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Monte Carlo study of phase transitions in the bond-diluted 3D 4-state Potts model

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Abstract

Large-scale Monte Carlo simulations of the bond-diluted three-dimensional 4-state Potts model are performed. The phase diagram and the physical properties at the phase transitions are studied using finite-size scaling techniques. Evidences are given for the existence of a tricritical point dividing the phase diagram into a regime where the transitions remain of first order and a second regime where the transitions are softened to continuous ones by the influence of disorder. In the former regime, the nature of the transition is essentially clarified through an analysis of the energy probability distribution. In the latter regime critical exponents are estimated. Rare and typical events are identified and their role is qualitatively discussed in both regimes.

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1. Introduction

The influence of disorder is of great interest in physics, since pure systems are rare in nature. It has been known for more than thirty years that the universality class associated with a continuous phase transition can be changed by the presence of quenched impurities [1]. According to the Harris criterion [2], uncorrelated randomness coupled to the energy density can only affect the critical behaviour of a system if the critical exponent α describing the divergence of the specific heat in the pure system is positive. This has been established in the case of the q-state Potts model in dimension $D = 2$ for example. For $2 < q \leqslant 4$, the pure system undergoes a continuous transition with a positive critical exponent α. As predicted by the Harris criterion, new universality classes have been observed both perturbatively and numerically [3] (for a review, see Ref. [4]). The special case $q = 2$, the Ising model, is particularly interesting since in the pure system, the specific heat displays a logarithmic divergence ($\alpha = 0$) making the Harris criterion inconclusive [5]. Based on perturbative and numerical studies, it is now generally believed that the critical behaviour remains unchanged apart from logarithmic corrections when introducing randomness in the system [6]. In three dimensions (3D), the disordered Ising model was subject of really extensive studies (see, e.g., Ref. [7] for an exhaustive list of references).

Less attention has been paid to first-order phase transitions. It is known that randomness coupled to the energy density softens any temperature-driven first-order phase transition [8]. Moreover, it has been rigorously proved [9] that in dimension $D \leqslant 2$ an infinitesimal amount of disorder is sufficient to *turn any first-order transition into a continuous one*. The first observation of such a change of the order of the transition was made in the 2D 8-state Potts model [10] where a new universality class was identified [11,12]. For higher dimensions, the first-order nature of the transition may persist up to a finite amount of disorder. A tricritical point at finite disorder between two regimes of respectively first-order and continuous transitions is expected [11,13]. The existence of such a tricritical point for the site-diluted 3D 3-state Potts model could only be suspected by simulations because the pure model already undergoes a very weak first-order phase transition [14]. On the other hand, the first-order phase transition of the pure 5-state Potts model is very strong and would hence make it rather difficult to study the role of disorder. As a consequence, we have turned our attention to the 3D 4-state Potts model and have shown that there exists a second-order transition regime for this model [15]. Our choice of bond dilution is motivated by the fact that for this model only high-temperature expansions results are available up to now which to our knowledge cannot be done for site-dilution or are at least more difficult [16].

In Section 2 we define the model and the observables, and remind the reader of how these quantities behave at first- and second-order phase transitions. Section 3 is devoted to the numerical procedure, first the description of and then the comparison between the algorithms which are used at low and high impurity concentrations, followed by a first discussion of the qualitative properties of the disorder average. A short characterisation of the nature of the phase transition—at a qualitative level—is reported in Section 4. The motivation of this section is to first convince ourselves that the transition does indeed undergo a qualitative change when the strength of disorder is varied. Then, we describe how the phase diagram is obtained and concentrate on the first-order regime in Section 5. In