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3D bond-diluted 4-state Potts model: a Monte Carlo study*

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We report on a Monte Carlo study of the three-dimensional bond-diluted 4-state Potts model which, in the pure case, undergoes a strong first-order phase transition. Subject to quenched, random disorder one expects a softening to a continuous transition from a certain disorder strength on. Employing a combination of cluster algorithms, multicanonical methods and reweighting techniques, we obtain strong numerical evidence for the existence of a tricritical point separating the first- and second-order regimes and give an estimate of its location.

1. INTRODUCTION

The influence of quenched, random disorder on phase transitions is of great importance in a large variety of fields, ranging from experiments with absorbed monolayers [1] in condensed matter physics to conceptual questions in non-perturbative quantum gravity [2]. For pure systems exhibiting a continuous phase transition, Harris [3] derived the criterion that random disorder is a relevant perturbation when the critical exponent of the specific heat of the pure system is positive, $\alpha > 0$. In this case one expects that the system falls into a new "disordered" universality class.

If a pure system with a first-order transition is subject to disorder, the transition is softened and may even turn into a continuous one [4]. This is always the case in two dimensions (2D) [5] (for numerical verifications see [6]). In higher dimensions, a tricritical point may appear at a finite concentration of impurities [7], separating "non-softened" first-order and "softened" second-order regimes. Numerically such a scenario has recently been observed for the 3D *site*-diluted 3-state Potts model [8]. Since here the first-order transition in the pure model is very weak [9], however, the characterization of the tricritical point is difficult. We, therefore, focussed in our study on the much stronger first-order transition of the 3D 4-state Potts model [10]. Moreover, we chose *bond*-dilution in order to facilitate comparison with recent high-temperature series expansions [11] for this model.

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2. MODEL AND SIMULATION SETUP

The model is defined by the Hamiltonian

$$-\beta H = \sum_{\langle ij \rangle} K_{ij} \delta_{\sigma_i,\sigma_j}; \quad \sigma_i = 1,\ldots,4, \tag{1}$$

where the sum extends over all pairs of neighbouring sites on a cubic lattice (with periodic boundary conditions) and the couplings K_{ij} are distributed according to the distribution $\wp(K_{ij}) = p\,\delta(K_{ij} - K) + (1-p)\,\delta(K_{ij})$, where $K \equiv J/k_B T$. The parameter p is thus the concentration of bonds in the system, i.e., $p = 1$ corresponds to the pure case with its strong first-order phase transition at $K_t = 0.62863(2)$ (and correlation length $\xi(K_t) \simeq 3$) [10]. Below the percolation threshold $p_c \simeq 0.2488$ one does not expect any finite-temperature phase transition since without any percolating cluster in the system long-range order is impossible.

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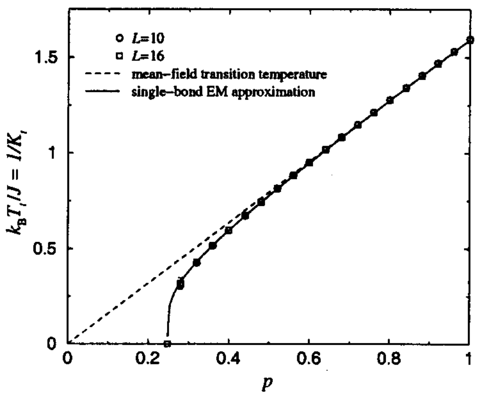

Figure 1. Phase diagram of the 3D bond-diluted 4-state Potts model.

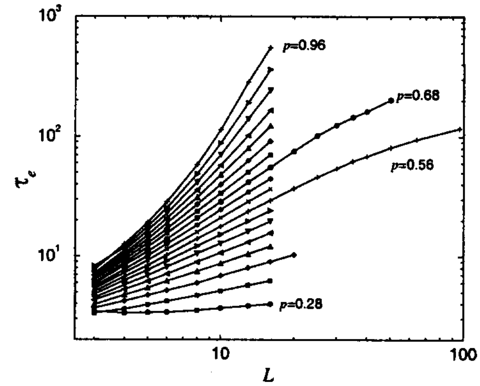

Figure 2. Autocorrelation time τ_e of the energy at $T_t(p)$ versus lattice size L (p in steps of 0.04).

The system was studied [12] by means of large-scale Monte Carlo (MC) simulations using the Swendsen-Wang cluster algorithm [13] in the regime of second-order transitions, and multicanonical simulations [14] in the regime of weak dilution where the first-order transition of the pure model persists. Thermodynamic quantities were averaged over a large number of disorder realisations, ranging between 2 000 and 5 000.

3. RESULTS

In order to map out the phase diagram of the model we considered all concentrations p in the interval $[0.28, 1]$ in steps of 0.04. As an estimate for the transition temperature $T_t(p)$ we took the location of the maximum of the magnetic susceptibility for a given lattice size L. The resulting phase diagram is depicted in Fig. 1, where we show for comparison also a simple mean-field prediction [12], $T_t(p) = pT_t(1)$, and the effective-medium approximation [15],

$$K_t(p) = \log \left[\frac{(1-p_c)e^{K_t(1)} - (1-p)}{(p-p_c)} \right], \qquad (2)$$

where in addition to the pure system limit ($p = 1$) also the percolation threshold p_c is built in, resulting in an extremely good approximation for all dilutions.

In a second step, the order of the phase transitions was investigated. A first indication is given by the finite-size scaling (FSS) behaviour of the autocorrelation time τ_e at $T_t(p)$. A glance on the log-log plot of Fig. 2 shows a qualitative change of the power-law behaviour for small p around $p = 0.80$. For weak disorder ($p \approx 1$), a clear exponential behaviour is observed, as one expects for a first-order transition where $\tau_e \propto \exp(2\sigma_{od}L^2)$, with the (reduced) interface tension σ_{od} parameterizing the free-energy barrier which separates the coexisting ordered and disordered phases.

Here we performed multicanonical simulations and estimated the interface tension from

$$\sigma_{od} = \frac{1}{2L^2} \log \frac{P_{\max}}{P_{\min}}, \qquad (3)$$

where $P_{\max}$ is the maximum of the probability density reweighted to the temperature where the two peaks are of equal height, and $P_{\min}$ is the minimum in between, see Fig. 3. The linear extrapolations of σ_{od} in $1/L$ in the lower part of Fig. 3 imply non-vanishing interface tensions only for $p = 0.84$ and above. For $p \leq 0.76$, σ_{od} seems to vanish in the infinite-volume limit, being indicative of the expected softening to a second-order phase transition. The tricritical point would thus be located around $p = 0.76 - 0.84$.

To confirm the softening for $p \leq 0.76$ we have performed a detailed FSS study at $p = 0.56$ with lattice sizes ranging up to $L = 96$ [12]. A log-log plot for $\bar{\chi}_{\max}$ shows that corrections to asymptotic FSS seem to become quite small above $L =$

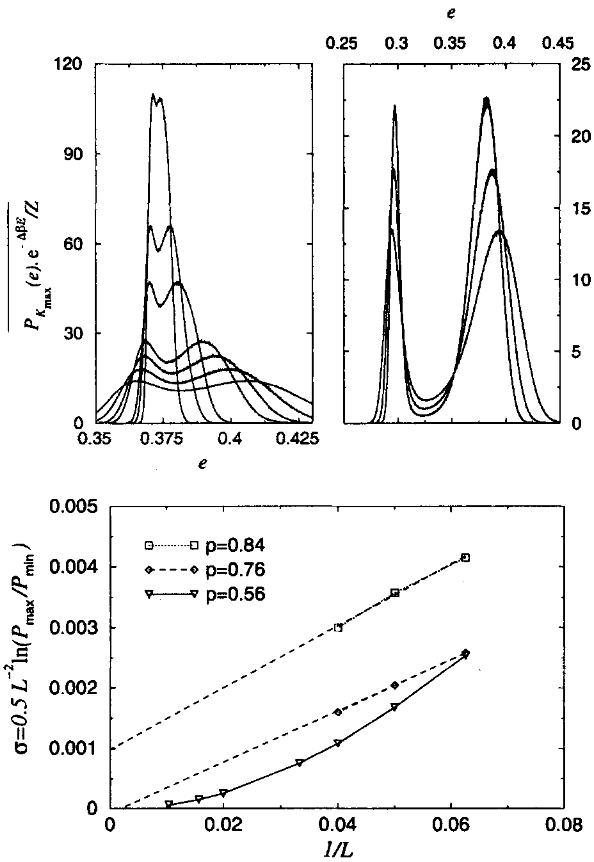

Figure 3. Probability density of the energy reweighted to equal peak height for $p = 0.56$ (top left) and $p = 0.84$ (top right). Interface tension versus inverse lattice size (bottom).

30, and linear fits of the form $a_\chi L^{\gamma/\nu}$ starting at $L_{\min} > 30$ yield $\gamma/\nu = 1.50(2)$. Similarly, the FSS of the quantity $(\partial_K \ln \bar{m})_{K_{\max}} \propto L^{1/\nu}$ gives an estimate of the exponent $1/\nu = 1.33(3)$, in agreement with the stability condition of the random fixed point ($1/\nu \leq D/2 = 1.5$). The same procedure was applied to the magnetization $\bar{m} \propto L^{-\beta/\nu}$, but here the associated critical exponent turned out to be not yet stable. We therefore also considered the FSS behaviour of higher (thermal) moments of the magnetization, $\overline{\langle \mu^n \rangle}$, which should scale with an exponent $n\beta/\nu$. The results for the first moments exhibit, however, again much stronger corrections to scaling than we observed for $\bar{\chi}$ or $\partial_K \ln \bar{m}$, leading to quite a conservative final estimate of $\beta/\nu = 0.65(5)$. We nevertheless note that our results do not fit satisfactorily the scaling law $2\beta/\nu = d - \gamma/\nu$.

4. CONCLUSIONS

From a large-scale Monte Carlo study of the 3D bond-diluted 4-state Potts model we obtain clear evidence for softening to a continuous transition at strong disorder, with estimates for the critical exponents of $\nu = 0.752(14)$, $\gamma = 1.13(4)$, and $\beta = 0.49(5)$ at $p = 0.56$. The analysis of both the autocorrelation time and the interface tension leads to the conclusion of a tricritical point around $p = 0.80$.

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