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DOI 10.1103/PhysRevE.97.040102
ISSN 1539-3755
ESSN 1550-2376

Publisher: American Physical Society -

Universality from disorder in the random–bond Blume–Capel model

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(Dated: April 7, 2018)

Using high-precision Monte Carlo simulations and finite-size scaling we study the effect of quenched disorder in the exchange couplings on the Blume-Capel model on the square lattice. The first-order transition for large crystal-field coupling is softened to become continuous, with a divergent correlation length. An analysis of the scaling of the correlation length as well as the susceptibility and specific heat reveals that it belongs to the universality class of the Ising model with additional logarithmic corrections observed for the Ising model itself if coupled to weak disorder. While the leading scaling behavior in the disordered system is therefore identical between the second-order and first-order segments of the phase diagram of the pure model, the finite-size scaling in the ex-first-order regime is affected by strong transient effects with a crossover length scale $L^* \approx 32$ for the chosen parameters.

PACS numbers: 75.10.Nr, 05.50.+q, 64.60.Cn, 75.10.Hk

The effect of random disorder on phase transitions is one of the basic problems in condensed-matter physics [1]. Examples include quantum Ising magnets such as $LiHo_xY_{1-x}F_x$ [2, 3], nematic liquid crystals in porous media [4], noise in high-temperature superconductors [5] and the anomalous Hall effect [6]. Understanding random disorder in classical, equilibrium systems is a crucial step towards solving the more involved problems in quantum systems [7], for example many-body localization with programmable random disorder [8], and in non-equilibrium phase transitions [9].

The case of weak disorder coupled to the energy density of systems with continuous transitions is rather well understood: Uncorrelated disorder is relevant and leads to new critical exponents if the specific-heat exponent α of the pure system is positive, a rule known as the Harris criterion [10]. If long-range correlations in the disorder are present, this rule can be generalized leading to interesting ramifications [11–16]. These effects, and in particular the marginal case of a vanishing specific-heat exponent as present in the two-dimensional Ising model, are intriguing and have attracted a large research effort over the past decades [17–24].

The situation is less clear for systems undergoing first-order phase transitions that are much more common in nature The observation that formally $\nu = 1/D$ and $\alpha = 1$ for such systems in D dimensions suggests that disorder is always relevant in this case, and the general observation is that it indeed softens transitions to become continuous [25]. Such a rounding of discontinuities has been rigorously established for systems in two dimensions [26], but is believed to be more general – a view that is supported by a mapping of the problem onto the random-field model [27–29]. This general picture is commonly accepted, and similar phenomena are recently studied in quantum systems [30–32] and for non-equilibrium phase transitions [33, 34]. Still, a number of important questions have not been answered in full generality: Is a finite strength of disorder required to soften a first-order transition? Is there a divergent correlation length? What is the universality class of the resulting continuous transition [29, 35, 36]?

While a softening must occur for arbitrarily small disorder strength in two dimensions [26–28], the situation is less clear in three dimensions [37, 38], but in both cases one finds divergent correlation lengths. The question of the universality class of softened transitions is perhaps the most intriguing one. This has been studied in some detail for the random-bond q-state Potts model [39–41]. It turns out to be difficult to determine the exponents with sufficient precision to arrive at decisive statements, but the most likely situation appears to be that $\nu \approx 1$ independent of q, while the magnetic ratio β/ν changes with q, a scenario that has recently also found additional support in perturbation theory [42].

A fertile testing ground for predictions relating to the behavior of first-order transitions under the influence of quenched disorder is the Blume-Capel model [43, 44]. It has been used to describe the prime nuclear fuel uranium dioxide [43], Mott insulators [45, 46], ^{3}He–^{4}He mixtures [48, 49] and more general multi-component fluids [50], as well as potentially the hardest piezomagnet known [47]. The pure system features a tricritical point separating second-order and first-order lines of transi-

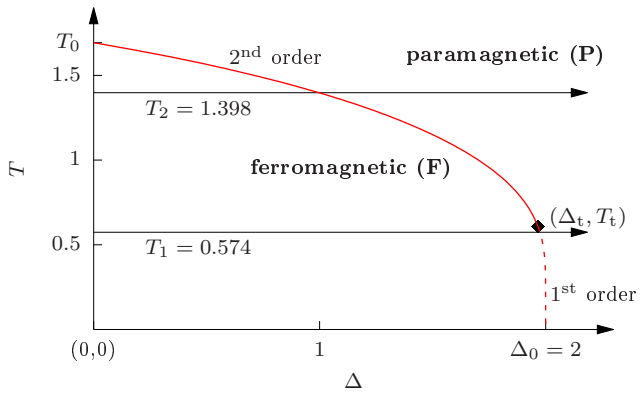

FIG. 1: (Color online) Phase diagram of the pure two-dimensional Blume-Capel model [51], showing the ferromagnetic (**F**) and paramagnetic (**P**) phases that are separated by a continuous transition for small Δ (solid line) and a first-order transition for large Δ (dotted line). The line segments meet at a tricritical point, as indicated by the black rhombus. The horizontal arrows indicate the paths of crossing the phase boundary implemented in the simulations of the present work.

tions [51]. There are many open questions concerning the behavior of this model in presence of quenched disorder, be it of random-bond type as considered here or in the form of random (crystal) fields [52, 53]. In particular, conflicting results have been found for the universality class of the ex-first-order segment of the transition line [54], and some authors have favored a scenario that contradicts universality [55, 56]. In the following, we present the results of high-statistics Monte Carlo simulations that demonstrate that the transitions in the second-order and the first-order segments of the transition line of the pure system are in the same universality class after coupling to the disorder, and this class is that of the two-dimensional (random) Ising model. Hence any doubts about the universality of critical behavior in this system are dispelled.

We study the spin-1 or Blume-Capel model [43, 44] with Hamiltonian

$$\mathcal{H} = -\sum_{\langle xy\rangle} J_{xy}\sigma_x\sigma_y + \Delta\sum_x \sigma_x^2 \;= E_J + \Delta E_\Delta = E, \quad (1)$$

where the spin variables $\sigma_x \in \{-1, 0, +1\}$ live on a square lattice with periodic boundaries and $\langle xy\rangle$ indicates summation over nearest neighbors. The couplings J_{xy} are drawn from a bimodal distribution

$$\mathcal{P}(J_{xy}) = \frac{1}{2}\,[\delta(J_{xy} - J_1) + \delta(J_{xy} - J_2)], \quad (2)$$

where following Refs. [55, 56] we choose $J_1 + J_2 = 2$ and $J_1 > J_2 > 0$, so that $r = J_2/J_1$ defines the disorder strength. The crystal field Δ controls the density of vacancies, *i.e.*, sites with $\sigma_x = 0$. The pure model has been studied extensively (for a review see Ref. [51]), the phase diagram in the (Δ, T)–plane is shown in Fig. 1: For small Δ there is a line of continuous transitions between the ferromagnetic and paramagnetic phases that crosses the $\Delta = 0$ axis at $T_0 \approx 1.693$ [56]. For large Δ, on the other hand, the transition becomes discontinuous and it meets the $T = 0$ line at $\Delta_0 = zJ/2$ [44], where $z = 4$ is the coordination number (here we set $J = 1$, and also $k_{\rm B} = 1$, to fix the temperature scale). The two line segments meet in a tricritical point estimated to be at $(\Delta_{\rm t} \approx 1.966, T_{\rm t} \approx 0.608)$ [57, 58]. It is well established that the second-order transitions belong to the universality class of the two-dimensional Ising model [51]. As $\alpha = 0$ there, the Harris criterion is inconclusive, but explicit studies of the Ising model indicate that the singularity is only logarithmically modified [17, 59, 60]. The first-order transition gets stronger as Δ_0 is approached and, in fact, the interface tension increases linearly with decreasing temperature [58]. According to the rigorous result of Aizenman and Wehr [26], the transitions must soften under the presence of even arbitrarily weak disorder, and we expect a second-order transition to emerge in this regime too.

As the phase boundary in the first-order regime is almost vertical, it is most convenient to cross it by varying the crystal field Δ while keeping the temperature constant. To this end we used a previously developed implementation of the multicanonical method [61, 62] applied only to the crystal-field energy E_Δ of Eq. (1) [63]. The method iteratively yields a flat histogram along E_Δ by replacing the canonical Monte Carlo weights $\exp(-\beta E)$ by $\exp(-\beta E_J)W(E_\Delta)$ and adapting $W(E_\Delta)$. Our calculations are implemented in a parallel fashion following the scheme discussed in Refs. [63–65]. This procedure allows us to directly study the probability distribution of E_Δ. The corresponding histogram for $T = T_1 = 0.574$ close to the transition point, averaged over $R = 256$ realizations of the random couplings for $r = 0.6$, is shown in Fig. 2. For small system sizes there is a clear double-peak structure, characteristic of a first-order phase transition. However, with increasing system size the distribution changes, exhibiting only a single, symmetric peak, clearly illustrating the second-order nature of the transition in the limit $L \to \infty$. In fact, the inset shows that the fraction of disorder samples with a double peak quickly decays to zero for increasing L, with $R_{\rm 2peaks}/R \approx 0$ for $L \geq L^* \approx 32$. This is clear evidence that bond disorder with $r = 0.6$ changes the pure first-order phase transition for $T = 0.574$ into a disorder-induced continuous one, yet, with a crossover behavior for small system sizes.

To reveal the universality class of the continuous transition resulting from the softening by disorder, we used an additional array of canonical Monte Carlo simulations, employing a combination of a Wolff single-cluster update [66] of the ± 1 spins and a single-spin flip Metropolis update [51, 67–69]. We restricted these simulations to

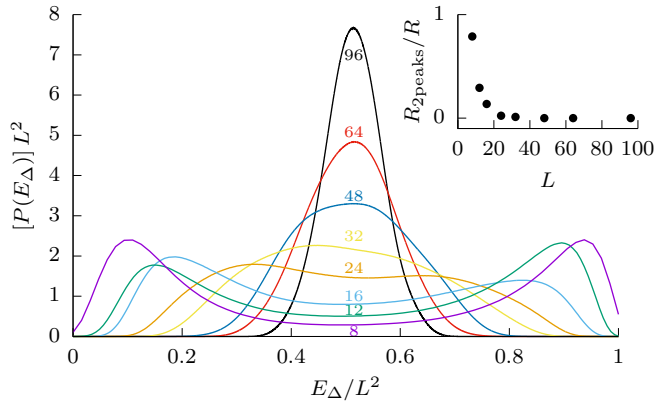

FIG. 2: (Color online) Probability distribution of crystal fields E_Δ of the random-bond Blume-Capel model at $T = 0.574$ and with disorder strength $r = 0.6$. The data are averaged over $R = 256$ disorder samples. With increasing system size, the double peak expected for a first-order transition changes to a single broad peak typical of a continuous transition. The inset shows the fraction of disorder samples exhibiting a double peak.

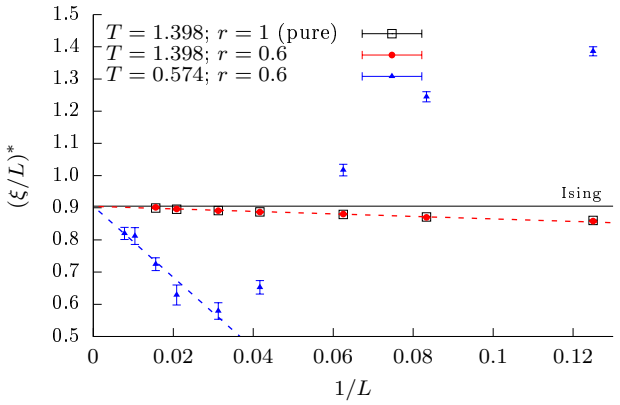

FIG. 3: (Color online) Finite-size scaling of the correlation-length ratios at their crossing points, $(\xi/L)^*$, for the pure and random model and the two temperatures considered in this work. Results are shown for the following pairs $(L, 2L)$ of system sizes: $(8, 16)$, $(12, 24)$, $(16, 32)$, $(24, 48)$, $(32, 64)$, $(48, 96)$, $(64, 128)$, $(96, 192)$, and $(128, 256)$. The horizontal line shows the asymptotic value for the square-lattice Ising model with periodic boundaries according to Eq. (3). The colored dashed lines show linear fits in $1/L$.

the two temperature points indicated by the arrows in Fig. 1, the case $T_1 = 0.574$ crossing the phase boundary in the first-order regime, and the choice $T_2 = 1.398$ in the second-order part of the transition line [51, 56]. Using this approach, we simulated the system sizes $L \in \{8, 12, 16, 24, 32, 48, 64, 96, 128, 192, 256\}$ for disorder strength $r = 0.6$. The ensemble sizes, R, of disorder realizations used are as follows: $R = 5 \times 10^3$ for $L = 8 - 32$, $R = 3 \times 10^3$ for $L = 48 - 96$, and $R = 1 \times 10^3$ for $L > 96$. Error bars were computed from the sample-to-sample fluctuations.

We first discuss the ratio of correlation length and system size, ξ/L. This is known to be universal for a given choice of boundary conditions and aspect ratio. For Ising spins on a square lattice with periodic boundary conditions as $L \to \infty$ it approaches the value [70]

$$\left(\frac{\xi}{L}\right)_\infty = 0.905\,048\,829\,2(4). \tag{3}$$

The behavior of the pure, square-lattice Blume-Capel model in the second-order regime is found to be perfectly consistent with Eq. (3) [51]. To determine ξ/L, we use the second-moment definition of the correlation length ξ [71, 72]. From the Fourier transform of the spin field, $\hat{\sigma}(\mathbf{k}) = \sum_{\mathbf{x}} \sigma_{\mathbf{x}} \exp(i\mathbf{kx})$, we determine $F = \left\langle |\hat{\sigma}(2\pi/L, 0)|^2 + |\hat{\sigma}(0, 2\pi/L)|^2 \right\rangle /2$ and obtain the correlation length via [72]

$$\xi \equiv \frac{1}{2\sin(\pi/L)} \sqrt{\frac{\langle M^2 \rangle}{F} - 1}, \tag{4}$$

where $M = \sum_x \sigma_x$. To estimate the limiting value of ξ/L we relied on the quotients method [73–75]: The crystal-field value where $\xi_{2L}/\xi_L = 2$, *i.e.*, where the curves of ξ/L for the sizes L and $2L$ cross, defines the finite-size pseudo-critical points Δ^{cross}. Let us denote the value of ξ/L at these crossing points as $(\xi/L)^*$. In Fig. 3 we show results of $(\xi/L)^*$ for three cases, namely the pure and random model at $T = 1.398$ and the random model at $T = 0.574$. The data for the pure case have been taken from Ref. [51], and the horizontal line shows the asymptotic value for the Ising model with periodic boundaries, cf. Eq. (3).

In the second-order regime of the pure model, for $T = 1.398$, the effect of the random bonds is extremely weak for $r = 0.6$, with the results for $(\xi/L)^*$ practically falling on top of the data for the pure system. For stronger disorder $r \to 0$ we expect numerically more pronounced effects, but no qualitatively different behavior. As is apparent from the data in Fig. 3, the results for the disordered and pure systems have consistent limiting values for $L \to \infty$. For the pure Blume-Capel model at the same temperature, it was previously found that $(\xi/L)_\infty = 0.906(2)$ [51], perfectly compatible with Eq. (3). For the disordered case a linear fit in $1/L$ for $L \geq 12$ (as shown by the red dashed line) yields

$$\left(\frac{\xi}{L}\right)^{T=1.398}_{\infty,\text{random}} = 0.905(2), \tag{5}$$

with goodness-of-fit parameter $Q \approx 0.3$. This is clearly consistent with the Ising value (3). An additional analysis of the scaling behavior of the magnetic susceptibility and specific heat (not shown) is also consistent with Ising universality, in line with previous analyses [55, 56].

We now turn to the temperature point $T_1 = 0.574$ in the first-order regime of the pure model. As it can be seen from the data of Fig. 3 the effect of disorder is

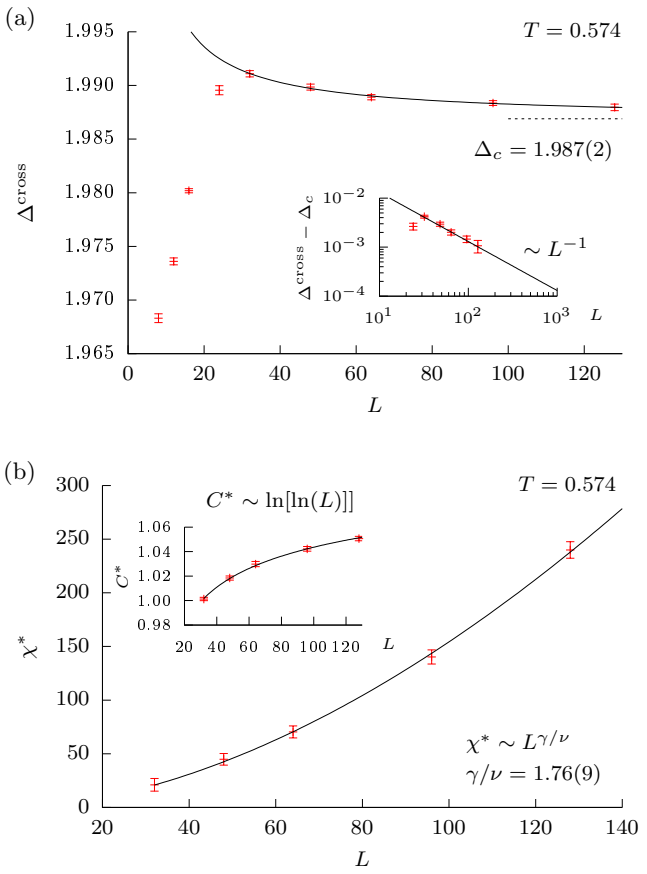

FIG. 4: (Color online) Finite-size scaling in the ex-first-order regime of the Blume-Capel model. (a): Shift behavior of the pseudo-critical points $\Delta^{\rm cross}$ estimated at the $(L, 2L)$ crossings of the ratio ξ/L shown in Fig. 3. (b): Scaling of the magnetic susceptibility $\chi^* = \chi(\Delta^{\rm cross})$ (main panel) and specific heat $C^* = C(\Delta^{\rm cross})$ (inset) evaluated at the pseudo-critical points for the smaller size of the pairs $(L, 2L)$ considered.

very strong there, leading to huge and non-monotonous scaling corrections. For smaller lattice sizes, the ratios $(\xi/L)^*$ do not show any tendency of converging to the universal Ising value until $L \approx 32$, when $(\xi/L)^*$ attains a minimum. Only for larger lattices the correlation length ratios start to approach the Ising limit approximately linearly in $1/L$. Taking lattice sizes $L \geq L^* \approx 32$ into account, a linear fit in $1/L$ (as shown by the blue dashed line) yields

$$\left(\frac{\xi}{L}\right)^{T=0.574}_{\infty,\text{random}} = 0.905(22), \qquad (6)$$

with $Q \approx 0.3$. The limit is again fully consistent with the Ising value. Note that the point $L \approx 32$ of the minimum corresponds to the crossover length scale L^* determined already as the size where the first-order nature of the transition disappears for the chosen disorder strength $r = 0.6$, see Fig. 2.

While the extrapolated value (6) of the correlation-length ratio $(\xi/L)^*$ is strong evidence for Ising behavior, universality classes are characterized by the entirety of their critical exponents and universal amplitude ratios. We therefore also considered the scaling of the pseudo-critical points $\Delta^{\rm cross}$, as well as the magnetic susceptibility χ and the specific heat C [76], both evaluated at $\Delta^{\rm cross}$. We first considered the scaling for the temperature $T_1 = 0.574$ in the first-order regime of the pure system. For large system sizes, the crossing points are expected to scale as

$$\Delta^{\rm cross} = \Delta_{\rm c} + bL^{-1/\nu}, \qquad (7)$$

where $\nu = 1$ for the two-dimensional Ising universality class. Our data for the pseudo-critical points are shown in Fig. 4(a), and we again observe strong scaling corrections with a pronounced turnaround in the behavior around the crossover length scale $L^* \approx 32$. As the inset illustrates, however, the behavior for $L \geq 32$ is in perfect agreement with the inversely linear behavior expected from Eq. (7) with $\nu = 1$. In fact, a fit of the form (7) for $L \geq 32$ with $Q \approx 0.8$ yields the critical crystal-field value $\Delta_{\rm c} = 1.987(2)$ and the estimate $\nu = 1.01(27)$.

Our results for the magnetic susceptibility χ and the specific heat C evaluated at the pseudo-critical points $\Delta^{\rm cross}$ at $T_1 = 0.574$ are shown in Fig. 4(b). Following the above analysis, we exclude small system sizes $L \leq 24$. For the magnetic susceptibility, a fit of the form $\chi^* \sim L^{\gamma/\nu}$ yields $\gamma/\nu = 1.76(9)$ with $Q \approx 0.9$, fully compatible within error bars to the Ising value 1.75. The specific heat, shown in the inset of Fig. 4(b), is well described by a double logarithm $C^* \sim \ln[\ln(L)]$ as predicted by Ref. [59], the corresponding fit quality being $Q \approx 0.9$. Similarly strong corrections to scaling in susceptibility data have also been reported for the diluted Ising model [21]. An analogous analysis of our data at the higher temperature $T_2 = 1.398$ in the second-order regime also yields values compatible to the Ising behavior, but without the strong scaling corrections observed for $T_1 = 0.574$.

To summarize, we have used the two-dimensional Blume-Capel model to investigate the effect of quenched bond disorder on originally second- and first-order phase transitions. We particularly focused on the effects in the originally first-order regime, a topic that has been controversial in the literature of disordered systems. We find that the disorder-induced continuous transitions in both segments of the phase diagram of the model belong to the universality class of the pure Ising ferromagnet with logarithmic corrections. This appears to be the physically most plausible scenario given that both transitions are between the same ferromagnetic and paramagnetic phases (Fig. 1), supporting the strong universality hypothesis [77–79]. While the leading behavior of the disordered system is hence consistent across the full transition line, there are dramatic differences in the scaling

corrections which appear to be minimal for the originally second-order transition but maximal and non-monotonic for the case of the originally first-order transition.

Although universality is a cornerstone in the theory of critical phenomena, it stands on a less solid foundation for the case of systems subject to quenched disorder. An explicit confirmation of the behavior of disordered models in this respect is therefore of fundamental importance for the theory as a whole (see also Ref. [75]). In this sense the unambiguous findings presented here set the stage for studies of similar systems in three dimensions, where one expects disorder to be relevant only beyond a finite threshold [27, 28, 37, 38]. A better understanding of the bond-disordered Blume-Capel model in three dimensions should be of relevance for a range of experimental systems including ^{3}He–^{4}He mixtures in porous media as well as impurities in uranium dioxide. Finally, when replacing the random bonds by random fields the Blume-Capel model might hold an answer to the intriguing question of whether first-order transitions can survive randomness if it couples to the order parameter instead of to the energy density [29, 52].

N.G.F is grateful to V. Martín-Mayor for his motivating comments that triggered this work. The project was financially supported by the Deutsch-Französische Hochschule (DFH-UFA) through the Doctoral College "$\mathbb{L}^4$" under Grant No. CDFA-02-07 as well as by the EU FP7 IRSES network DIONICOS under contract No. PIRSES-GA-2013-612707. J.Z. received financial support from the German Ministry of Education and Research (BMBF) via the Bernstein Center for Computational Neuroscience (BCCN) Göttingen under Grant No. 01GQ1005B. This research has been supported by the National Science Centre, Poland, under grant No. 2015/19/P/ST3/03541. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska–Curie grant agreement No. 665778. This research was supported in part by PLGrid Infrastructure.

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