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SECOND-ORDER PHASE TRANSITION INDUCED BY THE QUENCHED RANDOM DILUTION IN 3D

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Dedicated to Professor Boran Leontić on the occasion of his 70$^{\text{th}}$ birthday

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The effect of the quenched random dilution on the ferromagnetic transitions, in particular, the conversion from the first- to second-order transition is discussed. The new results are presented for the diluted three-dimensional three-state Potts model. The critical exponents of the disorder-induced second-order phase transition are derived by the finite-size scaling analysis of the moments of the energy and the largest cluster, obtained from the Monte Carlo simulations.

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1. *Introduction*

Over the past few years considerable attention has been turned to the effect of quenched random dilution on the phase transitions. Although the quenched randomness has for a long time been primarily discussed in the context of antiferromagnetic models, spin glasses, and competing interactions, a renewed interest has emerged for quenched disorder in models with purely ferromagnetic interactions. Many questions are still open, such as the consequences of strong disorder, the possibility of new disorder fixed points, and the related critical behaviour, to the extent that even the question of the critical behaviour of the dilute Ising model still has not been settled [1]). One of the problems which drew the attention recently is the striking effect of the change from the first- to second-order phase transition in presence of disorder.

From the experimental point of view the study of quenched random dilution is of obvious interest for understanding properties of the diluted magnetic materials, and, more generally, for dealing with the random inhomogeneities existing in all real materials. However, these studies were recently motivated by intensive and growing experimental activity focused on the phase transitions of fluids in confined media such as the aerogels, the highly porous silica glasses [2]. Such systems may be described with models where the particles of aerogel play the similar role as the quenched non-magnetic impurities within magnetic materials. Among other new phenomena, the broadening of the first-order phase transition, or its change to the second-order one was observed in extensive studies of the isotropic to nematic phase transition in nCB liquid crystals in aerogels [3] and also in the ^{3}He – ^{4}He mixtures in aerogels [4].

The idea that quenched disorder may change the first-order transition significantly and even lead to a continuous one was already formulated by Imry and Wortis in 1979 [5]. The Harris criterion [6], usually applied to determine the relevance of weak disorder to the second-order phase transitions from the positive sign of α, the critical exponent of the specific heat in the pure case, is not applicable when the transition in pure model is of the first order.

A phenomenological argument [7,8] which explains the onset of a second-order phase transition induced by randomness was presented for the case of a temperature-driven first-order phase transition with symmetry breaking. The underlining mechanism is the suppression of the interface free energy by a quenched disorder and is exactly opposite to the mechanism which explains the onset of the first-order phase transition in the pure q-state Potts model, by introducing vacancies as an annealed disorder [9,10]. The argument was supported by the renormalisation-group calculations [11,7] and also by independent rigorous results by Aizenman and Wehr [12]. Both approaches also show that the effect strongly depends on dimensionality d of the system, and that, in discrete models, an infinitesimal amount of disorder is sufficient to produce the conversion to the second-order transition when $d \leq 2$. In higher dimensions the conversion is still produced, but provided that some threshold amount of disorder is present.

These works have opened an intriguing question about the critical properties of the new second-order phase transition and its class of universality.

Among the arguments of general type, there is a rigorous result by Chayes et al. [13], derived on similar grounds as the Harris criterion, but which concerns the disorder fixed point instead. It requires that, in presence of disorder, the correlation length critical exponent ν obeys the inequality $1/\nu \leq d/2$.

The new transition was further explored in series of works, which were almost all done in two dimensions and on the Potts model, which is often taken as a paradigm in studies of a temperature-driven first-order phase transition. Its advantage in 2d are the analytic solutions for the pure case and the exact expressions for the critical temperature T_c and the critical exponents [14]. Furthermore, self-dual transformations for this model give the exact expression for T_c even for certain classes of random interactions [15]. For these reasons most of the studies were performed for a bimodal random bond distribution. However, the choice between site, or bond randomness, or random dilution, should not be of relevance for the critical behaviour alone as long as the frustration is absent.

The early Monte-Carlo (MC) simulations that have reproduced the effect on the 2d 8-state Potts model [16] support, together with some other works [17–19], the assumption that the new critical behaviour should be Ising-like, irrespective of the underlying symmetry.

More detailed analyses of the same models performed by MC simulations in combination with finite-size scaling (FSS) [20,21], by renormalisation-group (RG) [22,23], or by transfer-matrix and conformal invariance techniques [24–30] contradict this statement. They obtain clear continuous variation with q of the magnetic critical exponent β/ν, responsible for the correlation function decay at T_c, while the temperature critical exponent ν depends on q very weakly and is quite close to the Ising value, within the error limits.

It has been pointed out by many authors that in all the approaches used the important role is played by the disorder strength, which can be partially accounted for the contradictory results. The recent thorough analyses by Picco [25] show crossover effects due to the competition between the stable disorder fixed point and the two unstable fixed points corresponding to the pure system or the percolation limit [31] when the disorder strength is varied.

Although it has been shown that the new transition is a genuine second-order phase transition it has some peculiarities due to disorder. One of them is the lack of self-averaging of certain thermodynamic quantities at T_c [32–36], the effect otherwise characteristic for the low-temperature phase of spin-glasses. This has several consequences not yet completely investigated.

It was argued [34, 35] that, in the case of absence of self-averaging, the rigorous inequality by Chayes et al. may not hold since it is related to the finite-size correlation length and not the actual correlation length.

The absence of self-averaging leads also to the multifractality of local operators, which in the 2d Potts model with quenched randomness is found both for $q < 4$ [37–39] and for $q > 4$ [40]. In this later case, Olson and Young present, on the example of 8-state Potts model, the multi-fractal behaviour of the magnetic critical exponent and only a single temperature exponent ν, close to the Ising value.

Cardy and Jacobsen [23, 41] have given an appealing and new prospect to the problem of the first-order transition with quenched disorder by mapping it to the random-field Ising model, in general dimension. They have studied the interface energy by the perturbation RG approach establishing the correspondence between the latent heat and the magnetisation of these models, respectively. The fact that the random field destroys the spontaneous magnetisation for $d \leq 2$ [42] then explains the results of Aizenman and Wehr and Hui and Berker. In higher dimensions, where the latent heat may coexist with a finite amount of disorder this approach leads to the correspondence between the critical behaviour of the two models in the limit of the strong first-order transition ($q >> 1$).

In contrast to all this variety of results for $d = 2$ very roughly sketched above, in three dimensions very few calculations exist, although this case is much closer to the real systems that we have mentioned earlier. In three dimensions there are no exact results for the pure case, and the approximate approaches are technically more complicated. Monte Carlo simulations, although requiring significant numerical effort, since the computing time grows with linear size as L^3, are thus a useful tool there.

In three dimensions MC simulations have been applied [43] to the Blume-Emery-Griffiths model in order to reproduce the altering of the multi-critical phase diagram observed experimentally in ^{3}He – ^{4}He binary mixtures in aerogel [4]. The same result was later reproduced by the renormalisation-group calculations [44].

The MC study of the three- and four-state Potts model was undertaken [45] for the realistic model of aerogel obtained numerically by diffusion-limited cluster-cluster aggregation. The study has reproduced the onset of the second-order phase transition both for the aerogel type disorder and for simple dilution. In both cases it occurs above a certain threshold concentration. The extension of these studies to the calculation of critical exponents of the induced continuous transition requires intensive MC calculations with a more appropriate algorithm. We present here our first results in this direction.

2. Diluted Potts model

The diluted Potts model is described by the Hamiltonian

$$H = -J \sum_{i,j} n_i \, n_j \, \delta_{\sigma_i,\sigma_j} \, , \tag{1}$$

where σ_i denotes q-state Potts variable at lattice site i, $J > 0$ is a ferromagnetic coupling and the summation is taken over the nearest neighbors of the 3d cubic lattice. The dilution is introduced by the quenched random variables n_i which take values 0 or 1 for empty or occupied sites, respectively. They can represent simple vacancies, or impurities, which do not interact either with the Potts degrees of freedom, or with each other. Dilution obeys the canonical constraint, i.e. the number of empty sites N_0 is fixed. The concentration of non-occupied sites is then $c = N_0/L^3$, where L is the linear size of the lattice.

In a pure case ($c = 0$), the three-dimensional Potts model exhibits a second-order phase transition for low values of q, while for $q \geq 3$ it is of a first-order. The threshold separating the two regimes lies slightly below $q = 3$ [14].

The gradual effect of finite concentrations of disorder is illustrated in Fig. 1. It was obtained by MC simulations for a 4-state Potts model, where n_i's are set according to the realistic model of aerogel structure obtained numerically by diffusion-limited cluster-cluster aggregation. The figure represents plots of the free energy versus energy at the critical temperature calculated from single disorder configurations for three different concentrations. For $c = 0.05$ it has two pronounced maxima which correspond to the coexistence of the ordered and disordered phases. The barrier between them which increases with lattice size L represents the interface free energy which scales as a surface and is the evidence for the first-order phase transition. For $c = 0.15$ the barrier disappears with increasing L and for the still higher concentration $c = 0.3$ the barrier is absent as an indication of the onset of the continuous transition.

This illustrates the existence of the finite threshold for the onset of the second-order phase transition in three dimensions.

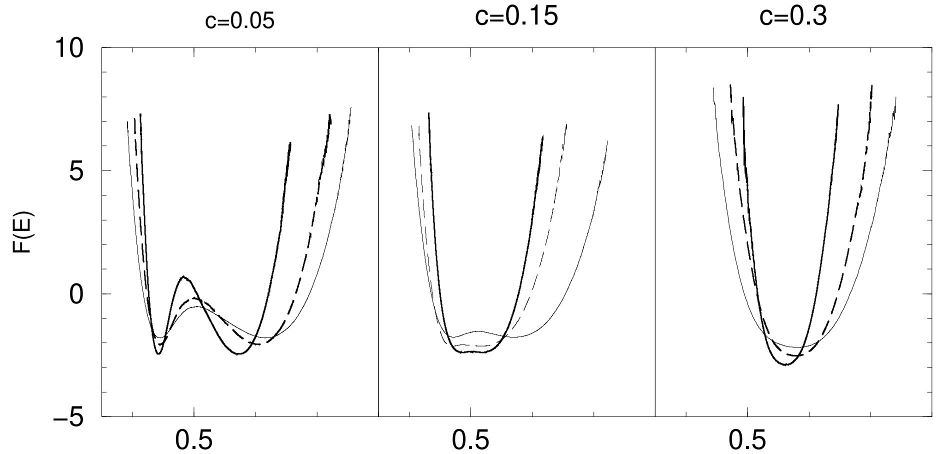

Fig. 1 Metropolis results for the free energy $F_L(E)$ versus E/E_{max} (E_{max} is the energy at $T = 0$) of the four-state Potts model for three different concentrations of aerogel. Thin, dashed, and thick line denote lattice sizes $L = 12, 15$ and 20, respectively.

While the results of Fig. 1 refer to the random but strongly correlated dilution characteristic for an aerogel, qualitatively similar behaviour is obtained for the simple random dilution.

We present in the following paragraphs the recent MC simulations focused on the critical behaviour of the disorder-induced second-order transition and performed for the case of simple random dilution.

We consider the three-dimensional three-state Potts model. Due to the small latent heat, the continuous phase transition sets on there at low dilution, which is of technical convenience to reduce the dispersion of data by disorder.

3. *Simulations and finite-size scaling*

The Monte Carlo simulations were performed on the $L \times L \times L$ simple cubic lattices with fully periodic boundary conditions by using the Swendsen-Wang cluster algorithm [46], efficient in suppressing the critical slowing down at criticality.

Starting with an arbitrary configuration of spins, it consists of two steps: (i) identification of all clusters by the following rule: two neighbouring spins belong to the same cluster if they are in the same state and if the link between them is active. The later is completed with the probability $p_{\rm add} = 1 - \exp(-J/k_b T)$. (ii) all clusters are independently flipped to randomly chosen states. Single spins are considered as clusters. In order to obtain a good statistics, one has to perform at least 10^5 such Monte Carlo swaps (MCS) of the system. For quenched disorder, it is also necessary to perform independent MC runs for a large number of individual realisations of disorder and average over the calculated thermodynamic quantities in the end. In the present paper we denote this average by [...], while the thermal average is denoted by $\langle ... \rangle$.

Simulations provide the distributions of energy and order parameter, but also those related to the clusters, since the Swendsen-Wang algorithm gives a direct insight into the cluster statistics.

Thermodynamic quantities of interest are then expressed through the moments of energy and the order parameter.

The specific heat is expressed by

$$C_L(T) \ = \ \frac{L^3}{k_B T^2} \ [\ \langle E^2 \rangle_L - \langle E \rangle_L^2 \ ], \tag{2}$$

where the moments of energy are given by

$$\langle E^k \rangle_L \ = \ \sum_E \ E^k \ P_L(E), \tag{3}$$

where $E = \sum_{<l,l'>} \delta_{\sigma_l, \sigma_{l'}}$ and $P_L(E)$ is the energy probability distribution. The label L denotes the finite size.

The order parameter of the Potts model is usually defined as

$$M = (q \langle max\{m_\alpha\} \rangle - 1)/(q-1); \qquad m_\alpha = \sum_i \delta_{\sigma_i, \alpha}, \quad \alpha = 1, 2, 3. \tag{4}$$

In simulations, the average is taken over the largest components $max\{m_\alpha\}$ of each configuration in order to break the symmetry in a finite system.

Instead of using the expression (4) we calculate the order parameter as an average over the largest cluster. It follows from the graph expansion by Kasteleyn and Fortuin [47], the very basis of the Swendsen-Wang algorithm, that the distribution of clusters constructed from active bonds can also be used to calculate the thermodynamic properties [48,49] in a similar way as the purely geometric clusters are used to describe geometrical transitions like percolation.

The probability of the largest cluster is defined by

$$P_L(n_{max}) = \ \frac{1}{mcs} \ N_L(n_{max}) \tag{5}$$

where $N_L(n_{max})$ is the total number of occurrences of the largest cluster of the size n_{max} during mcs Monte Carlo swaps.

The related moments

$$\langle n_{max}^k \rangle_L = \sum_{n_{max}} n_{max}^k P_L(n_{max}). \tag{6}$$

are used to express the order parameter as

$$\langle n_{max} \rangle_L = \sum_{n_{max}} n_{max} P_L(n_{max}) \tag{7}$$

and the susceptibility, by the second moment, as

$$\chi_L(T) \;=\; L^3 \;\; [\, \langle n^2_{max} \rangle_L - \langle n_{max} \rangle^2_L \,] \tag{8}$$

In the thermodynamic limit, the quantities $C_L(T)$ and $\chi_L(T)$ have a singularity at the critical temperature T_c. For the first-order phase transition it is trivial and given by the δ function, while for the second order phase transition the singularities have the form power-laws described by the critical exponents α and γ, respectively. In the finite-size quantities $C_L(T)$ and $\chi_L(T)$ these singularities are rounded, with the finite maxima near T_c and the finite-size scaling (FSS) analysis (see e.g. [50]) is used to recover the critical exponents. In the case of δ function the maxima will scale as L^d. In the case of a second-order phase transition the maxima scale as $L^{\alpha/\nu}$ and $L^{\gamma/\nu}$ for $C_L(T)$ and $\chi_L(T)$, respectively.

4. *Results*

The simulations were performed on lattices of linear sizes $L = 10, 12, 15, 20$ and 30 by considering two cases: the pure model ($c = 0$) and the diluted model in the regime of a second-order phase transition ($c = 0.3$).

Results for $c = 0$ are obtained with runs between 10^5 and 10^6 MCS, those for $c = 0.3$ with 10^5 MCS. For the diluted case, all the plots versus temperature presented in figures below (for $C_L(T)$, $\chi_L(T)$ and $R_L(T)$) have been obtained by averaging over 30 realisations of disorder. The data used for the FSS fits (given in the insets of these figures) have been averaged over 300 configurations of disorder. The total computing time consumed for the presented material is approximately six months of CPU time on a 400MHz Pentium II processor.

4.1. *Specific heat*

The plots of the specific heat versus temperature are presented for various sizes in Figs. 2a and 2b for the pure and the diluted case, respectively.

According to the FSS arguments [50] for the 1^{st}-order phase transition the maxima should scale as L^d, while for the 2^{nd}-order one they scale with $L^{\alpha/\nu}$. The data of the specific heat maxima $C_{Lmax}(T_{cL})$ were fitted to the power-law form with an additional constant term present to eliminate nonsingular contributions to $C_L(T)$.

For $c = 0$, the fitted value 2.461 is quite distant from $d = 3$. The major reason for the discrepancy comes from the extremely weak first-order character of this transition, which requires very large lattice sizes to be detected correctly.

For $c = 0.3$, the scaling exponent is drastically lowered as a clear indication of the disappearance of the 1^{st}-order phase transition. Since it is very close to 0, we limit here to examine only its sign by drawing the plot of the maxima of the $C_L(T)$ versus $ln(L)$. As it can be seen from the inset of the Fig 2b, the data are almost linear in $ln(L)$, while the restriction to larger sizes suggests a positive exponent α.

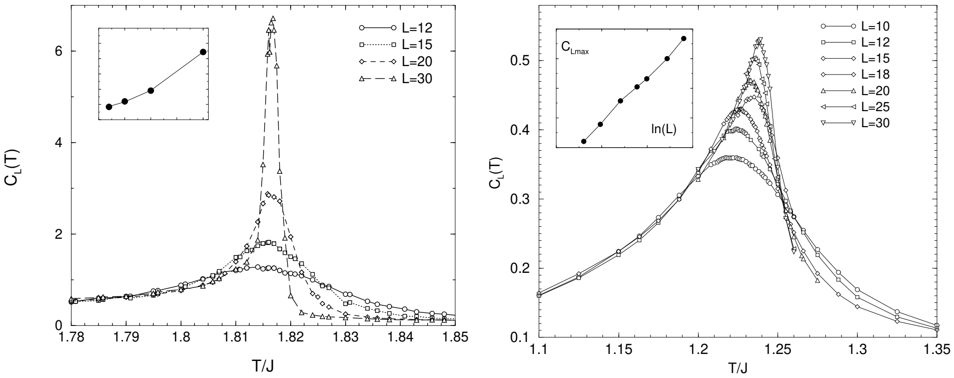

Fig. 2. Plots of the specific heat $C_L(T)$ versus temperature compared for the pure and diluted models. (a) the pure model (c=0). The inset gives plot of the maxima versus size: the fit to the form $C_L(T) = C_0 + C_1 * L^x$ contains $C_0 = 2.223$, $C_1 = 0.0046$, $x = 2.461$; (b) diluted model ($c = 0.3$): The inset contains the plot of the maxima of the $C_L(T)$ versus lnL.

4.2. Susceptibility

The plots of the susceptibility (Eq. (8)) versus temperature are presented for the pure and the diluted case, in Figs. 3a and b, respectively. In the insets of the two figures are illustrated the log-log plots of the maxima $\chi_{Lmax}(T_{cL})$ versus size.

For $c = 0$ the scaling exponent is equal to 2.82 ± 0.05. The discrepancy from $d = 3$ should again be attributed to the weak first-order transition, as discussed earlier.

The slope of the log-log plot for $c = 0.3$ gives the ratio $\gamma/\nu = 1.92 \pm 0.02$, or, expressed by the correlation function exponent, $\eta = 0.08 \pm 0.02$.

4.3. The ratio of moments

The thermal critical exponent ν may be derived directly from the moment ratio

$$R_L = \frac{\langle n_{max}^4 \rangle}{\langle n_{max}^2 \rangle^2} \tag{9}$$

related to the Binder's fourth-order cumulant [51]. Similar to the Binder's fourth-order cumulant for magnetisation, it is almost size-independent at T_c. Consequently, all finite-size curves for $R_L(T)$ versus T cross at the same point which corresponds to the critical temperature (see Fig. 4).

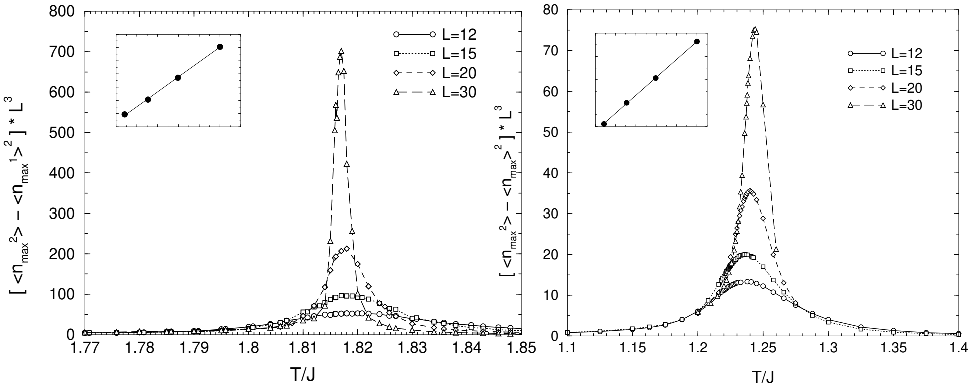

Fig. 3. Plots of susceptibility $\chi_L(T)$ versus temperature compared for pure and dilute models with $q = 3$. In the insets are the log-log plots of the maxima versus size. (a) $c = 0$: the log-log plot in the inset gives the slope 2.82; (b) $c = 0.3$: the log-log plot in the inset gives the slope 1.92.

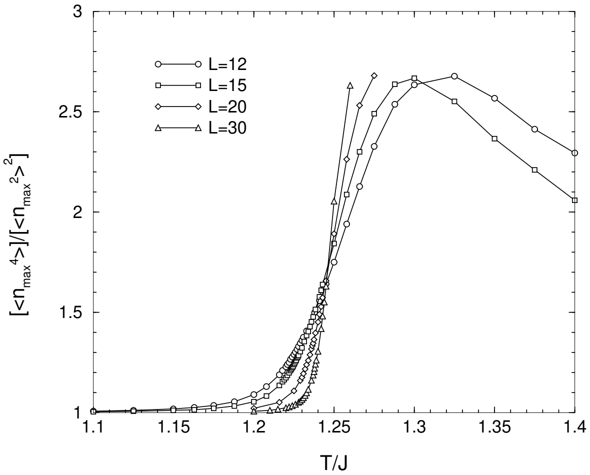

Fig. 4. Plots of moment ratio R_L versus temperature. The curves for all sizes L have the common crossing at $T = 1.245$.

The ratio $R_L(T)$ also satisfies the scaling relation [48, 49]

$$R_L(\tau) = L^x \ f(L^{1/\nu} \ \tau), \qquad \tau = \frac{T - T_c}{T_c}. \tag{10}$$

The critical exponent ν can be determined by collapsing the curves with precision up to a few percent. In Fig. 5 are shown the curves collapsed by scaling the reduced temperature τ with $L^{1/\nu}$. The scaling exponent was found to be equal to 1.50 ± 0.08, so that the resulting exponent is estimated as $\nu = 0.67 \pm 0.05$. Within the given error limits, this value is consistent with the behaviuor obtained for the specific heat.

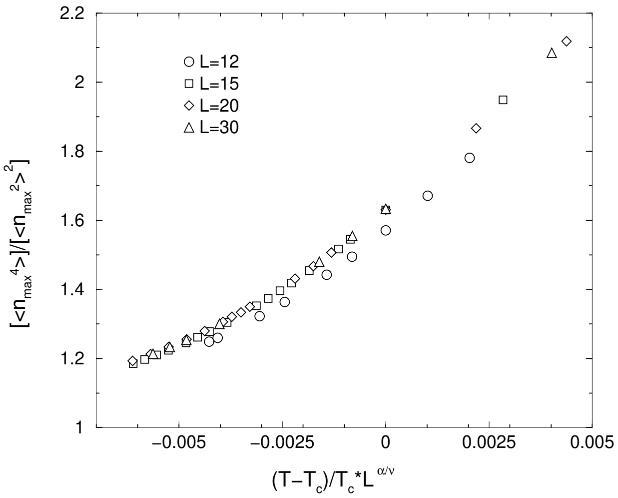

Fig. 5. The collapsed curves of the moment ratio R_L when ploted versus the reduced temperature scaled with $L^{1.5}$.

5. Discussion and conclusion

The effect of dilution on the critical behaviour of ferromagnetic models is a complex problem which still rises a number of fundamental questions: the difference between weak and strong randomness, the degree of universality of the disorder critical exponents, in particular when a new second-order phase transition is induced by disorder from a first-order one.

We have presented new results for the critical behaviour of the second-order phase transition induced by random dilution in $3d$ three-state Potts model. The critical exponents α, η and ν were studied by the FSS analysis of the moments of energy and the largest cluster. As expected, the maxima of the pure model ($c = 0$) do not scale so well with d, due to the weak first-order character of the transition. This, in contrast, presents an advantage for the diluted case. Clear evidence for the second-order phase transition has been obtained for the diluted case when $c = 0.3$. As it concerns the critical exponents, two mayor points should be discussed. The first one is the possible crossover effect dependent on the concentration c. As pointed out in $2d$ [25], for very low or very high concentrations, the obtained critical exponents can be influenced by the unstable fixed points corresponding to these two respective limits. Since the concentration studied in this paper is rather low, further calculations with higher concentrations are needed to examine the possible crossover effects. The second point is the possible comparison to the critical exponents of other models related to the problem, in particular those for the pure $3d$ Ising model ($\nu = 0.63$, $\eta = 0.037$, $\alpha = 0.11$) [52], the diluted $3d$ Ising model ($\nu = 0.684$, $\eta = 0.0375$) [53] and for the percolation in $3d$ ($\nu = 0.875$ and $\eta = 0.051$) [54]. According to the early conjectures, the new exponents should be compared to those of the pure Ising model, or, since the pure Ising model has $\alpha > 0$, with those of the diluted Ising model. The percolation exponent should be important in the limit of large c close to the percolation threshold. The calculated exponents are clearly different from the percolation exponent, which is not unexpected. As for the other two cited classes of universality, the present calculation cannot give a conclusive answer, since all the three values involved are close to each other, the difference between them being smaller than the error margins. The results are also inconclusive with respect to possible violation of the Chayes inequality. Although the Chayes inequality is a rigorous result, it may be interpreted as a consequence of the way of averaging [34] and this does not excludes the possibility that the exponent α eventually indeed turns out to be positive.

The presented numerical approach may be extended along several directions. The work is in preparation including a systematic FSS analysis of a larger number of quantities, which, together with some additional data, should improve the accuracy in the calculation of the exponents [55]. In future it would be interesting to examine the dependence of the calculated exponents on the number of Potts states. Another, more important question, in particular for the present approach, is to examine the possible crossover effects in the model by varying the concentration of dilution. A more difficult task for the Monte Carlo approach would be to find the critical exponents of the tricritical point for large values of q and compare them to the to the corresponding exponents of the random field Ising model.

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FAZNI PRIJELAZ DRUGOG REDA IZAZVAN ZAMRZNUTIM NASUMIČNIM RAZRJEĐENJEM U 3D

Raspravlja se učinak nasumičnog, zamrznutog razrjeđenja na feromagnetske prijelaze, posebice na promjenu iz prijelaza prvog u onaj drugog reda. Prikazani su novi rezultati za razrijeđeni trodimenzijski Pottsov model s tri stanja. Kritični eksponenti faznog prijelaza drugog reda izazvanog neredom izvedeni su ljestvičnom analizom momenata energije i najvećeg grozda, dobivenih Monte Carlo simulacijama.