

Uncovering the secrets of the 2d random-bond Blume-Capel model

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The effects of bond randomness on the ground-state structure, phase diagram and critical behavior of the square lattice ferromagnetic Blume-Capel (BC) model are discussed. The calculation of ground states at strong disorder and large values of the crystal field is carried out by mapping the system onto a network and we search for a minimum cut by a maximum flow method. In finite temperatures the system is studied by an efficient two-stage Wang-Landau (WL) method for several values of the crystal field, including both the first- and second-order phase transition regimes of the pure model. We attempt to explain the enhancement of ferromagnetic order and we discuss the critical behavior of the random-bond model. Our results provide evidence for a strong violation of universality along the second-order phase transition line of the random-bond version.

1. INTRODUCTION

Although originally thought to play a rather innocuous role, quenched bond randomness may (or may not) modify the critical exponents of second-order phase transitions [1], whereas in 2d it always affects first-order phase transitions by conversion to second-order phase transitions even for infinitesimal strength [2, 3, 4]. These predictions have been confirmed by various Monte Carlo simulations and they have been also well verified by our recent numerical studies via a two-stage WL method [5, 6, 7]. The random-bond version of the BC model is defined by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} s_i s_j + \Delta \sum_i s_i^2 ; P(J_{ij}) = \frac{1}{2} [\delta(J_{ij} - J_1) + \delta(J_{ij} - J_2)] ; r = J_2/J_1, \quad (1)$$

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where the spin variables s_i take on the values $-1, 0$, or $+1$, $\langle ij \rangle$ indicates summation over all nearest-neighbor pairs of sites and Δ is the value of the crystal field. The above bimodal distribution describes our choice for the quenched random interactions corresponding to disorder strength $r = J_2/J_1$, where both J_1 and J_2 are taken positive and the temperature scale may be set by fixing $2k_B/(J_1 + J_2) = 1$. The pure square lattice model exhibits a phase diagram with ordered ferromagnetic and disordered paramagnetic phases separated by a transition line that changes from an Ising-like phase transition to a first-order transition at a tricritical point $(T_t, \Delta_t) = (0.609(4), 1.965(5))$ [8, 9, 10, 11].

The present paper considers further interesting aspects of the random-bond version of the 2d BC model. In particular we will report on the effects of bond randomness on the ground-state structure, the phase diagram and the critical behavior of the square lattice ferromagnetic BC model. The ground-state problem is briefly discussed in the next Section and the order-parameter behavior, as a function of the disorder strength for several values of the crystal field, is illustrated. Then, in Section 3, we report on the effects of bond randomness on the phase diagram of the model and the enhancement of ferromagnetic order is clarified. We continue with a study of the conversion to a second-order phase transition, due to the introduction of bond-randomness of the first-order transition of the pure model at the value $\Delta = 1.975$. The more general critical behavior of the second-order phase transition of the random-bond 2d BC model is also briefly discussed. The implemented two-stage method of a restricted entropic WL sampling has been described in our recent studies [6, 7]. Finally, our conclusions are summarized in Section 4.

2. UNSATURATED FERROMAGNETIC GROUND STATES

In the presence of bond randomness the competition between the ferromagnetic interactions with the crystal field may result in destabilization of the ferromagnetic ground state. This phenomenon occurs for strong disorder and sufficiently large values of the crystal field giving rise to unsaturated ground states. To clarify this possibility, we observe that there will be on the average (in a large sample of disorder realizations) a finite portion of about 6.25% of lattice sites with all their connections being weak couplings (J_2). Thus, at strong disorder (small J_2) these lattice sites will be, at $T = 0$, in the $s_i = 0$ state provided that $\Delta > 4J_2$. Consequently, for strong disorder and for any $\Delta > 4J_2$, vacant sites ($s_i = 0$) will be distributed in the ground state of any given disorder realization. The complexity of this phenomenon may be further illuminated by defining weak clusters such that, in $T = 0$, these weak clusters will be in the all $s_i = 0$ state.

This subject has not been studied before and the consequences of the unsaturated ground state on the critical behavior of the 2d (and 3d) random-bond BC model are not known. The calculation of the ground states can be carried out in polynomially bounded computing time by mapping the system into a network and searching for a minimum cut by using a maximum flow algorithm. The results shown in figure 1, obtained via the FORD-FULKERSON method (see for instance [12]), illustrate the ground-state behavior of the order parameter $[M(T = 0)]_{av}$ as a function of the disorder strength r , for several values of the crystal field $\Delta = 0.5, 1.5, 1.95$, and 1.99 using a square lattice of linear size $L = 30$. The growing importance of the $s_i = 0$ state as we increase the value of the crystal field reflects the weak clusters complexity mentioned above and it will be very interesting to

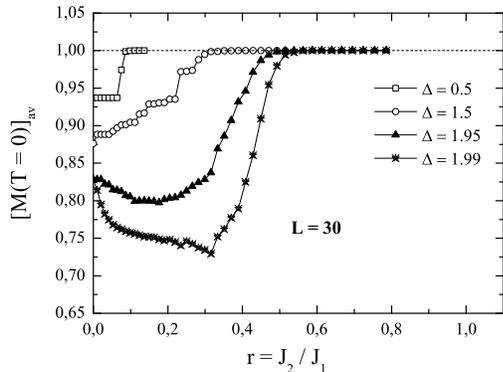


Figure 1. Ground-state behavior of the order parameter of the random-bond 2d BC model versus r for various values of Δ averaged over 250 disorder realizations.

find any possible interconnections with the critical properties of the random-bond model.

3. ENHANCEMENT OF FERROMAGNETIC ORDER AND CRITICAL BEHAVIOR

In general, the introduction of bond randomness is expected to decrease the phase-transition temperatures which at the percolation limit of randomness ($r = 0$ and $J_2 = 0$) should tend to zero. However, for weak randomness only a slight decrease is expected, if the average bond strength is maintained, as implemented here. Such a slight decrease in the critical temperature (by 1%) was reported earlier, for $\Delta = 1$, whereas, in sharp contrast and for the same disorder strength ($r = 0.6$), for $\Delta = 1.975$ (first-order regime of the pure model) we have found a considerable increase of the critical temperature, by 9% [7]. A microscopic explanation of this phenomenon was attempted in [7] by discussing the behavior of the connectivity spin densities, $Q_n = \langle s_i^2 \rangle_n$, where the subscript $n = 0, 1, 2, 3, 4$ denotes the class of lattice sites and is the number of the quenched strong couplings (J_1) connecting to each site in this class. For $\Delta = 1.975$, a pronounced preference was observed for the $s_i = 0$ state on the low strong-coupling connectivity sites whereas the $s_i = \pm 1$ states preferentially occurred with strong-coupling connectivity. It was then pointed out that this naturally leads to a higher transition temperature and effectively carries the ordering system to higher non-zero spin densities, the domain of second-order phase transitions. A similar microsegregation phenomenon, of the $s_i = \pm 1$ states and of the $s_i = 0$ state, has been seen in the low-temperature second-order transition between different ordered phases under quenched randomness [13].

As verified by our subsequent studies (for $r = 0.6$) this enhancement of the ferromagnetic order takes place in the neighborhood of $\Delta = 1.64$, where the phase diagrams of the pure and the random-bond models cross each other. Figure 2(a) illustrates the temperature behavior of the connectivity densities. The illustration gives the behavior for two values of Δ , namely $\Delta = 1.5$ and $\Delta = 1.75$ which lie below and above the estimated phase

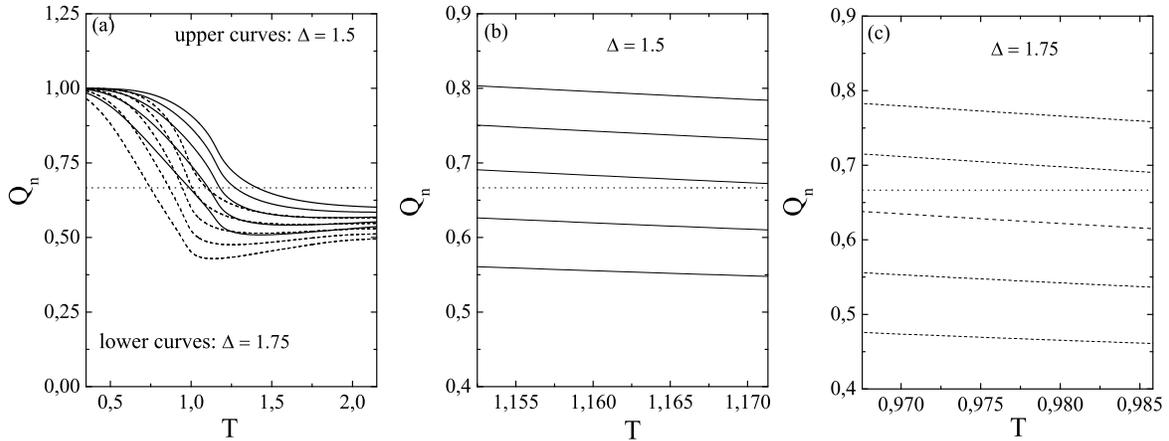


Figure 2. Average (10 realizations) behavior of the connectivity spin densities $Q_n = \langle s_i^2 \rangle_n$ for $\Delta = 1.5$ and for $\Delta = 1.75$. The lattice linear size used is $L = 40$.

diagrams crossing. Furthermore, figures 2(b) and (c) illustrate the heights and the differences (between the smallest $n = 0$ and the largest $n = 4$) of the connectivity densities in the corresponding pseudocritical region, defined by the specific heat and magnetic susceptibility finite-size peaks. For $\Delta = 1.75$, the difference is roughly 0.32, whereas for $\Delta = 1.5$ the difference between the smallest and the largest of the connectivity densities is only 0.239. The middle curves correspond to the leading connectivity density defined on the lattice sites with two strong and two weak couplings ($n = 2$). These sites amount on the average to a relative majority of 37.5% of the lattice sites. The height of the middle curve falls below the value $2/3$ (shown by the dot-line parallel to T -axis) as we move from the value $\Delta = 1.5$ to the value $\Delta = 1.75$ signaling that the preference on the $s_i = 0$ state is now extended even to the relative majority connectivity sites. This observation may be related to the enhancement of the ferromagnetic order as we pass through the crossing point of the two phase diagrams at $\Delta = 1.64$. Thus, in agreement with our previous conclusion microsegregation does occur in the first-order regime of the pure model where macrosegregation occurs in the absence of bond randomness. However, the enhancement of ferromagnetic order has already appeared before the first-order regime of the pure model as a kind of a precursor effect induced by weak randomness.

We now consider the critical behavior at $\Delta = 1.975$ [7]. Figure 3(a) contrasts the specific heat results for the pure 2d BC model and two strengths of disorder, $r = 17/23 \simeq 0.74$ and $r = 3/5 = 0.6$. The saturation of the specific heat is clear and signals the conversion of the first-order transition to a second-order transition with a negative critical exponent α . Figures 3(b) - (d) summarize our finite-size scaling (FSS) analysis for the disorder strength $r = 3/5 = 0.6$. The behavior of five pseudocritical temperatures $T_{[Z]_{av}^*}$, $T_{[Z]_{av}^*} = T_c + bL^{-1/\nu}$ (corresponding to the peaks of susceptibility, derivative of the absolute order parameter with respect to the inverse temperature ($K = 1/T$) and first-, second-, and fourth-order logarithmic derivatives of the order parameter with respect to the inverse

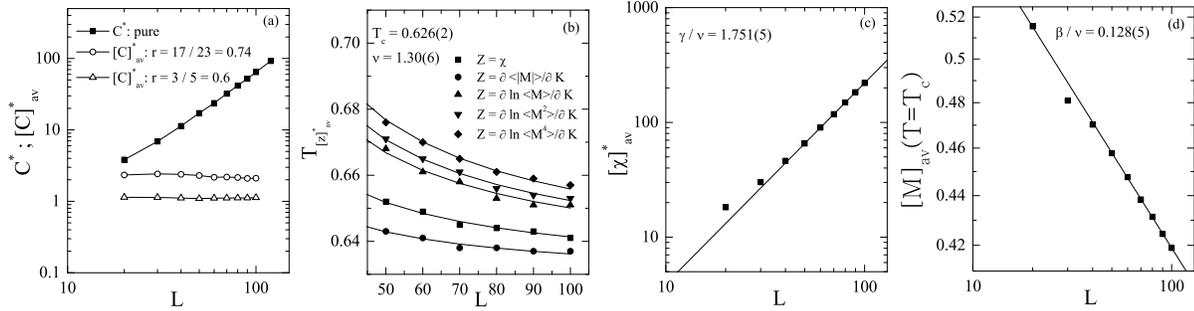


Figure 3. Behavior of the 2d BC model at $\Delta = 1.975$: (a) Illustration of the saturation of the specific heat for the random-bond model (open symbols). FSS behavior, for $r = 0.6$, of (b) pseudocritical temperatures, (c) susceptibility peaks, and (d) order parameter at T_c . Linear fits are applied for $L \geq 50$.

temperature) is presented in figure 3(b) and allow us to estimate $T_c = 0.626(2)$ and for the correlation length exponent $\nu = 1.30(6)$. From the peaks of the average susceptibility and the values of the average order parameter at $T_c = 0.626$, we have estimated, as shown in Figures 3(c) and (d), that the values of the exponent ratios $\gamma/\nu = 1.751$ and $\beta/\nu = 0.128$ are very close to the exact values of the Ising model. This “weak universality” is well obeyed for several pure and disordered models, including the pure and random-bond version of the square Ising model with nearest- and next-nearest-neighbor competing interactions [6].

At $\Delta = 1$ the random version should be comparable with the random Ising model, a model that has been extensively investigated and debated [6, 14, 15, 16, 17, 18, 19, 20]. Fitting our data for the corresponding pseudocritical temperatures in the range $L = 50 - 100$ to the expected power-law behavior mentioned above, we find that the critical temperature is $T_c = 1.3812(4)$ and the shift exponent is $1/\nu = 1.011(22)$. This last estimate is a strong indication that the random-bond 2d BC at $\Delta = 1$ and weak disorder has the same value of the correlation’s length critical exponent as the 2d Ising model. Furthermore, our data for the specific heat maxima averaged over disorder, $[C]_{av}^*$, showed that the expected double-logarithmic divergence scenario is well obeyed. Finally, the FSS behavior of the susceptibility peaks (giving the estimate 1.749(7) for γ/ν) and the order-parameter values at the estimated critical temperature $T_c = 1.3812$ (giving an estimate $\beta/\nu = 0.126(4)$) are in good agreement with the expected 2d Ising universality class behavior.

4. CONCLUSIONS

The effects of bond randomness on the ground-state structure of the 2d BC model have been briefly illustrated by mapping the system onto a network and searching for a minimum cut by using a maximum flow algorithm. Furthermore, we clarified some aspects

of the enhancement of ferromagnetic order, due to bond randomness, and we found that this appears before the first-order regime of the pure model. Our study at $\Delta = 1.975$ shows a conversion of the first-order transition of the pure model to a second-order phase transition, giving a distinctive universality class with $\nu = 1.30(6)$ and supporting an extensive but weak universality as in a wide variety of 2d systems without [21] and with [6, 22] quenched disorder. At $\Delta = 1$, our study of the random-bond 2d BC model indicates that for weak disorder the random system belongs to the same universality class as the random Ising model and the effect of the bond disorder on the specific heat is well described by the double logarithmic scenario. These results amount to a strong violation of universality since the two second-order phase transitions mentioned above, with different sets of critical exponents, are between the same ferromagnetic and paramagnetic phases. A more complete presentation of the effects of strong disorder on the ground-state structure and also on the critical behavior of the 2d BC model will appear in a forthcoming paper.

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