Critical Behavior of the Spin-$3/2$ Blume-Capel Model on a Random Two-Dimensional Lattice

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We investigate the critical properties of the spin-$3/2$ Blume-Capel model in two dimensions on a random lattice with quenched connectivity disorder. The disordered system is simulated by applying the cluster hybrid Monte Carlo update algorithm and re-weighting techniques. We calculate the critical temperature as well as the critical point exponents γ/ν, β/ν, α/ν, and ν. We find that, contrary of what happens to the spin-$1/2$ case, this random system does not belong to the same universality class as the regular two-dimensional ferromagnetic model.

Keywords: Random lattices; Blume-Capel model; Hybrid Monte Carlo; Universality

I. INTRODUCTION

Experimental studies of the critical behavior of real materials are often confronted with the influence of impurities and inhomogeneities [1]. For a proper interpretation of the measurements it is, therefore, important to develop a firm theoretical understanding of the effect of such random perturbations. In many situations the typical time scale of the thermal fluctuations in the idealized "pure" systems is clearly separated from the time scale of the impurity dynamics, such that to a very good approximation the impurities can be treated as quenched. The importance of the effect of quenched random disorder on the critical behavior of a physical system can be classified by the specific heat exponent of the pure system, α_{pure}. The criterion due to Harris [2] asserts that for $\alpha_{pure} > 0$ quenched random disorder is a relevant perturbation, leading to a different critical behavior than in the pure case (which is the case of the three-dimensional Ising model). In particular, one expects [3] in the disordered system that $\nu \geq 2/D$, where ν is the correlation length exponent and D is the dimension of the system. Assuming hyper-scaling to be valid, this implies $\alpha = 2 - D\nu \leq 0$. On the other hand for $\alpha_{pure} < 0$ disorder is irrelevant (as is the case of the three-dimensional Heisenberg model) and, in the marginal case $\alpha_{pure} = 0$, no prediction can be made. For the case of (non-critical) first-order phase transitions it is known that the influence of quenched random disorder can lead to a softening of the transition [4]. Recently, the predicted softening effect at first-order phase transitions has been confirmed for 3D q-state Potts models with $q \geq 3$ using Monte Carlo [5–7] and high temperature series expansion [8] techniques. The overall picture is even better in two dimensions ($2D$) where several models with $\alpha_{pure} > 0$ [9–12] and the marginal ($\alpha_{pure} = 0$) [13–17] have been investigated.

In this paper we study another type of quenched random disorder, namely *connectivity disorder*, a generic property of random lattices whose local coordination number varies randomly from site to site. Specifically, we consider $2D$ Poissonian random lattices of Voronoi-Delaunay type, and performed an extensive computer simulation study of a Blume-Capel model. We concentrated on the close vicinity of the transition point and applied finite-size scaling (FSS) techniques to extract the exponents and the "renormalized charges" U_2^* and U_4^*. To achieve the desired accuracy of the data in reasonable computer time we applied the single-cluster hybrid algorithm [18] to update the spins and furthermore made extensively use of the re-weighting technique [19]. Previous studies of connectivity disorder focusing mainly on $2D$ lattices have been realized by Monte Carlo simulations of q-state Potts models on quenched random lattices of Voronoi-Delaunay type for $q = 2$ [20–22], $q = 3$ [23] and $q = 8$ [24, 25]. In particular, it has been shown that for $q = 2$ [20–22] and $q = 3$ [23] the critical exponents are the same as those for the model on a regular $2D$ lattice. This is indeed a surprising result since the relevance criterion of the Delaunay triangulations reduces to the well known Harris criterion such that disorder of this type should be relevant for any model with positive specific heat exponent [26]. This means that for $q = 3$, where $\alpha_{pure} > 0$, one would expect a different universality class. On the other hand, for the present spin-3/2 model, where $\alpha_{pure} = 0$, we show that the exponents indeed change in the Voronoi-Delaunay lattice type, turning out the situation still more bizarre . In the next section we present the model and the simulation background. The results and conclusions are discussed in the last section.

II. MODEL AND SIMULATION

The Voronoi construction or tessellation for a given set of points in the plane is defined as follows [27]. Initially, for each point one determines the polygonal cell consisting of the region of space nearer to that point than any other point. Then one considers that the two cells are neighboring when they possess an extremity in common. From the Voronoi tessellation the dual lattice can be obtained by the following procedure: (a) when two cells are neighbors, a link is placed between the two points located in the cells; (b) from the links one obtains the triangulation of space that is called the Delaunay lattice; (c) the Delaunay lattice is dual to the Voronoi tessellation in the sense that points corresponding to cells link to edges, and triangles to the vertices of the Voronoi tessella-

tion.

We consider now the two-dimensional spin-3/2 Blume-Capel model on this Poissonian random lattice. The Blume-Capel Model is a generalization of the standard Ising model [28] and was originally proposed for spin-1 to account for first-order phase transition in magnetic systems [29, 30]. The Hamiltonian can be written as

$$H = -J \sum_{<i,j>} S_i S_j + \Delta \sum_i S_i^2, \tag{1}$$

where the first sum runs over all nearest-neighbor pairs of sites (points in the Voronoi construction) and the spin-3/2 variables S_i assume values $\pm 3/2, \pm 1/2$. In eq. (1) J is the exchange coupling and Δ is the single ion anisotropy parameter. The second sum is taken over the N spins on a D-dimensional lattice. The case where $S = 1$ has been extensively studied by several approximate techniques in two- and three-dimensions and its phase diagram is well established [29–35]. The case $S > 1$ has also been investigated according to several procedures [36–42].

The simulations have been performed for $\Delta = 0$, which is the simplest case, on different lattice sizes comprising a number $N = 1000, 2000, 4000, 8000,$ 16000 and 32000 of sites. For simplicity, the length of the system is defined here in terms of the size of a regular lattice $L = N^{1/2}$. For each system size quenched averages over the connectivity disorder are approximated by averaging over $R = 100$ ($N = 1000$ to 4000), $R = 50$ ($N = 8000$) and $R = 25$ ($N = 16000$ and 32000) independent realizations. For each simulation we have started with a uniform configuration of spins (the results are however independent of the initial configuration). We ran 2.52×10^6 Monte Carlo steps (MCS) per spin with 1.2×10^5 configurations discarded for thermalization using the "perfect" random-number generator [43]. We have employed the hybrid algorithm [18] where we included n Wolff clusters (here $n = 5$) intercalated by one Metropolis single-spin flip sweep. This algorithm has been shown to be quite effective for spin-3/2 models [18]. For every 12th MCS, the energy per spin, $e = E/N$, and magnetization per spin, $m = \sum_i S_i/N$, were measured and recorded in a time series file.

From the series of the energy measurements we can compute, by re-weighting over a controllable temperature interval ΔT, the average energy and specific heat

$$e(K) = [< E >]_{av}/N, \tag{2}$$

$$C(K) = K^2 N[< e^2 > - < e >^2]_{av}, \tag{3}$$

where $K = J/k_B T$, with $J = 1$, and k_B is the Boltzmann constant. In the above equations $< ... >$ stands for thermodynamic averages and $[...]_{av}$ for averages over the different realizations. Similarly, we can derive from the magnetization measurements the average magnetization, the susceptibility, and the magnetic cumulants,

$$m(K) = [< |m| >]_{av}, \tag{4}$$

$$\chi(K) = KN[< m^2 > - < |m| >^2]_{av}, \tag{5}$$

$$U_2(K) = [1 - \frac{< m^2 >}{3 < |m| >^2}]_{av}, \tag{6}$$

$$U_4(K) = [1 - \frac{< m^4 >}{3 < |m| >^2}]_{av}. \tag{7}$$

Further useful quantities involving both the energy and magnetization are their derivatives

$$\frac{d[< |m| >]_{av}}{dK} = [< |m|E > - < |m| >< E >]_{av}, \tag{8}$$

$$\frac{d \ln[< |m| >]_{av}}{dK} = [\frac{< |m|E >}{< |m| >} - < E >]_{av}, \tag{9}$$

$$\frac{d \ln[< |m^2| >]_{av}}{dK} = [\frac{< |m^2|E >}{< |m^2| >} - < E >]_{av}. \tag{10}$$

In the infinite-volume limit these quantities exhibit singularities at the transition point. In finite systems the singularities are smeared out and scale in the critical region according to

$$C = C_{reg} + L^{\alpha/\nu} f_C(x)[1 + ...], \tag{11}$$

$$[< |m| >]_{av} = L^{-\beta/\nu} f_m(x)[1 + ...], \tag{12}$$

$$\chi = L^{\gamma/\nu} f_\chi(x)[1 + ...], \tag{13}$$

$$\frac{d \ln[< |m|^p >]_{av}}{dK} = L^{1/\nu} f_p(x)[1 + ...], \tag{14}$$

where C_{reg} is a regular background term, ν, α, β, and γ are the usual critical exponents, and $f_i(x)$ are FSS functions with $x = (K - K_c)L^{1/\nu}$ being the scaling variable, and the brackets $[1 + ...]$ indicate corrections-to-scaling terms. We calculated the error bars from the fluctuations among the different realizations. Note that these errors contain both, the average thermodynamic error for a given realization and the theoretical variance for infinitely accurate thermodynamic averages which are caused by the variation of the quenched, random geometry of the lattices.

III. RESULTS AND CONCLUSION

By applying standard re-weighting techniques to each of the R time-series data we first determined the temperature dependence of $C_i(K)$, $\chi_i(K)$,..., $i = 1,...,R$, in the neighborhood of the simulation point K_0. Once the temperature dependence is known for each realization, we can easily compute the disorder average, e.g., $C(K) = \sum_{i=1}^{R} C_i(K)/R$, and then determine the maxima of the averaged quantities, e.g., $C_{max}(K_{max}) = max_K C(K)$. The variable R represents the number of replicas in our simulations.

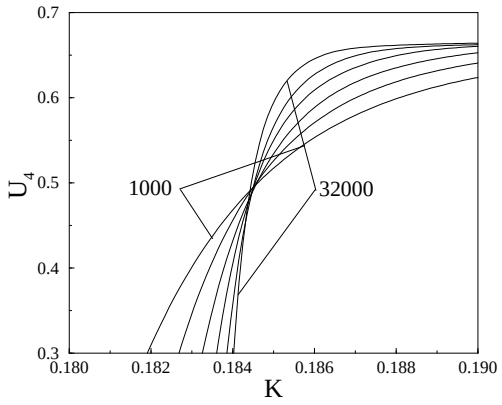

FIG. 1: Fourth-order Binder cumulant as a function of K for several values of the system size $N = 1000, 2000, 4000, 8000, 16000$ and 32000.

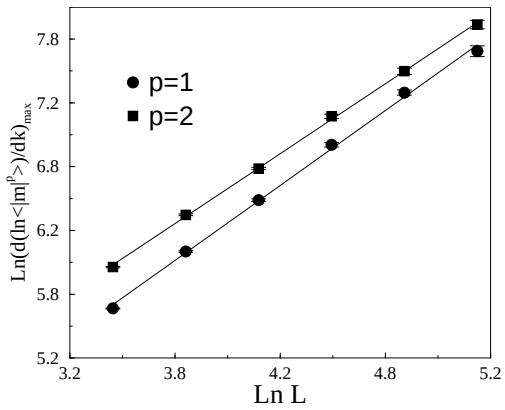

FIG. 2: Log-log plot of the maxima of the logarithmic derivative $\frac{d\ln[<|m|^p>]}{dK}$ versus the lattice size $L = N^{1/2}$ for $p = 1$ (circle) and $p = 2$ (square). The solid lines are the best linear fits.

In order to estimate the critical temperature we calculate the second and fourth-order Binder cumulants given by eqs. (7) and (8), respectively. It is well known that these quantities are independent of the system size and should intercept at the critical temperature [44]. In Fig. 1 the fourth-order Binder cumulant is shown as a function of the K for several values of N. Taking the largest lattices we have $K_c = 0.1844(1)$. To estimate U_4^* we note that it varies little at K_c so we have $U_4^* = 0.482(6)$. From the second-order cumulant we similarly get $K_c = 0.1845(1)$ and $U_2^* = 0.579(8)$. One can see that the agreement of the critical temperature is quite good and U_4^* is definitely far from the universal value $U_4^* \sim 0.61$ for the same model on the regular $2D$ lattice.

The correlation length exponent can be estimated from the derivatives given by eq. (15). Fig. 2 shows the maxima of the logarithm derivatives as a function of the logarithm of the lattice size L for $p = 1$ and $p = 2$. From the linear fitting one gets $\nu = 0.85(2)$ ($p = 1$) and $\nu = 0.917(8)$ ($p = 2$), which is again different from the regular lattice exponent $\nu = 1$.

In order to go further in our analysis we also computed

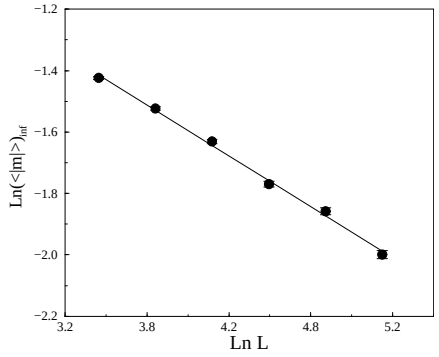

FIG. 3: Plot of the logarithm of the modulus of the magnetization at the inflection point as a function of the logarithm of $L = N^{1/2}$. The solid line is the best linear fit.

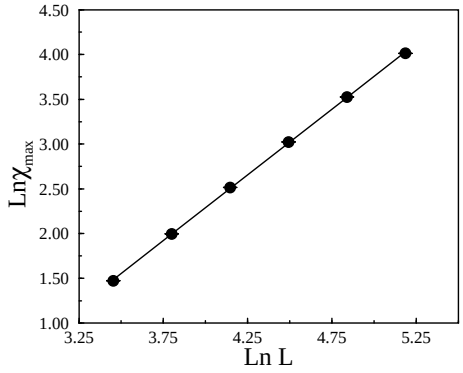

FIG. 4: Log-log plot of the susceptibility maxima χ_{max} as a function of the logarithm of $L = N^{1/2}$. The solid line is the best linear fit.

the modulus of the magnetization at the inflection point and the maximum of the magnetic susceptibility. The logarithm of these quantities as a function of the logarithm of L are presented in Figs. 3 and 4, respectively. A linear fit of these data gives $\beta/\nu = 0.331(9)$ from the magnetization and $\gamma/\nu = 1.467(9)$ from the susceptibility which should be compared to $\beta/\nu = 0.125$ and $\gamma/\nu = 1.75$ obtained for a regular $2D$ lattice.

The specific heat can also be analysed in this case but, as it happens in other models [21, 23], we cannot find a clear unambiguous support for a definite scaling. Fig. 5 shows the maximum of the specific heat C_{max} as a function of L. Least-squares fits to a logarithmic Ansatz $C_{max} = B_0 + B_1 \ln L$ give $B_0 = 0.44(6)$, $B_1 = 0.72(1)$ and is shown by the full line in Fig. 5. The dashed line in this figure corresponds to a pure power-law Ansatz, $C_{max} = cL^{\alpha/\nu}$ with $c = 1.475(5)$ and $\alpha/\nu = 0.202(5)$. From these results one can slightly see a better agreement with the logarithmic Ansatz.

Thus, from the above results, there is a strong indication that the spin-3/2 Blume-Capel model on a Voronoi lattice is in a different universality class than its regular lattice counterpart. This poses, in addition to the $q = 3$ Potts model in two dimensions, and taking into account the extensive study

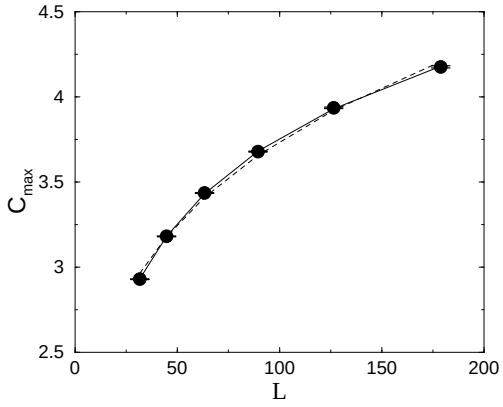

FIG. 5: Specific heat maxima C_{max} as function of $L = N^{1/2}$. The solid line is the best fit to an $\alpha \sim 0$ (Log) Ansatz and the dashed line to a power law Ansatz.

done Janke and Weigel on the Harris-Luck criterion for random lattices [26], another open question to be answered in more general terms.

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