Influence of dilution on the strong first-order phase transition of the 3D 4-state Potts model

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Abstract

We investigate the phase diagram of the bond-diluted three-dimensional 4-state Potts model which undergoes a strong first-order phase transition in the pure case. We used standard large-scale Monte Carlo simulations with a cluster algorithm coupled to multicanonical methods in the regime of low dilution where the transition is supposed to be first order. We present strong numerical evidence for the existence of a tricritical point and we give an estimate of its location. © 2002 Published by Elsevier Science B.V.

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1. Introduction

The unavoidable presence of impurities in any experimental sample has motivated for several decades a lot of experimental and theoretical studies of the influence of disorder. Twenty-five years ago, Harris showed that quenched randomness modifies the universality class of a second-order phase transition only when the critical exponent α associated with the divergence of the specific heat of the pure system is positive [1]. This criterion has been checked experimentally many times as for example in the order-disorder transition of hydrogen adsorbed on the (111)-surface of nickel [2]. Randomness softens first-order phase transitions and may even turn a discontinuous transition into a con-

tinuous one [3]. Aizenman and Wehr showed that in dimension $d = 2$ an infinitesimal amount of disorder is sufficient to erase any discontinuity [4]. This was verified numerically for the q-state Potts model which undergoes in dimension $d = 2$ a first-order phase transition when $q > 4$ [5]. In higher dimensions ($d > 2$), a tricritical point may appear at a finite concentration of impurities, separating two regimes of discontinuous and continuous transitions. Such a tricritical point has been observed for the site-diluted 3-state Potts model in dimension $d = 3$ [6]. The pure system undergoes a very weak first-order phase transition which makes the determination of the location of the tricritical point very difficult. We therefore focused on the diluted 4-state Potts model which presents the advantage of exhibiting a strong first-order phase transition making clearly visible a regime of discontinuous transitions at low dilution.

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2. Model and simulation setup

More precisely, we studied the bond-diluted 3D 4-state Potts model defined by the following Hamiltonian:

$$-\beta H = \sum_{(i,j)} K_{ij}\delta_{\sigma_i,\sigma_j} \quad (\sigma_i = 0,\dots,3), \quad (1)$$

where the sum extends over all pairs of neighboring sites on the lattice and the couplings K_{ij} are distributed according to the distribution

$$\wp(K_{ij}) = p\delta(K - K_{ij}) + (1-p)\delta(K_{ij}). \quad (2)$$

The parameter p is thus the concentration of bonds in the system. $p = 1$ corresponds to the pure 3D 4-state Potts model which undergoes a strong first-order phase transition with a correlation length $\xi \simeq 3$ at the transition temperature [8]. One does not expect any finite-temperature phase transition for concentrations below the percolation threshold $p_c \simeq 0.2488$ since the absence of any percolating cluster in the system forbids long-range order. We considered all concentrations p multiple of 0.04 in the interval [0.28, 1].

The system is studied using large-scale Monte Carlo simulations with the Swendsen–Wang cluster algorithm [7], which reduces the critical slowing-down encountered at second-order phase transitions when local update algorithms are used. A regime of first-order phase transitions being expected at weak disorder, we checked that the number of Monte Carlo iterations were sufficient in the neighbourhood of the transition temperature to observe several tunneling events between the ordered and disordered phases. Nevertheless, once the transition point was approximately located, we then performed multicanonical simulations to get refined estimates of the free-energy barrier. Thermodynamic quantities were averaged over a large number of disorder realizations, between 2000 and 5000. The stability of the averages over randomness has been checked by plotting the averages with respect to the number of random samples. Indeed, a too small number of disorder realizations would lead to typical values instead of average ones [9]. These two values are different as can be seen in the probability distribution which presents a long tail that prevents the most probable event and the average one being the same.

3. Transition line

We defined the location of the maximum of the magnetic susceptibility as the transition temperature $T_t(L)$ for a given lattice size L. This choice was motivated by the observation that the specific heat presents larger error bars than the magnetic susceptibility and because the stability of a possible second-order regime implies a negative specific heat exponent (and thus a non-diverging specific heat) at the random fixed point. Canonical simulations for lattice sizes $L = 2$ to 16 have been performed for all concentrations p to get a rough estimate of the location of these maxima. Then a larger simulation combined with histogram reweighting was used to refine these estimates. The transition line is plotted in Fig. 1. Mean-field theory for the Potts model states that the transition temperature should be in any dimension a linear function of the number of neighbors, thus in the case of the bond-diluted Potts model proportional to the concentration of bonds p. Such a linear behaviour is indeed observed at weak disorder over a quite large interval of concentration, say [0.6, 1]. At stronger disorder, however, the mean-field approximation fails to reproduce the correct behaviour.

The phase diagrams of quenched bond disordered Ising and Potts models were studied by Turban [10] using an effective-medium approximation. Limiting the approximation to a single bond, the following estimate for the transition temperature is obtained:
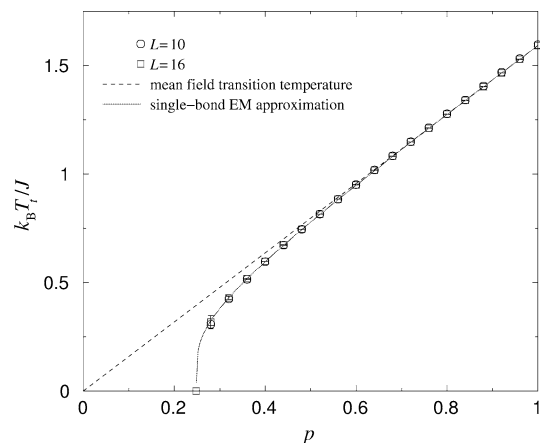

Fig. 1. Phase diagram of the bond-diluted 3D 4-state Potts model. The dashed line corresponds to the mean-field prediction and the solid line to an effective-medium (EM) approximation.

$$1/T_t(p) = \log\left[\frac{(1 - p_c)\mathrm{e}^{1/T_t(p=1)} - (1 - p)}{(p - p_c)}\right], \quad (3)$$

which is exact in the limits of the pure system ($p = 1$) and the percolation threshold ($p_c \simeq 0.2488$). As can be seen in Fig. 1, the transition line is extremely well reproduced by this approximation.

4. Nature of the transitions

In a second step, the order of the phase transition was investigated. A first insight is given by the behaviour of the autocorrelation time at the transition temperature with the lattice size. Indeed, the autocorrelation time is the characteristic time of the Monte Carlo dynamics that one can interpret as the number of iterations required to get two statistically independent spin configurations. When one uses local update algorithms, the Monte Carlo simulation is essentially a random walk in configuration space for a second-order phase transition, and the autocorrelation time is expected to behave like L^z with $z \simeq 2$. Cluster algorithms speed up the dynamics, i.e. reduce the dynamical exponent z. In the case of a first-order phase transition, a free-energy barrier separates the two phases in coexistence. The characteristic time of the dynamics is thus the tunneling time through this barrier. Tunneling is only possible by growing an interface between the two phases, thus the autocorrelation time grows exponentially with the energy σL^2 of this surface where σ is the interface tension.

The behaviour of the integrated autocorrelation time of the energy is plotted with respect to the lattice size and for all dilutions in Fig. 2. For weak disorder, a clear exponential behaviour is observed providing evidence for a first-order phase transition. At strong disorder, a power-law dependence is observed which is a signal for a continuous phase transition. As can be seen in Fig. 2, strong corrections to scaling seem to be present in the case of the concentration $p = 0.56$. One cannot exclude the possibility of a weak first-order phase transition for which the correlation length is larger than the considered lattice sizes, resulting thus in a continuous-like behaviour. Nevertheless, this would mean a correlation length at the transition temperature larger than $L = 96$ in the case of $p = 0.56$. A finite-size scaling study has been performed at $p = 0.56$ that gives critical exponents
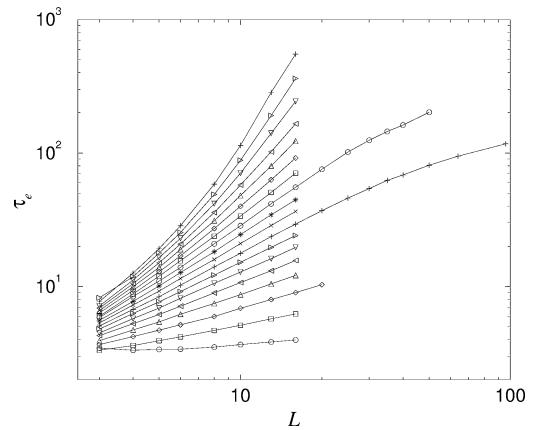

Fig. 2. Autocorrelation time of the energy τ_e at the transition temperature with respect to the lattice size L for all considered concentrations ranging from $p = 0.28$ (bottom) to $p = 0.96$ (top) in steps of 0.04.

clearly supporting the picture of a second-order phase transition [11].

We then performed large-scale multicanonical simulations in the supposed first-order regime for lattice sizes between $L = 13$ and 25 and calculated the interface tension as defined by:

$$\sigma = \frac{1}{2L^2} \log\frac{P_{\max}}{P_{\min}}, \quad (4)$$

where $P_{\max}$ is the probability at the top of the two peaks corresponding to the two coexisting phases and $P_{\min}$ that at the minimum of the gap between them. The simulations were performed at the transition temperature $T_t(L)$ previously determined. The collected data were then reweighted using the Boltzmann weight corresponding to the temperature for which the two peaks have equal height. It is then easier to apply Eq. (4) and define an interface tension. Fig. 3 presents an example of such a reweighting procedure. Preliminary results show an interface tension which is clearly vanishing for $p = 0.56$ as expected for a continuous transition. As presented in Fig. 4, a linear interpolation in $1/L$ of the data for $p = 0.84$ and $p = 0.76$ leads to the conclusion of a non-vanishing interface tension only for $p = 0.84$. The tricritical point would then be between $p = 0.76$ and $p = 0.84$. It is also around $p = 0.80$ that the autocorrelation times seem to switch from an exponential to a power-law behaviour. Nevertheless, data for larger lattice sizes would be necessary to confirm this picture but this would need a computation time unreachable for us.
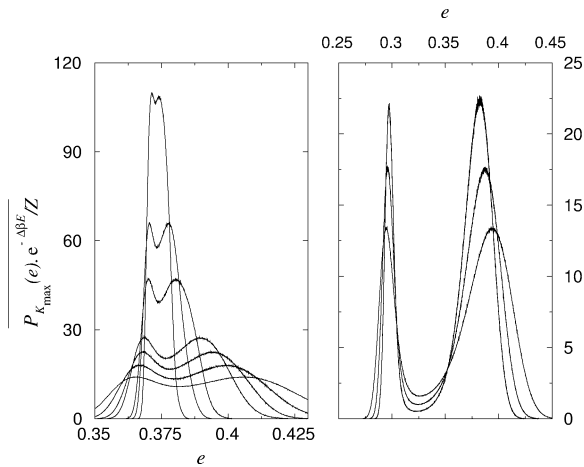
Fig. 3. Probability density of the energy reweighted at the temperature for which the two peaks have equal height. The two plots correspond to $p = 0.56$ (left) and $p = 0.84$ (right).
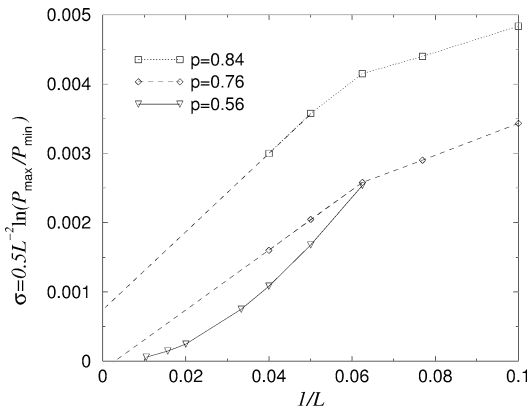

Fig. 4. Free-energy density barrier with respect to the inverse lattice size for three different concentrations.

5. Conclusion

We have presented a large-scale Monte Carlo simulation of the 3D bond-diluted 4-state Potts model. The strong first-order phase transition of the pure system is softened by randomness and clear evidence for a continuous transition at strong disorder is found. The analysis of both the autocorrelation time and the interface tension leads to the conclusion of a tricritical point around $p = 0.80$.

Acknowledgements

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