Effects of quenched disorder in the two-dimensional Potts model: A Monte Carlo study

Ricardo Paredes V.[1] and Johnny Valbuena[2]
[1]*Laboratorio de Física Estadística de Sistemas Desordenados, Centro de Física, IVIC, Apartado 21827, Caracas 1020A, Venezuela*
[2]*PDVSA Intevep, Apartado 76343, Caracas 1070A, Venezuela*
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Motivated by recent experiments on phase behavior of systems confined in porous media, we have studied the effect of randomness on the nature of the phase transition in the two-dimensional Potts model. To model the effects of the porous matrix we introduce a random distribution of couplings $\mathcal{P}(J_{ij})=p\,\delta(J_{ij}-J_1)+(1-p)\,\delta(J_{ij}-J_2)$ in the q state Potts Hamiltonian. An extensive Monte Carlo study is made on this system for $q=5$. We studied two different cases of disorder (a) $J_1/J_2\to\infty$ and $p=0.8$ and (b) $J_1/J_2=10$ and $p=0.5$. We observed, in both cases, that the weak first order transition that appears in the pure case, changes to a second-order transition. A finite size scaling analysis shows that the correlation length exponent ν is close to 1 and the best fit to the dependence of the specific heat on system size is logarithmic. This suggests that both cases belong to the universality class of the Ising model. In contrast, the magnetic exponents point to a different universality class. [S1063-651X(99)02204-7]

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I. INTRODUCTION

During the past few years a great deal of effort has been devoted to the study of the effect of quenched randomness on phase transitions [1–10,12–28]. Bond and field randomness can produce drastic effects in a phase transition. For example, critical exponents change in systems with positive heat capacity exponent α if bond randomness is introduced [1]. Schwenger *et al.* [2] found experimentally that the order-disorder phase transition of the (2×2)-$2H$ structure on Ni(111) yields critical exponents for the pure layers which are compatible with those of the four-state Potts universality class ($\alpha>0$). Nevertheless, they found that these critical exponents are modified when the system has 3% of preadsorbed atomic oxygen, resulting close to those of the Ising universality class. Additionally, it has been argued that the introduction of quenched bond randomness has drastic effects on all temperature driven first-order phase transitions [3]. There is also some experimental evidence that disorder produced by porous media affects phase transitions of systems within them. An extensive study of the isotropic to nematic phase transition of nCB liquid crystals in aerogel shows that the transition temperature is lowered compared to the pure situation, and that the order of this transition changes from first to second [4–7]. The same effect has been observed in ^{3}He-^{4}He mixtures in aerogels [8]. Using renormalization group calculations [9] and Monte Carlo simulations [10] Falicov *et al.* explained the latter experiment introducing bond randomness in a lattice model of ^{3}He-^{4}He mixtures.

The q-state Potts model [11] is a simple model that, depending on q, exhibits temperature-driven first or second order phase transitions. For this reason it has been a good candidate to study the influence of quenched disorder on phase transitions. The random bond [13–27] and the random field [28] Potts model have been studied recently using, mainly, double peak distributions of couplings and magnetic field, respectively.

Most recent works have focused on disorder where couplings can get any of two finite values J_1 and J_2 with equal probability. The strength of the disorder is given by the ratio of the two values $r=J_1/J_2$ [14–21]. The system in this case is, on average, self-dual. The main advantage of such a choice is that the critical temperature can be obtained analytically, leaving one less parameter to fit. In this paper, the system with this type of disorder will be called the self-dual (SD) model and in the following the main results reported using this model will be summarized.

Chen *et al.* made an extensive Monte Carlo study on the random-bond eight-state Potts model in two-dimensions (2D) [14,15]. They found a second-order phase transition instead of the first-order one found in the pure case. Additionally, they found that this second-order transition belongs to the same universality class as the pure Ising model. Wiseman and Domany arrived at the same result for the random-bond Ashkin-Teller and four-state Potts model finding that the specific heat has a logarithmic type divergence at criticality [16].

Recently Chatelain and Berche [17] reported results for large-scale Monte Carlo simulations on the SD random-bond eight-state Potts model. They found, contradicting Chen and collaborators, that the exponents γ/ν and β/ν are quite different from the Ising values. Their results are closer to the prediction made by Cardy and Jacobsen [18] using transfer matrix methods. In this last work, it was reported that the ratio β/ν changes to a value different to that of the Ising model, and depends continuously on q. They also obtained that the correlation length exponent ν is consistent, within error bars, with the pure Ising values.

Kim [19] reported the results of Monte Carlo simulations on the $q=3$ random-bond Potts model using the SD model with r equal to 10/9, 2, and 4. He concluded that, while the ratios γ/ν and β/ν remain unchanged, the exponents ν, γ and β change continuously with the strength of disorder. In the same year, Picco [20] reported results of Monte Carlo simulations on the same system as Kim but with stronger disorder ($r=10$) and he found that while the values of β/ν and γ/ν do not change significantly from the pure case, the value of ν is clearly different.

The strong disorder limit for the SD model was

TABLE I. The table shows the number of samples used in the simulations. RD denotes the random dilution model and SD the self-dual model. The first set of simulations for the RD model (first row) were used to estimate the critical coupling J_c using histogram techniques [31].

Lattice size	12	16	24	32	48	64	96	128	192	256	512
RD		287	288	166	137	194	43	43			
RD (J_c)		180	360	180	358	90	179	90	92		
SD (J_c)	899	899	979	998	799	400	450	399	204	151	91

studied theoretically by Coniglio [21] some time ago. He analyzed the random diluted q-state Potts model in any dimension at the percolation threshold. On a square lattice, this is the SD model in the limit $r\to\infty$. He found that the Potts thermal exponent ν equals the percolation correlation length exponent ν_p when $T\to T_c=0$.

Random quenched impurities and its effect on the Potts model is another case discussed in the literature. In an earlier work, Novotny and Landau [22], using Monte Carlo simulations, studied the effects of impurities on the Baxter-Wu model. In the absence of disorder the latter model is in the same universality class as the four-state Potts model. Introducing disorder in the form of random dilution caused drastic effects in the critical behavior, changing the critical exponents upon the addition of only a few impurities. They found that this random Baxter-Wu model possibly belongs to the same universality class as the Ising model.

In 3D Uzelac *et al.* [23] performed Monte Carlo simulations to study the three- and four-state Potts model with impurities. These models have temperature driven first-order phase transition for the pure case. In their simulations, lattice sites were eliminated according to a dilution model emulating (a) the structure of aerogels and (b) site percolation. They found, in both cases, a change in the order of the transition only if a finite amount of disorder was present. They also observed that the new specific heat exponent is close to the Ising value. In Refs. [22] and [23] the Potts lattice sites do not interact with the impurities. That is, the ratio r between couplings tends to ∞. In both references the fraction of impurities are far away from the percolation threshold.

Monte Carlo simulations reported using a model of disorder different to that of the SD model have given rough estimates of the critical exponents and in general disagree with the SD results [22,23]. For this reason it is really important to do intensive Monte Carlo simulation studies considering other disorder models. In what follows, we describe our results using a random dilution bond model with a ratio $r\to\infty$ but with a fraction of nonzero couplings equal to 0.8. We chose an intermediate value to reduce finite size effects close the pure case ($p=1$) [26,27] and strong fluctuations close the percolation threshold ($p=0.5$). Traditionally, in $d=2$, Monte Carlo studies for the random bond Potts model, have been performed in the second order region ($q\leqslant 4$) or in the strong first-order region ($q=8$). We focused the $q=5$ Potts model exhibiting a weak first-order phase transition. To compare with the previous reported results, an extensive Monte Carlo study for the SD model was also considered.

In the next section we discuss the random-bond Potts model used. Then, in Sec. III we discuss the finite size scaling methodology followed by us to estimate the exponents. In Sec. IV, the results are discussed and finally, in the last section, we draw conclusions.

II. THE RANDOM-BOND POTTS MODEL

The q-state Potts model [11] is described by the Hamiltonian

$$-\beta H=\sum_{\langle ij\rangle} J_{ij}\delta_{s_i s_j}, \tag{1}$$

where $\beta=1/k_BT$. The spin s can take the values $1,2,\ldots,q$ and δ is the Kroneker delta function. The sum runs over all nearest-neighbor bonds in the system and J_{ij} is the strength of the interaction between s_i and s_j. In a pure system, J_{ij} is constant for all bonds. The q-state Potts model is a simple generalization of the Ising model which has the advantage of exhibiting first-order phase transitions for $q>q_c(d)$ and second-order transitions for $q\leqslant q_c(d)$. In two dimensions ($d=2$), q_c is equal to 4 and in three dimensions ($d=3$), q_c is equal to 2.

The random-bond Potts model used is described by the above Hamiltonian with couplings randomly selected from the distribution

$$\mathcal{P}(J_{ij})=p\,\delta(J_{ij}-J)+(1-p)\,\delta(J_{ij}-rJ). \tag{2}$$

We studied two different cases: the most commonly used, $p=0.5$ and $r=10$ (or SD model) and the random dilution (RD) case where $r\to\infty$ and $p=0.8$. The advantage of the SD model is that the critical value of J can be derived by duality relations. In particular the critical value J_c can be obtained solving the equation [29]

$$(e^{J_c}-1)(e^{rJ_c}-1)=q. \tag{3}$$

III. METHODS

We performed extensive simulations of $L\times L$ lattices with periodic boundary conditions using the Swendsen-Wang multiple spin flip method [30]. Histogram techniques were used to determine several thermodynamic quantities over a range of J [31]. For each distribution of couplings 2×10^5 Monte Carlo steps per spin were performed. This number of steps is 10^4 times the correlation time, enough to produce reliable thermal averages. The number of disorder realizations performed for each model and lattice size are displayed in Table I. Due to fluctuations smaller lattice sizes require larger number of configurations.

The configurational average value of a thermodynamic quantity A is obtained by first calculating the thermal average

$\langle A\rangle$ for a given disorder configuration, and then averaging over the bond distribution

$$[\langle A\rangle]=\frac{\sum_{i=1}^{N_\sigma}\langle A\rangle}{N_\sigma}, \tag{4}$$

where N_σ is the number of bond configurations. We denote the configurational average by $[\langle A\rangle]$.

As in previous works, the order parameter for the Potts model has been taken as

$$M=\frac{q\rho-1}{q-1}, \tag{5}$$

where

$$\rho=L^{-d}\max(M_1,M_2,\ldots,M_q) \tag{6}$$

and M_j is the number of spins in state j [14,17,19]. We computed the moments of the magnetization $\langle M\rangle$, $\langle M^2\rangle$, and $\langle M^4\rangle$ and used their values at the critical J_c to obtain the exponent combination given by

$$[\langle M^k\rangle(J_c)]\propto L^{k\beta/\nu}. \tag{7}$$

Using these momenta we also calculated the magnetic susceptibility

$$\chi_L(J)=JL^d(\langle M^2\rangle_L-\langle M\rangle_L^2). \tag{8}$$

The magnetic susceptibility maximum and its value at J_c scales as

$$[\chi_L(J_c)],[\chi_{L,\max}]\propto L^{\gamma/\nu}, \tag{9}$$

permitting the evaluation of γ/ν.

To compute the correlation length exponent we estimated the logarithmic derivatives of an integer power of the order parameter M,

$$\frac{\partial\ln\langle M^n\rangle}{\partial J}=\frac{\langle M^nE\rangle}{\langle M^n\rangle}-\langle E\rangle, \tag{10}$$

where $E=\Sigma_{\langle ij\rangle}\delta_{sisj}$. The configurational averages of these derivatives scale with system size as $L^{1/\nu}$ [32], which allows us to directly calculate the correlation length exponent ν.

We also calculate the specific heat which involves the variance of the energy distribution

$$C_L(J)=\left(\frac{J}{L}\right)^2(\langle E^2\rangle_L-\langle E\rangle_L^2). \tag{11}$$

According to finite size scaling theory, the maximum of the specific heat and its value at J_c scale with system size as

$$[C_{L,\max}],[C_L(J_c)]\propto L^{\alpha/\nu}. \tag{12}$$

For a first order transition, the specific heat grows as L^d, so a measure of the scaling behavior of C will provide additional evidence of the order of the transition.

To calculate the critical temperature for the RD model we used the finite size scaling relation

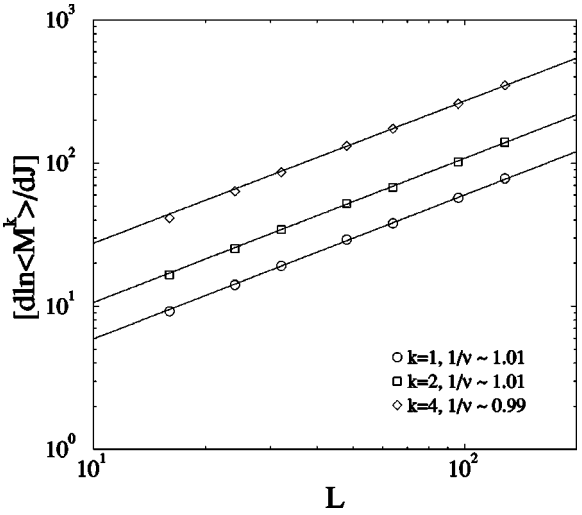

FIG. 1. The maxima of the logarithmic derivatives of powers of the order parameter M versus system size L for the random dilution model (RD). The correlation length exponent obtained from the fit of the momenta $k=1$ and $k=2$ do not follow the inequality shown in Eq. (15). This is, presumably, due to finite size effects.

$$J_c=J_c(L)+aL^{-1/\nu}(1+bL^{-\omega}), \tag{13}$$

where $J_c(L)$ is identified by the position of the maxima of the specific heat, the magnetic susceptibility, the logarithmic derivatives of the moments of the magnetization or the position of the minimum of the Binder cumulant [33]

$$V_B=1-\frac{\langle E^4\rangle}{3\langle E^2\rangle^2}. \tag{14}$$

IV. RESULTS AND DISCUSSION

The correlation length exponent was obtained from Eq. (10). For the RD model the maxima of these derivatives as a function of L are estimated using histogram techniques. Then, configurational averages are taken. Figure 1 depicts the dependence of these quantities on the system size. The behavior is asymptotically a power law and the exponent obtained fitting the curves are close to the Ising value $\nu=1$. It is clear that some corrections to scaling should be included because the value obtained for the correlation length exponent does not follow, exactly, the inequality [34]

$$\nu\geqslant 2/d, \tag{15}$$

where d is the space dimension. The exponent obtained averaging the results corresponding to each one of the moments is $\nu=1.00\pm0.01$.

Using the same procedure, the maxima of the specific heat, the magnetic susceptibility and the minimum of the Binder cumulant are estimated for the RD model. Additionally, the corresponding J_x values for these extreme values are obtained. In Fig. 2 we show the dependence of J_x as a function of $L^{-1/\nu}$, taking $\nu=1$. A regression using the expression given in Eq. (13) is shown in the figure as continuous lines. The value estimated using this regression is $J_c=1.564\pm0.001$. This result agrees qualitatively with numerical results reported previously [26]. In this reference, a linear

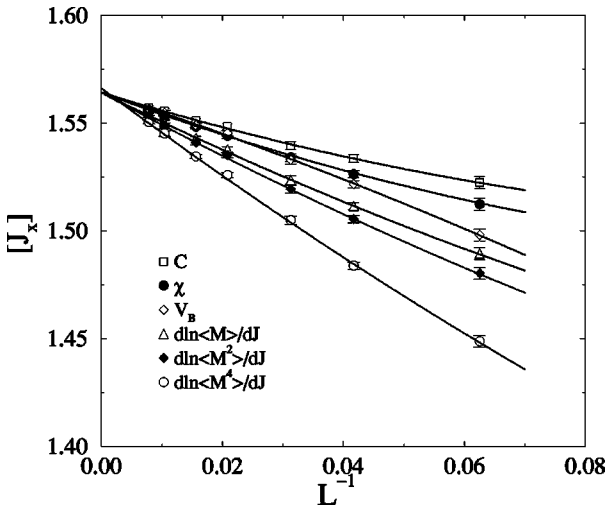

FIG. 2. The position of the maxima of the specific heat C, magnetic susceptibility χ, $d\ln\langle M^k\rangle/dJ$, and the minimum of the Binder cumulant V_B versus $L^{-1/\nu}$ for the random dilution model. The correlation length exponent is assumed to be 1. The continuous lines are the fit of the data to Eq. (13). The critical coupling obtained by taking the limit $L\to\infty$ is $J_c=1.564\pm0.001$.

behavior $1/J_c(p)=p/J_c(1)$ was observed close to $p=1$. On the other hand, when p is decreased the critical coupling tends to be larger than what the linear formula predicts. Far away from the percolation threshold p_c a mean field result is expected. In contrast, when p tends to this critical value the critical coupling increases systematically [23] and should approach infinity at p_c. For the SD model the critical coupling J_c is calculated exactly from Eq. (3). The value obtained is $J_c=0.2801273049\cdots$.

In Fig. 3 we plot the derivatives of the logarithm of the moments $k=1,2,4$ of the magnetization at J_c, versus the system size, for the SD and RD models. The exponent obtained using the maxima of these quantities for the RD model, are confirmed. The average value of the correlation length exponent fitting the data shown in Fig. 3 (RD) is $\nu=1.00\pm0.01$, that is, the same value as in the pure Ising

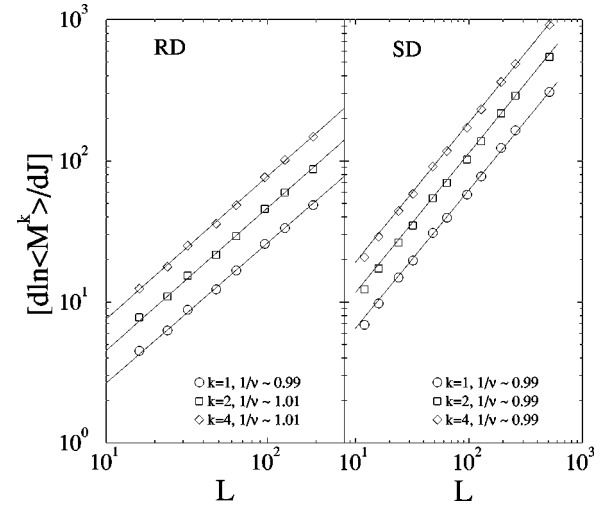

FIG. 3. $d\ln\langle M^k\rangle/dJ$ at the critical coupling J_c versus system size L for the random dilution and the self-dual models . The correlation length exponent obtained by fitting is close to 1 for both types of disorder.

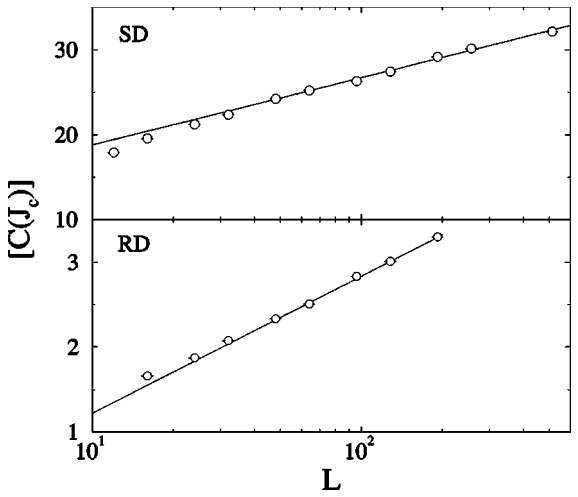

FIG. 4. The specific heat C at the critical coupling J_c versus system size L for the random dilution and the self-dual models. The continuous lines represent a logarithmic fit to the data. It is possible to fit the data using a power law function but a better fit is obtained by using $C\sim\ln L$. Additionally, in this way the hyperscaling relation given by Eq. (16) is satisfied.

model. On the other hand, for the SD model, the value obtained is $\nu=1.01\pm0.01$ [see Fig. 3 (SD)].

In Fig. 4 we show a plot of the specific heat at J_c versus L. $[C(J_c)]$ has a logarithmic behavior in both RD and SD models. The solid lines in the figure represent linear regressions for $L\geqslant48$. It is clear that finite size effects are present in the data. Obviously, it is possible to fit the data using a power-law function. However, to be consistent with the hyperscaling relation

$$\alpha=2-d\nu, \tag{16}$$

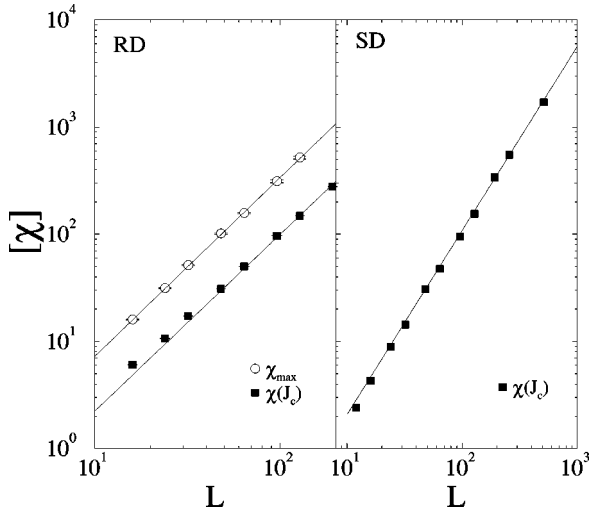

FIG. 5. The magnetic susceptibility χ at J_c versus system size L for the random dilution and the self-dual models. Additionally, the susceptibility maximum vs L is shown for the RD model. Power law fits to each of the data sets are shown as continuous lines. RD model: the values obtained from the fit are $\gamma/\nu=1.67\pm0.05$ and $\gamma/\nu=1.6\pm0.1$ for $\chi_{\max}$ and $\chi(J_c)$, respectively. These results are clearly different for the corresponding Ising value (1.75). SD model: the exponent obtained is $\gamma/\nu=1.72\pm0.01$ for $\chi(J_c)$. This value is closer to 1.75 but the tendency of the curve is that in the limit $L\to\infty$ a lower value must be obtained.

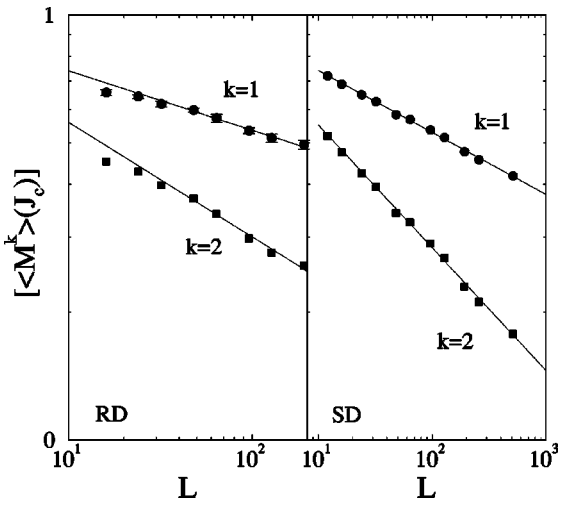

FIG. 6. The momenta $k=1$ and $k=2$ for the magnetization M at J_c versus system size L for the random dilution and the self-dual models. Power-law fits to each of the data sets are shown as continuous lines. The values obtained from the fit are $\beta/\nu=0.14 \pm 0.01$ and $\beta/\nu=0.146\pm 0.001$ for the RD and SD models, respectively. These results are clearly different for the corresponding Ising value (0.125).

and with the result for the correlation length exponent shown before, a logarithmic behavior should be expected. We then conclude that the results for α and ν for the five-state random bonds Potts model point to the Ising model universality class. Such conclusion is independent of the type of disorder used in the simulations.

The question now is what happens with the magnetic exponents? We now estimate the susceptibility and the magnetization exponents γ and β and check the hyperscaling relation

$$d\nu=2\beta-\gamma. \tag{17}$$

The scaling of the magnetic susceptibility is shown in Fig. 5 for the RD and SD models. For the RD model the exponent γ/ν is estimated in two different ways. First, using the maxima obtained from the histogram technique and second, simulating the system at the J_c estimated previously. The exponent obtained are, respectively, $\gamma/\nu=1.67\pm 0.05$ and $\gamma/\nu=1.6\pm 0.1$. Figure 5 (RD) depicts the results of the simulation and the fit using the data for $L\geqslant 48$. The results are clearly different from the Ising values ($\gamma/\nu=1.75$). For the SD model the simulations were performed at the theoretical critical value J_c and the value obtained is $\gamma/\nu=1.72\pm 0.01$. The value is close to the Ising one, but working out the data and the fit in Fig. 5 (SD), the tendency of the exponent is to separate from the corresponding Ising value. As you fit taking into account more of the larger L behavior the exponent decreases.

Figure 6 shows the magnetization and its second moment at J_c, versus the system size L. The results from the fit with a power law are $\beta/\nu=0.14\pm 0.01$ for the RD model and $\beta/\nu=0.146\pm 0.001$ for the SD model. Both results are clearly different from the Ising value $\beta/\nu=0.125$. All the regressions were made for $L\geqslant 48$, observing the finite size effects for the RD model [see Fig. 6(RD)]. Again, the results tend to separate from the Ising value. The hyperscaling relation given in Eq. (17) is satisfied, within error bars, for the RD and the SD models. In Table II we show a summary of the results for the exponents.

TABLE II. The table summarizes the results obtained in this work and their comparison with the corresponding Ising values. The results from the RD model come from the average of exponents obtained using the maxima of the associated thermodynamic quantities (histogram techniques [31]) and from simulations at the estimated value of J_c. The SD exponents come from simulations at the critical coupling J_c calculated from Eq. (3). The $\alpha/\nu=0$ results assume a logarithmic scaling behavior for the specific heat (best fit).

Exponent	ν	α/ν	γ/ν	β/ν
RD	1.00 ± 0.01	0 ($\log L$)	1.64 ± 0.08	0.14 ± 0.01
SD	1.01 ± 0.01	0 ($\log L$)	1.72 ± 0.01	0.146 ± 0.001
Ising	1	0 ($\log L$)	1.75	0.125

V. CONCLUSIONS

From the results above it is clear that introducing bond randomness, in the $q=5$ Potts model, changes the nature of the transition. The weak first-order transition observed in the pure case changes to a continuous one. The presence of disorder also decreases the transition temperature as seen in liquid crystal systems. The results obtained for the correlation length ν and specific heat α exponent are close to the corresponding Ising values. To be sure that the specific heat behavior is logarithmic one must be able to go to larger system sizes. However, the magnetization and susceptibility exponents β and γ clearly indicate that the random bond Potts model belongs to a universality class other than the Ising model. This conclusion is reached for both types of disorder used in the present work. The change observed in the magnetic exponent follows the tendency reported by Cardy and Jacobsen [18] and agrees qualitatively with Monte Carlo simulations performed for the $q=8$ SD Potts model [17]. The random dilution model was difficult to simulate because the critical coupling must also be estimated. However, it is clear for our simulations, that the tendency is that random magnetic exponents γ and β are different from the corresponding exponents of the Ising model. These results disagree with the Monte Carlo simulations performed for the Potts model with random impurities [22,23] and with the experimental results of Schwenger and collaborators [2]. We assume that the discrepancy is due to the small sizes simulated in the previous numerical works. On the other hand, if one watch carefully the experimental results it will be noticed that the exponents reported by us fall inside the experimental errors. In conclusion, regardless of the type of disorder considered, the five-state random bond Potts model belongs to a new universality class.

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