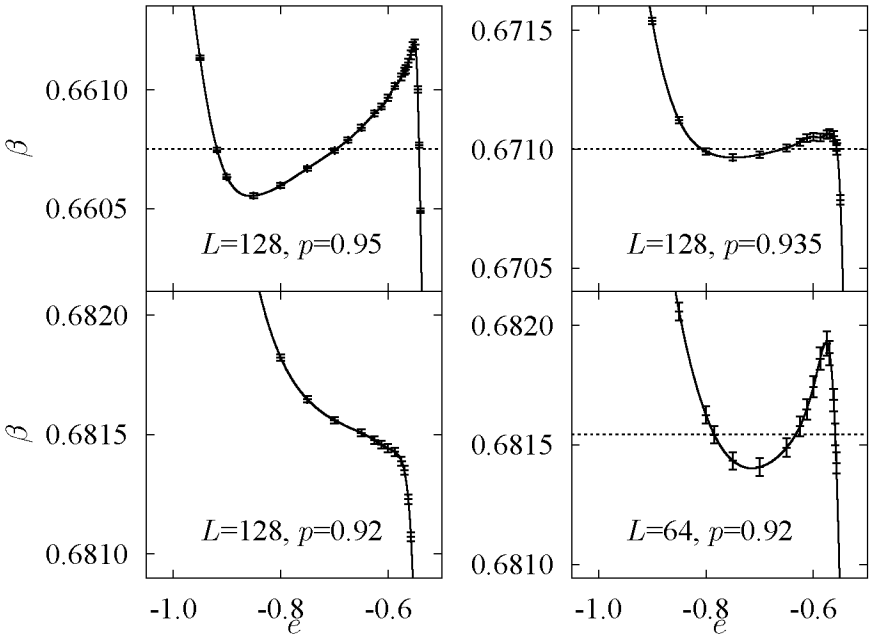

FIGURE 1. Sample-averaged e-derivative of the entropy, $\beta(e)$, for several lattice sizes, L, and spins concentrations, p. Metastability requires a non-decreasing $\beta(e)$. The horizontal dotted line marks the critical (inverse) temperature $1/T_c$, obtained through Maxwell's construction. At fixed 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).

The alternative possibility is to compute the sample-average $\beta(e) = \overline{\beta_{\{\varepsilon\}}(e)}$, and then to perform on it the Maxwell construction (i.e. take the sample average of $s(e)$, rather than the sample average of the free-energy at fixed T).

We have empirically found that the two sample-averaging 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.

While the first method offers more information, 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 are yet to be researched [16].

RESULTS

Simulation Details

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 (p, L) we simulated 128 samples. Besides, some intermediate L values were added for the Finite Size Scaling study below (see Figs. 5 and 4), and we also 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 [12]. For disordered systems, SW updates properly loosely connected regions [17] 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 maximise the acceptance of the SW attempt (SWA), κ should be chosen as close as possible to $\beta_{\{\varepsilon\}}(e)$. 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 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*[12]).

Latent heat and Surface tension

The PDFs for Δe and Σ, Fig. 2, display an interesting L evolution. When the $\beta(e)$ changes behaviour from non-monotonic ($L = 64$, Fig. 1, bottom-right) to monotonic ($L = 128$, Fig. 1, bottom-left), the two PDFs becomes enormously wide[2], see top panels in Fig 2. This arises because for many $L = 128$ samples, the curve $\beta_{\{\varepsilon\}}(e)$ is becoming flat, or even monotonically decreasing (i.e. $\Delta e = \Sigma = 0$), while no such behaviour 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.

Additional results for the latent-heat, Eq. 11, and the surface tension are shown 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 a sizeable value $p_t^{L=16} \approx 0.75$, but the estimate of p_t increases very fast with L.

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[2] The estimates for Δe and Σ are consistent with the *median* of their (non-Gaussian) PDFs.

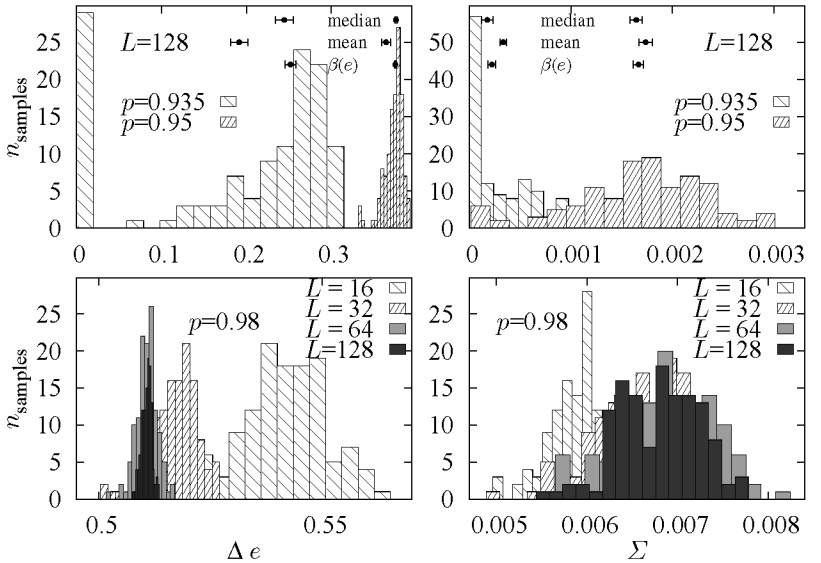

FIGURE 2. Histograms for the sample-dependent latent-heat $\Delta_{\{e\}}e = e_d - e_o$ (**left**) and surface-tension (**right**). In the top panels we show results in the largest lattice, where two very close spin concentrations behaves very differently. The three types of drawn horizontal lines (indicating central value and statistical error) correspond, from top to bottom, to the median, the mean and values 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). As can be seen, the latent-heat is self-averaging while the surface tension is not.

Finite Size Scaling Study

From Figs. 1, 2 and 3 one cannot state unambiguously that $p_t \neq 1$: a disordered first-order transition would not exist at the thermodynamic limit. Fortunately we can solve this dilemma by considering the correlation-length, obtained from the *sample-averaged* correlation function, Eq. 4.

We take the correlation-length in units of the lattice size at e_d (Fig.4), and e_o (Fig.5), as obtained from $\beta(e)$ (a jackknife method [15] 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 non-vanishing and different limits for large L[3]. 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 behaviour goes from second-order like to first-order (see Fig 1). Hence, a Finite-Size Scaling approach [15] is needed.

Consider the curves of $\xi(e_d)/L$ versus p, for different L, Figs. 4 and 5. There is

[3] We have numerically checked that this is indeed the case for the $D = 2$, $Q = 4$, pure Potts model (a prototypical example of a second-order phase transition with a double peaked canonical PDF for e at T_c).

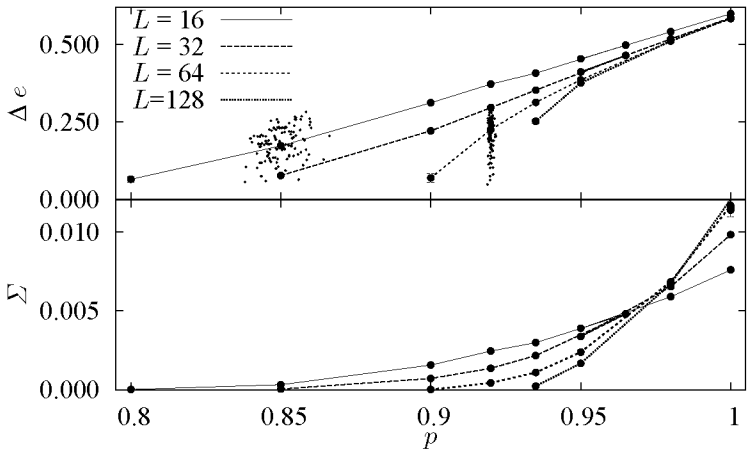

FIGURE 3. **Top:** Latent heat as obtained from $\beta(e)$ vs. spins concentration for several lattice sizes (lines are linear interpolations). Data for $p = 1$ and $L = 128$ were taken from Ref. [12]. To illustrate the sample dispersion, we plot as well the scatter-plot of $(N/L^D, \Delta_{\{\varepsilon\}}e)$ for the 128 samples at $L = 16$ $p = 0.85$ and $L = 64$ $p = 0.92$. **Bottom:** as top part, for the surface tension.

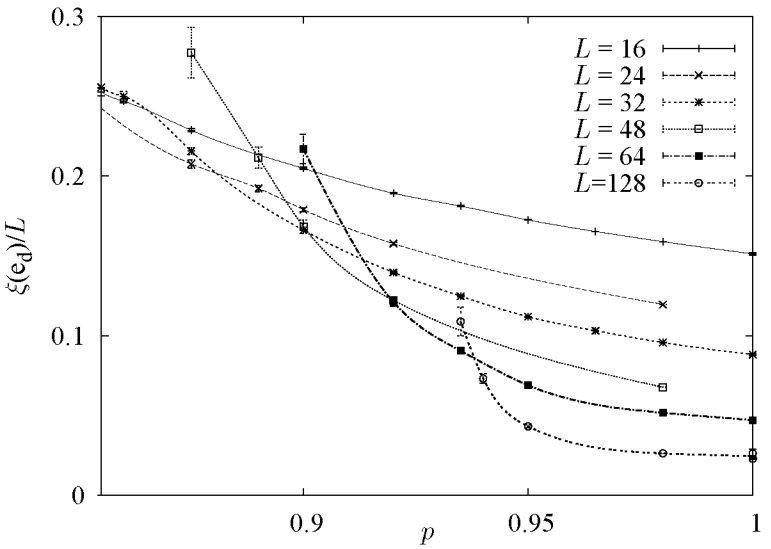

FIGURE 4. Correlation length in units of the lattice size, at phase-coexistence for the paramagnetic phases , as a function of concentration for several L (lines are cubic spline interpolations for data at fixed L).

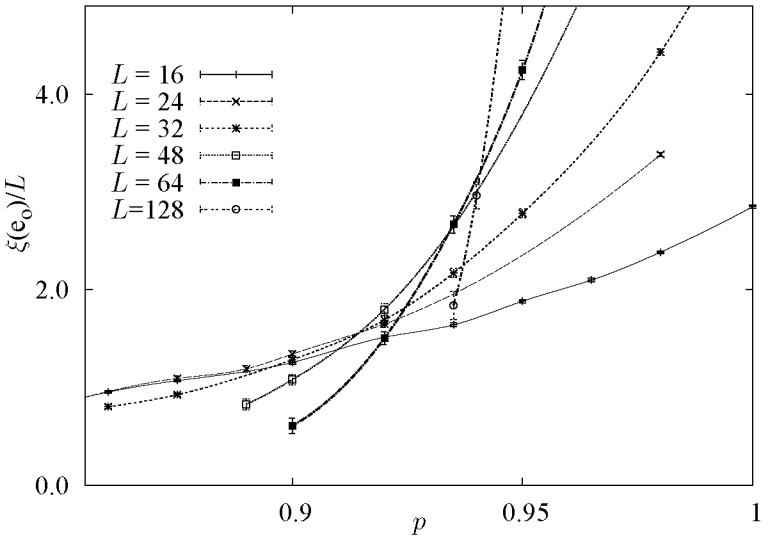

FIGURE 5. Correlation length in units of the lattice size, at phase-coexistence for the ferromagnetic phases , as a function of concentration for several L (lines are cubic spline interpolations for data at fixed L).

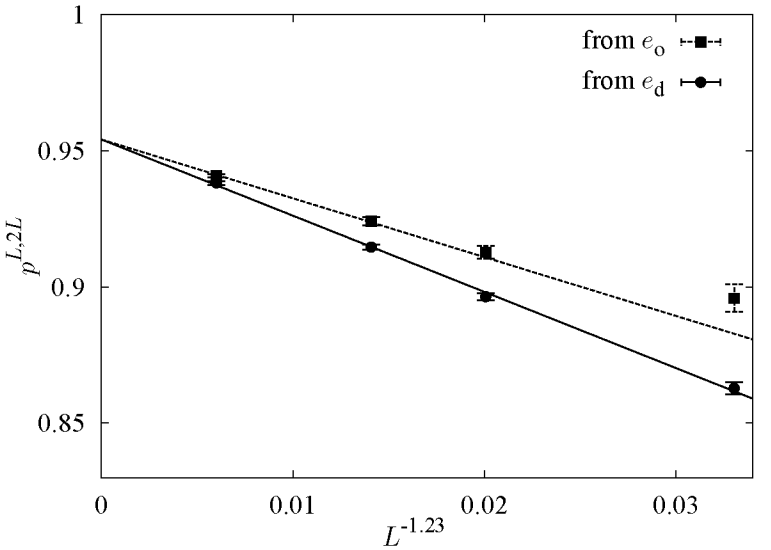

FIGURE 6. Spin concentration where ξ/L (data from Figs. 4 and 5) coincide for lattices L and $2L$ versus $1/L^x$, see Eqs.(12, 13). Lines are a joined fit for x, p_t, A_d and A_o.

a unique concentration, $p^{L,2L}$, where the correlation length in units of the lattice size coincides for lattices L and $2L$. One has [4]

$$p^{L,2L} \approx p_t + A_d L^{-x}, \tag{12}$$

An analogous result holds for $\xi(e_o)/L$. Since A_d and A_o are rather different, see Fig. 6—right, a join fit of all data yields an accurate estimate for the location of the tricritical point:

$$p_t = 0.954(3), \quad x = 1.23(9), \quad \frac{\chi^2}{\text{dof}} = \frac{4.23}{3} \tag{13}$$

Of course, due to higher-order scaling corrections, Eq.(12) should be used only for lattices larger than some $L^{\min}$ [18]. The fit χ^2 was acceptable taking $L_d^{\min} = 12$ and $L_o^{\min} = 16$ (for the sake of clarity we do not display data for $L = 12$ in the figures). Therefore we can conclude that $p = 0.98$ is definitively in the first-order part of the critical line.

We now look at ξ/L at $p^{L,2L}$, Figs. 4 and 5. Consider $\xi(e_d)/L$ 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, $L_{cr}(p)$, that separates the first-order like behaviour from the second order one, see Figs. 4 and 5; (iii) at the crossing point $p^{L,2L}$ we have $L < L_{cr}(p^{L,2L}) < 2L$; (iv) at least within the range of our simulations, $L_{cr}(p)$ 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 $1/L_{cr}(p^{L,2L})$ ($\xi(e_o)/L \sim L_{cr}^{D/2}$). If $L_{cr}(p)$ 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.

CONCLUSIONS

To summarise, in this work we have performed a detailed study of the effects of the quenched disorder on a system undergoing a first-order transition in $D = 3$, by site-diluting the $Q = 4$ Potts model, a model suffering a prototypically strong first-order transition. A 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 has allowed to firmly conclude that $p_t < 1$. We are able to claim that (quenched) disordered first-order transitions do exist in $D = 3$, although quenched disorder is unreasonably effective in smoothing the transition (we speculate that the percolative mechanism for colossal magnetorresistance proposed in [3] could be fairly common in $D = 3$). We also observe that, for a given $p < p_t$, a crossover length scale $L_{cr}(p)$ exists such that for $L < L_{cr}(p)$ the behaviour is first order like. The asymptotic second-order behaviour appears only for $L > L_{cr}(p)$. This has been made possible by new definitions of the quenched average that

[4] The tricritical point has no basin of attraction for the Renormalization Group flow in the (T,p) plane. Although two relevant scaling fields are to be expected, the Maxwell construction allows us to eliminate one of them and hence we borrow the formulas for a standard critical point.

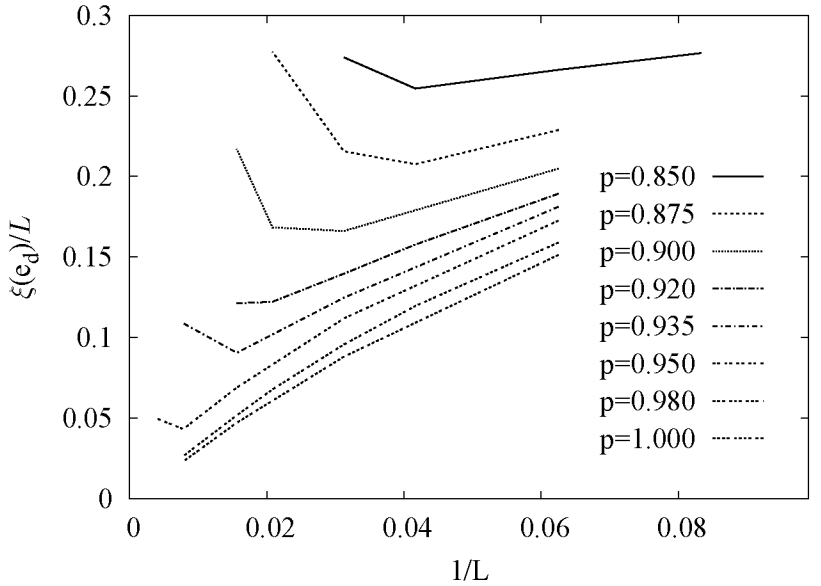

FIGURE 7. Correlation length at e_d in units of the lattice size, for fixed dilutions as a function of the inverse lattice size. For fixed $p < p_t$, $\xi(e_d)/L$ has a minimum at a crossover length scale, $L_{cr}(p)$, that separates the first-order like behaviour from the second order.

avoids long-tailed PDF [10]. It was crucial to achieve these results a recently introduced microcanonical Monte Carlo method that features the entropy density rather than the free energy [12].

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