Critical behavior in the site-diluted three-dimensional three-state Potts model

H. G. Ballesteros* and L. A. Fernández†
Departamento de Física Teórica I, Universidad Complutense de Madrid, 28040 Madrid, Spain

V. Martín-Mayor‡
Departamento de Física Teórica I, Universidad Complutense de Madrid, 28040 Madrid, Spain and Dipartimento di Fisica, Università di Roma I ''La Sapienza'' and INFN, 00185 Roma, Italy

A. Muñoz Sudupe§
Departamento de Física Teórica I, Universidad Complutense de Madrid, 28040 Madrid, Spain

G. Parisi**
Dipartimento di Fisica, Università di Roma I ''La Sapienza'' and INFN, 00185 Roma, Italy

J. J. Ruiz-Lorenzo††
Departamento de Física Teórica I, Universidad Complutense de Madrid, 28040 Madrid, Spain
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We have studied numerically the effect of quenched site dilution on a weak first-order phase transition in three dimensions. We have simulated the site diluted three-states Potts model studying in detail the second-order region of its phase diagram. We have found that the ν exponent is compatible with the one of the three-dimensional diluted Ising model, whereas the η exponent is definitely different.

I. INTRODUCTION

The effect of impurities on the critical behavior of a pure material is an important issue, since frequently real systems cannot be considered as pure. Nowadays the effect of dilution (disorder coupled to the energy density) on second-order phase transitions is well understood. The phase transition keeps being second order, and the eventual modification of the universality class is governed by the specific heat divergence, as stated by the Harris criterion.[1] When the pure model shows a first-order phase transition the situation is more complicated. However, in two dimensions there is a set of important results, both numerical and analytical. For instance, Aizenman and Wehr[2] showed rigorously that when introducing disorder, its conjugated density becomes a continuous function of the thermodynamic parameters.

In three dimensions the scenario is different. Let us briefly describe a plausible phase diagram in the temperature–concentration plane (T,p) of a Potts spin system. The pure model undergoes a first-order phase transition, at a critical temperature $T_c(p=1)$, separating the paramagnetic high-temperature phase from the low temperature ordered one. This first-order transition can be, in principle, continued inside the (T,p) plane, where the critical temperature $T_c(p)$ will lower for smaller p. The latent-heat for the first-order phase transition will decrease until the tricritical point. At this point the model suffers a second-order phase transition that continues (belonging to another universality class) until the $T_c(p_c)=0$ percolation limit. We remark that this phase diagram would present three different universality classes: site percolation in three dimensions (which has been studied in the literature, e.g. in Ref. 3), the universality class of the tricritical point (conjectured in Ref. 4) and the universality class that controls the critical behavior in the line between the tricritical point and the percolation point.

In this paper we will restrict ourselves to the study of the second-order line. The three-state Potts model is a good choice since it presents a weak first-order transition in the pure version. In addition, the pure $q=3$ Potts model shows some experimental realizations appearing in very distant fields. We can cite the deconfining phase transition in quenched quantum chromodynamics or some systems in condensed matter physics. For instance, a cubic ferromagnet with three easy axes of magnetization when a magnetic field in the diagonal of the cubic lattice is turned on (e.g., $DyAl_2$), structural phase transitions (e.g., $SrTiO_3$), and some fluid mixtures of five (suitably chosen) components.[5]

Although an experimental realization of the site diluted Potts model is not yet known (disorder tends to couple with the order parameter rather than with the energy), whenever it will appear it will be interesting to have clear theoretical predictions at hand.

The techniques used in this paper are well suited for second-order transitions, but they should be modified in the concentration range for which the phase transition is first order. Nevertheless, the three state Potts model is difficult to study in this region, since an asymptotic behavior is only reached with very large lattices. Work is in progress[6] to study this region in a five-state Potts that presents, without dilution, a very stronger transition.

II. THE MODEL AND OBSERVABLES

We have studied the three-dimensional site diluted three-state Potts model, whose Hamiltonian defined on a cubic lattice with volume $V=L^3$ is

$$\mathcal{H}=\mathrm{Re}\left[\sum_{\langle i,j\rangle}\epsilon_i\epsilon_j z_i z_j^*\right], \tag{1}$$

and periodic boundary conditions are applied. In Eq. (1) z_i's are complex roots of $z^3=1$, and ϵ_i's are uncorrelated quenched random variables, which are 1 with probability p, and 0 with probability $1-p$. The Boltzmann weight is proportional to $\exp(-\beta\mathcal{H})$.

We have used clusters algorithms in order to update the system. In a diluted system, the set of occupied sites can present regions that are lightly connected to the percolating cluster. These regions are very difficult to equilibrate just with a single-cluster algorithm.[7] We have found that a single-cluster algorithm combined with a heat bath sweep per measure is efficient for large concentrations. However, for small concentrations ($p<0.6$) the previous method is not efficient enough due to the presence of intermediate-sized clusters, and we have used the Swendsen-Wang algorithm.[8]

We have simulated at $p=1.0$, 0.9, 0.8, 0.7, 0.6, 0.5006, and 0.4005 at $\beta=0.5505$, 0.6117, 0.690, 0.803, 0.969, 1.247, and 1.855, respectively, in lattices $L=8,16,32$, and 64. We will refer in the rest of the paper to the dilutions $p=0.4005$ and 0.5006 as $p=0.4$ and 0.5, respectively. For $p=0.8,0.7,0.4$ we have also run in $L=128$ lattices. We have performed $N_I=200$ nearly independent measures in every single disorder realization. For $p\leqslant 0.8$ the number of these realizations has been $N_S=10000$, except for $p=0.8$, $L=128$, where we have fixed $N_S=1000$. In the $p=0.9$ case we have measured in 2000 different disorder realizations. The total amount of CPU time has been the equivalent of 16 years of 200 MHz Pentium-Pro processor. For small dilutions we have performed the usual β extrapolation,[9] while for $p<0.6$ we used a p extrapolation method.[10] Let us recall that when planning a disordered model simulation, one should balance two competing effects. First, to minimize statistical errors, it is better to work in a $N_I\ll N_S$ regime. On the other hand, if N_I is too small, the usual calculation of β derivatives and extrapolations is biased. We follow the same procedure of Ref. 11 to eliminate the bias. With our simulation strategy ($N_I\ll N_S$), it is crucial to check that the system is sufficiently thermalized while taking measures. In order to ensure this, we have systematically compared the results coming from hot and cold starts: half of our statistics for the largest lattices have been obtained with hot starts, while the other half comes from cold starts.

Regarding the observables, in addition to the energy we have measured the complex magnetization and the (real) susceptibility as

$$M=\sum_i \epsilon_i z_i, \quad \chi=\frac{1}{V}\overline{\langle|M|^2\rangle}. \tag{2}$$

We have denoted with $\langle(\cdots)\rangle$ the thermodynamical average with fixed disorder and with $\overline{(\cdots)}$ the average over the disorder.

The formulas for the cumulants read

$$g_2=\frac{\overline{\langle|M|^2\rangle^2}-\overline{\langle|M|^2\rangle}^2}{\overline{\langle|M|^2\rangle}^2}, \tag{3}$$

$$g_3=\frac{\overline{\langle M^3\rangle}}{\overline{\langle|M|^2\rangle}^{3/2}}, \tag{4}$$

$$g_4=2-\frac{\overline{\langle|M|^4\rangle}}{\overline{\langle|M|^2\rangle}^2}, \tag{5}$$

g_4 being the standard Binder cumulant, g_2 measures whether the susceptibility is or not a self-averaging quantity, and g_3 has been introduced since the three-states Potts model is invariant under a global transformation of the Z_3 group. The other cumulants, g_2 and g_4, are also trivially invariant since we have used the modulus of the complex magnetization in their construction.

We have used a quotient method,[12] in order to compute the critical exponents. We recall briefly the basis of this method. Let O be a quantity diverging as t^{-x_O} (t being the reduced temperature) in the thermodynamical limit. We can write the dependence of O on L and t in the following way:

$$O(L,t)=L^{x_O/\nu}\left[G_O\left(\frac{\xi(L,t)}{L}\right)+\mathcal{O}(L^{-\omega})\right], \tag{6}$$

where G_O is a (smooth) scaling function and $(-\omega)$ is the biggest nonpositive eigenvalue of the Renormalization Group transformation (the corrections-to-scaling exponent). The definition of the correlation length on a finite box, $\xi(L,t)$, that we use is the second momentum one.[13]

The main formula of the quotient method is

$$Q_O|_{Q_\xi=s}=\frac{O(sL,t)}{O(L,t)}=s^{x_O/\nu}+\mathcal{O}(L^{-\omega}), \tag{7}$$

e.g., we compute the quotient between $O(sL,t)$ and $O(L,t)$ at the reduced temperature, t, in which $\xi(sL,t)/\xi(L,t)=s$. As particular cases of interest we cite the susceptibility, χ, and the β derivative of the correlation length, $\partial_\beta\xi$, whose associated exponents are

$$x_{\partial_\beta\xi}=1+\nu, \quad x_\chi=(2-\eta)\nu, \tag{8}$$

respectively.

A clean measure of scale invariance is provided by $(\xi/L)|_{Q_\xi=s}$. Let us recall that ξ/L is a monotonically growing function of the inverse temperature. In the ordered phase it grows as $L^{d/2}$, while in the disordered phase decreases with growing lattice size. Therefore, for any pair of lattice sizes, there is a crossing temperature where $Q_\xi=2$. In a second-order transition, ξ/L at the crossing point should tend to a nonvanishing universal value. For a first-order transition, the crossing temperatures tend to the transition point but ξ/L at the crossing diverges due to the coexistence of ordered and disordered phases.

We finally analyze the quotient of the cumulants g_2, g_3, or g_4 at two different lattices, L and sL, computed at the temperature where $Q_\xi=s$. Notice that for a second-order phase transition the asymptotic limit ($L\to\infty$) of these quotients is 1 corrected by terms like $L^{-\omega}$ [see Eq. (7)].

The quotient method, Eq. (7), has several interesting fea-

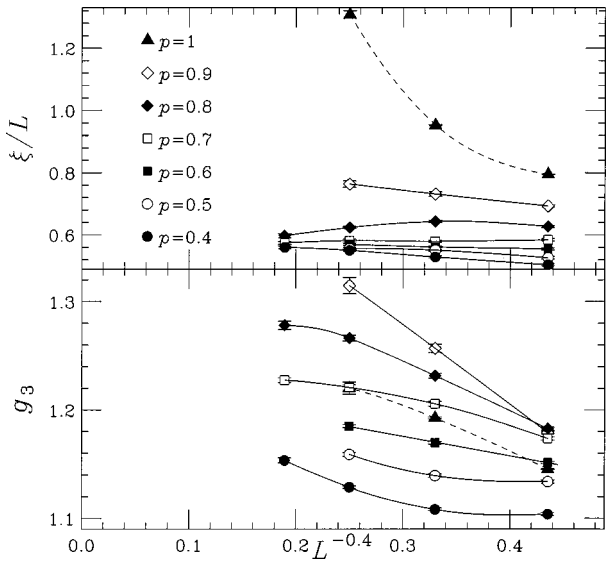

FIG. 1. The ratio ξ/L and the cumulant g_3 when $\xi(2L,t)=2\xi(L,t)$ as a function of $L^{-0.4}$ for different values of the concentration p.

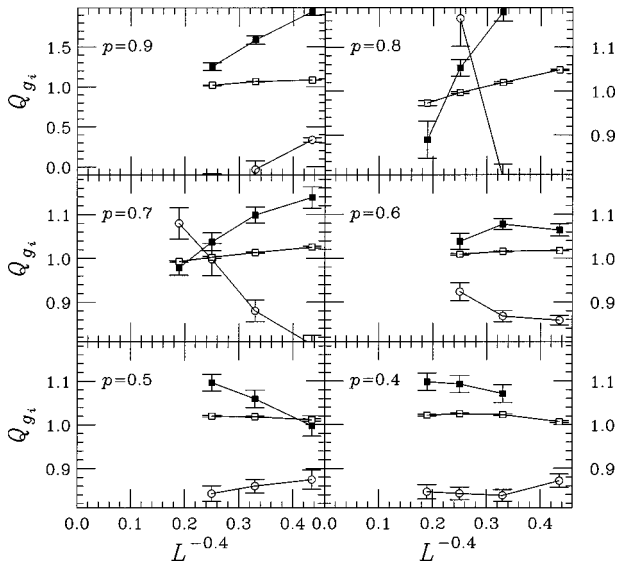

FIG. 2. Quotients of the cumulants g_2, g_3, and g_4 (filled squares, open squares, and open circles, respectively) as a function of $L^{-0.4}$. Notice the different y scale in the $p=0.9$ case.

tures. First, we profit of the large statistical correlation between Q_O and Q_ξ. Next, one does not need a previous estimate of the infinite volume critical point. Finally, it allows a simple control of the scaling corrections. All of this makes the method specially efficient for the measures of anomalous dimensions.

III. NUMERICAL RESULTS

Our scope is now to compute the critical exponents in the region in which the transition is clearly second order, i.e., the study of the universality class between the tricritical and percolation limits. The first stage is to determine where an asymptotic second-order behavior has been reached with lattice sizes up to $L=128$.

In Fig. 1 we show the value of ξ/L, at the points for which $Q_\xi=2$ for the different $(L,2L)$ lattice pairs and as functions of $L^{-\omega}$. We have used for ω the corresponding value of the site diluted Ising model.[14] For $p\leqslant 0.7$ we find that ξ/L seems to tend to a dilution-independent value. Notice the clear divergence for $p=1$, where the transition is known to be first order. For $p=0.9$ we find a similar trend that for the pure case, while for $p=0.8$ we find a transient behavior: for small lattices ξ/L grows, while in the largest lattices it seems to approach the universal value. We also guess from this figure that the ω value cannot be much larger than 0.4.

Another interesting quantity is the cumulant g_3 (lower part of Fig. 1). In this case we see a different scaling behavior por $p=0.9$ and $p=0.8$ up to the studied lattice sizes. We also guess that the ω value cannot be much larger than 0.4. We have next considered the quotients of the different cumulants g_i at the points where $Q_\xi=2$. We recall that these quantities should go to 1 as L tends to infinity in a second-order phase transition. We present our results in Fig. 2. At concentrations $p=0.9$ and $p=0.8$ we do not find an asymptotic behavior. For $p=0.7$, the behavior is not yet monotonous. Only for $p=0.4$, 0.5, and 0.6 it seems that the asymptotic behavior is reached. Unfortunately, a reliable estimate of ω cannot be obtained but our results point to a value near 0.4. Moreover, the higher-order scaling corrections are rather strong for these quantities. Finally, let us remark that the corrections to scaling and statistical errors are much larger for g_2 and g_4 than for g_3. Therefore, for the study the second-order region, we conclude that only for $p\leqslant 0.6$ an asymptotic scaling behavior for the considered lattice sizes has been found.

We report the results for the critical exponents as functions of p and L in Tables I and II. We have applied Eq. (7) with $s=2$ to $\partial_\beta\xi$ for computing ν and to χ for extracting η. We can observe that the asymptotic behavior of these estimates for $p\geqslant 0.7$ is not clear.

However, we have been able to extrapolate (using a $1/L$ law) the apparent critical exponents $\nu(L)$ and $\eta(L)$ for $p=0.4$, 0.5, and 0.6 to the infinite volume limit. We have obtained:

TABLE I. Apparent critical exponent ν, obtained from $Q_{\partial_\beta\xi}$ measured where $Q_\xi=2$ for all the concentrations studied.

L	$p=0.9$	$p=0.8$	$p=0.7$	$p=0.6$	$p=0.5$	$p=0.4$
8	0.571(4)	0.633(3)	0.662(4)	0.685(3)	0.706(4)	0.738(5)
16	0.592(7)	0.659(3)	0.686(3)	0.692(3)	0.698(4)	0.711(5)
32	0.664(12)	0.700(4)	0.695(4)	0.688(4)	0.694(4)	0.696(4)
64		0.711(13)	0.707(4)			0.692(4)

TABLE II. Apparent critical exponent η, computed using Q_χ, for all the considered concentrations.

L	$p=0.9$	$p=0.8$	$p=0.7$	$p=0.6$	$p=0.5$	$p=0.4$
8	0.048(2)	0.057(2)	0.065(2)	0.0745(15)	0.079(4)	0.072(4)
16	0.036(4)	0.045(2)	0.068(2)	0.0773(14)	0.079(2)	0.077(3)
32	−0.029(9)	0.050(3)	0.074(3)	0.077(2)	0.079(2)	0.077(3)
64		0.064(6)	0.071(3)			0.080(3)

$$\nu = 0.690(5), \quad \eta = 0.078(4). \tag{9}$$

We can compare this estimate for the critical exponents with that of the three-dimensional diluted Ising model: $\nu = 0.684(5)$ and $\eta = 0.037(5)$.[14] It is clear that the Potts value for ν agrees in the error bars with the Ising's value, but, on the contrary the η-values are definitively different.

From the extrapolation of the apparent critical exponents we can guess that $\omega = 1$ for the leading scaling-corrections term could be a reasonable choice in this case. We recall that we have found a $\omega \approx 0.4$ value for the cumulants. A possible explanation of this contradiction could be that for the observables used for computing the critical exponents the leading term ($\omega \approx 0.4$) vanishes. In any case we should remark that we have no precise control over the scaling corrections unlike, for example, in the investigation of the three dimensional site diluted Ising model.[14] Fortunately, the scaling corrections for the critical exponents are rather small. Thus, it is not essential in this model to perform an infinite-volume extrapolation of our estimates. This is in marked contrast with the Ising case, where the extrapolation procedure was crucial to correctly compute the critical exponents.

IV. CONCLUSIONS

We have numerically studied the three-dimensional site diluted three-state Potts model. The phase diagram in the temperature-concentration plane consists of a ferromagnetically ordered phase separated from a paramagnetic, high-temperature one. Between both regions there is a critical line, which is (weakly) first order in the limit of pure samples. For small concentrations, a clear second-order behavior is found, while the region with $p \gtrsim 0.9$ shows a different behavior, probably corresponding to a crossover, more difficult to analyze.

We have found that the exponents are dilution independent, and that they show a very mild evolution with the lattice size. That is why a sound estimate of the critical exponents can be given, in spite of the fact that we have been unable to measure the scaling-corrections exponent ω. This is in marked contrast with the situation in the site-diluted Ising model, where the scaling-corrections are severe but ω can be obtained with a 15% accuracy.

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*Electronic address: hector@lattice.fis.ucm.es
†Electronic address: laf@lattice.fis.ucm.es
‡Electronic address: victor@chimera.roma1.infn.it
§Electronic address: sudupe@lattice.fis.ucm.es
**Electronic address: giorgio.parisi@roma1.infn.it
††Electronic address: ruiz@lattice.fis.ucm.es

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