Critical line of honeycomb-lattice anisotropic Ising antiferromagnets in a field

S. L. A. de Queiroz*

Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, 21941-972 Rio de Janeiro, Rio de Janeiro, Brazil

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Numerical transfer-matrix methods are used to discuss the shape of the phase diagram, in field-temperature parameter space, of two-dimensional honeycomb-lattice Ising spin-$\frac{1}{2}$ magnets, with antiferromagnetic couplings along at least one lattice axis, in a uniform external field. Both the order and universality class of the underlying phase transition are examined as well. Our results indicate that in one particular case, the critical line has, at least to a very good approximation, a horizontal section (i.e., at constant field) of finite length, starting at the zero-temperature end of the phase boundary. Other than that, we find no evidence of unusual behavior, at variance with the re-entrant features predicted in earlier studies.

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Here we study Ising spin-$\frac{1}{2}$ systems on a honeycomb (HC) lattice, with ferro- (F) and antiferromagnetic (AF) interactions, in the presence of a uniform magnetic field. Denoting by $k = 1$, 2, and 3 the three lattice directions, the Hamiltonian reads

$$\mathcal{H} = -\sum_k J_k \sum_{\langle i,j\rangle_k} \sigma_i\,\sigma_j - H\sum_i \sigma_i \ , \qquad (1)$$

where $\langle i,j\rangle_k$ denotes nearest-neighbor spins along lattice direction k, and $\sigma_{i,j} = \pm 1$. All fields H, coupling strengths J_k, and temperatures T are given in units of J_1. We always take at least one of the $J_k < 0$.

For a two-dimensional Ising AF system in a uniform field, an ordered phase is found at suitably low H, T. For the triangular-lattice isotropic AF the zero-field critical temperature vanishes, reflecting the macroscopic entropy of the ground state; the phase diagram in H-T space exhibits re-entrant behavior [1]. The second-order transition along the critical line belongs to the ferromagnetic three-state Potts universality class [2–4]; near $T = H = 0$ there is crossover toward a Kosterlitz-Thouless phase whose existence has been well established *on* the $T = 0$ axis for a finite range of H [5]. For isotropic AFs on both the square [6–9] and HC [9–11] lattices, the Ising character is preserved everywhere along the critical line on the H-T plane. For anisotropic square-lattice Ising systems with mixed interactions (F along one lattice direction, AF along the other) in a field (see, e.g., Refs. [12,13]), re-entrant behavior was found at low temperatures in some numerical or analytic treatments. The results of Ref. [13] indicate that re-entrant behavior is not present in this system and that the critical line starts horizontally at the zero-temperature end of the phase boundary. While for the triangular-lattice Ising AF the re-entrant shape of the critical curve is connected to its nontrivial ground-state structure, the vanishing ground-state entropy per spin of its square and HC-lattice counterparts does not, by itself, rule out this sort of behavior. Therefore, one must proceed to a case-by-case analysis. For HC lattices with anisotropy, the existence of re-entrances has been predicted [14] for a variety of combinations of F and AF interactions, depending also on their relative strength. In Ref. [14], an approach was used which considers the zeros of the partition function on an elementary lattice cycle and their connection to the free energy singularity at the transition [9]. The same approach also predicted a re-entrant critical curve for the mixed square-lattice model [14].

We use numerical transfer-matrix (TM) methods, plus finite-size scaling (FSS) and conformal invariance ideas, to establish the shape of the phase diagrams of systems described by Eq. (1), especially as regards the existence (or not) of re-entrancies. Our underlying hypotheses are that (i) the phase transition is second order all along the critical line and (ii) it is in the Ising universality class. Both assumptions are critically reviewed toward the end of the paper, in light of the numerical results obtained while assuming their validity. We consider combinations of interaction signs in which either one, two, or all three of the J_k in Eq. (1) are AF. The respective strengths reproduce points in $\{J_k\}$ parameter space for which Ref. [14] predicts sizable re-entrant sections of the critical line. In the following we keep the couplings along two directions with the same sign and strength, while bonds along the third direction (to be denoted as *inhomogeneous*) differ from the other two in strength and/or sign. Strips of width N sites with periodic boundary conditions across were used, with two distinct orientations: in (a) the TM proceeds perpendicularly to one lattice direction [15] (only N even is allowed by periodicity); in (b) it goes parallel to one lattice direction [11] (N even or odd). We used $4 \leqslant N \leqslant 20$, which (together with suitable extrapolation techniques) generally proved enough to yield accurate estimates of the critical lines. The following variants are considered:

(a1), (a2) denote choice (a), with the inhomogeneous bond: (a1) perpendicular to the TM's direction of advance or (a2) along either of the remaining two directions.

(b1), (b2) denote choice (b), with the inhomogeneous bond: (b1) parallel to the TM's direction of advance or (b2) along either of the remaining two directions.

In such weakly anisotropic systems [16,17], estimates of critical quantities should converge to the same orientation-independent limit for $N \gg 1$, albeit with differing finite-size corrections. However, in this case where spin couplings differ along the lattice axes, and the strips used in our calculations are essentially one dimensional, iteration of the TM along a fixed direction may introduce subtle biases. We used two distinct

*sldq@if.ufrj.br

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procedures, of which the latter is expected to be less prone to such biases than the former:

Procedure A: Keeping $\eta = 1/4$. Following earlier work on similar problems [6,8,11,13], our finite-N estimates for the critical line are found by requiring that the amplitude-exponent relation of conformal invariance on strips [18] be satisfied, with the Ising decay-of-correlations exponent $\eta = 1/4$:

$$4N\kappa_N(T,H) = \zeta\pi \ , \tag{2}$$

where $\kappa_N(T,H) = \ln|\lambda_1/\lambda_2|$ is the inverse correlation length on a strip of width N sites, λ_1 and λ_2 are the two largest eigenvalues (in absolute value) of the TM, and ζ compensates for the fact that on the HC lattice the strip width, in lattice parameter units, is not equal to N. For orientation (a) $\zeta = 2/\sqrt{3}$, and $\zeta = 1/\sqrt{3}$ for (b).

Procedure B: Phenomenological renormalization. The assumption of Ising behavior in Eq. (2) can be relaxed by demanding only that the transition remains second order. From FSS, the basic equation of the phenomenological renormalization group (PRG) [19] for the critical line is

$$N\kappa_N(T,H) = N'\kappa_{N'}(T,H), \tag{3}$$

with N and N' as close as possible for improved convergence of results against increasing N. In Eq. (3) one compares correlation lengths evaluated along the same lattice direction, so the likely biases mentioned above tend to cancel out [13]. PRG results can also be used as a test of the internal consistency of the Ising-universality class assumption; also, should additional, non-Ising, transitions be present elsewhere in parameter space, they should be detected by PRG.

Case I: $J_1 = J_2 < 0$; $J_3 > 0$. In this case, analysis of the zero-field ground state shows that N must be a multiple of 4 for choice (a2) above and even for choice (b2). We take $J_3 = 1$, so (i) ground-state considerations show that $H = 2$ is the zero-T critical field, and (ii) the zero-field critical temperature is the same as for pure AF (or F) systems: $T_c(H=0) = 2/\ln(2+\sqrt{3}) = 1.5186514\ldots$. Reference [14] finds that for $J_2/J_1 = |J_3/J_1| \gtrsim 0.6725$ the critical curve starts from $H = 0$ going towards higher temperatures, forming a "bulge," and then turns towards lower T, monotonically approaching its limiting intercept at $H = H_c(T=0)$. Furthermore, the critical curve is predicted to reach the point $T = 0, H = H_c(T=0)$ horizontally. For $H \ll 1$, the approximate critical curves, solutions of Eqs. (2) and (3), leave the T axis vertically and are very close to each other, for all choices (a1)–(b2). We find no evidence of a "bulge": $T_c(H)$ decreases monotonically with increasing H. As H increases, differences between curves generated by the various procedures become slightly more pronounced, as illustrated in Fig. 1. With increasing N, all four families of solutions of Eq. (2) converge towards approximately the same intermediate location, which also coincides with the single solution of Eq. (3) shown. The solutions of Eq. (3) converge much faster with increasing N than those of Eq. (2), so the single PRG curve depicted accurately represents the $N \to \infty$ limit of its family, to the scale of the figure. At low $T \lesssim 0.2$–0.3, numerical difficulties arise, because of the very large ratio between the TM states' Boltzmann weights. Even accounting for this, all approximate critical curves unequivocally point toward $(T,H) = (0,2)$ at finite angles, as illustrated by the dashed straight-line

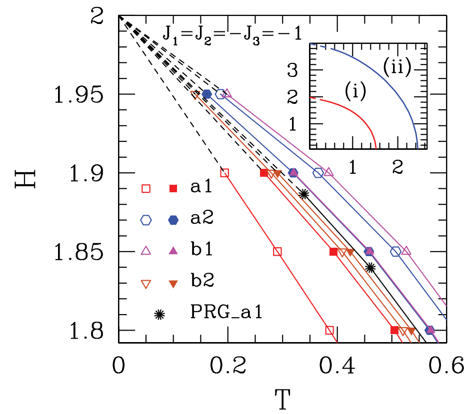

FIG. 1. (Color online) For $J_1 = J_2 = -J_3 = -1$, low-temperature approximate critical boundaries given by solutions of Eq. (2) [hollow symbols: $N = 4$; solid symbols, $N = 14$ (a1, b1), 12 (a2,b2)], or Eq. (3) [PRG_a1: strips of widths N, $N-2$, $N = 12$, geometry (a1)]. Large-N curves for (a2) and (b1) practically coincide on the scale shown. Inset: approximate phase diagrams generated by the solutions of Eq. (2), in geometry (a1) for $N = 16$. Curve (i) [red]: $J_1 = J_2 = -J_3 = -1$; curve (ii) [blue]: $2J_1 = -J_2 = -J_3 = 2$. Same axis labels as in main figure. See text.

segments (guides to the eye, only) in Fig. 1. In conclusion, no evidence is found that the critical curves approach $T = 0$ horizontally.

Returning to the "bulge" behavior predicted at higher temperatures, the inset of Fig. 1 shows the full phase diagram generated by the solutions of Eq. (2), in geometry (a1) for $N = 16$, both for $J_1 = J_2 = -J_3 = -1$ (discussed above) and for $2J_1 = -J_2 = -J_3 = 2$. This second combination allows direct comparison with one of the diagrams shown in Fig. 12 of Ref. [14], corresponding to the same coupling values. The phase diagram obtained there exhibits a horizontal portion at $H = 4$, from $T = 0$ to $T \approx 1$, as well as a "bulge" with maximum extent at $T \approx 2.7$, $H \approx 2.3$. Here, both features are absent from the numerically evaluated critical lines.

Case II: $J_1 = J_2 > 0$; $J_3 < 0$. As in case I, here N must be a multiple of 4 for (a2) and even for (b2). We assume $J_3 = -1$, so (i) $H_c(T=0) = 1$ and (ii) $T_c(H=0) = 2/\ln(2+\sqrt{3})$ as in case I. Reference [14] predicts that, for $J_2/J_1 = |J_3/J_1| > 1/3$, the critical line should leave the $T = 0$ axis with positive slope. For $J_3 = -1$, Fig. 11 of Ref. [14] shows that the peak of the corresponding reentrance is expected to occur at $T \approx 0.45$, $H \approx 1.05$. No "bulge" (i.e., a section of the critical curve extending to $T > T_c(H=0)$ at low H) is predicted. Figure 2 shows our results for low T, encompassing the region of the predicted reentrance. For (a1), (a2), and (b2), our numerical results indeed show re-entrant-like behavior in the predicted range of T. However, in all three cases the excess peak heights (i.e., above the $H = 1$ level) become smaller as N increases, as illustrated in Fig. 3. The trend followed in all cases certainly excludes a positive limiting height; rather, slightly negative values ($\approx$0.005 in modulus) appear more likely. The solutions of Eq. (2) in geometry (b1) do not show re-entrances; their low-temperature sections approach straight lines homing in towards $(T,H) = (0,1)$. Upon increasing N, the slope of such straight-line sections of the $T_c \times H$ curves becomes closer to zero. A similar trend is followed by the solutions of Eq. (3)

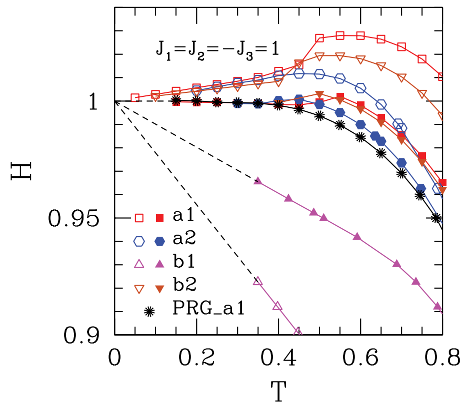

FIG. 2. (Color online) For $J_1 = J_2 = -J_3 = 1$, low-temperature approximate critical boundaries given by solutions of Eq. (2) [hollow symbols: $N = 4$; solid symbols, $N = 14$ (a1), 16 (a2) and (b1), 12 (b2)], or Eq. (3) [PRG_a1: strips of widths N, $N-2$, $N = 12$, geometry (a1)]. See text.

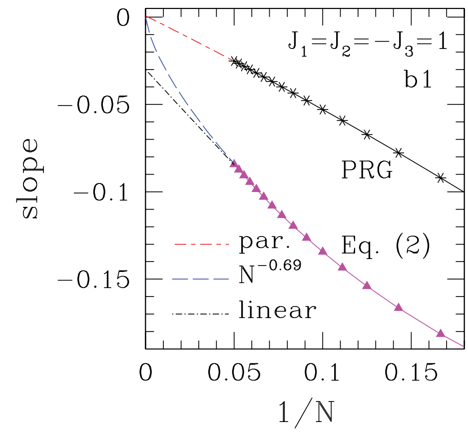

FIG. 4. (Color online) For $J_1 = J_2 = -J_3 = 1$, slopes of the low-temperature straight-line sections of approximate critical boundaries given in geometry (b1), by the solutions of Eq. (2) or Eq. (3) (PRG), against inverse strip width. Data points are for $N = 6$–20. Lines for $N^{-1} < 0.05$ are fits of $15 \leqslant N \leqslant 20$ data to forms shown ["par." stands for "parabolic"].

in the same geometry. Figure 4 shows both sets of slope values. For the solutions of Eq. (2), linearly extrapolating large-N data gives a negative limiting slope of approximately -0.030. Including a quadratic term (not shown) results in a limiting value around -0.015. Fitting to a single-power form $\sim N^{-x}$ requires $x \approx 0.69$. Though not altogether implausible, an exponent $x < 1$ means a growing amount of curvature with increasing N. In summary, a positive initial slope of the critical curve appears unlikely. The solutions of Eq. (3) in geometry (b1) behave smoothly and a parabolic fit gives a limiting slope equal to $(6 \pm 2) \times 10^{-4}$, which essentially equates to zero in the present context. On the other hand, PRG estimates in geometry (a1) (shown in Fig. 2), and also in geometries (a2) and (b2) (not shown) consistently give the approximate critical boundary lying slightly below the $H = 1$ line (within less than 0.1% of it) for all $T \lesssim 0.4$. Similarly to case I, here too the solutions of Eq. (3) [other than those for geometry (b1)] exhibit very little N dependence: for geometry (a1), differences between results for $N = 6$ and $N = 12$ are at most of order 1–2 parts in 10^3, with the largest values occurring midway between the phase diagram's end points. Thus, one cannot discard the possibility that the critical curve starts horizontally from $(T, H) = (0, 1)$ and remains flat for a finite extent, up to $T \approx 0.4$.

Case III: $J_1 = J_2 < 0$; $J_3 < 0$. In this case, the zero-field ground state is the same as for the pure AF. We use $J_3 = -0.4$, so (i) $H_c(T = 0) = 2.4$, and (ii) $T_c^{\,0} \equiv T_c(H = 0)$ does not take on the exact value $2/\ln(2 + \sqrt{3})$ any longer. For these coupling values, Ref. [14] predicts that the critical curve should leave the $T = 0$ axis with a positive slope, $S = \frac{3}{2}\ln 2$; see their Eq. (38). The eight sets of finite-N estimates, from solving Eqs. (2) and (3) in geometries (a1)–(b2), give very similar results, as depicted in Fig. 5. In contrast with cases I and II, the largest variations among differing calculational schemes are found for $H \ll 1$. At $H = 0$ we quote $T_c^{\,0} = 1.1170(5)$, where the error bar reflects the scatter among extrapolations of finite-N sequences for each of the eight sets available. At $T = 0$ the critical curve starts with a negative slope, in contrast to the prediction of Ref. [14].

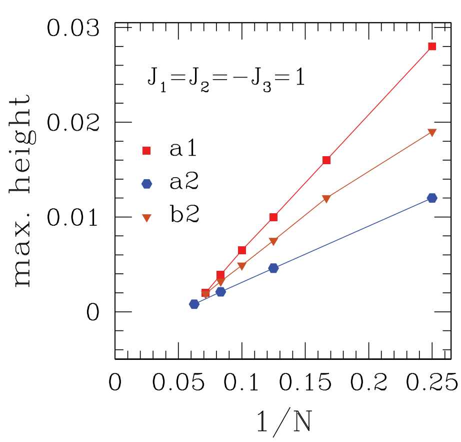

FIG. 3. (Color online) For $J_1 = J_2 = -J_3 = 1$, excess peak heights (above $H = 1$) of numerically obtained phase diagrams from solutions of Eq. (2), for geometries (a1), (a2), and (b2), against $1/N$. See Fig. 2 for reference.

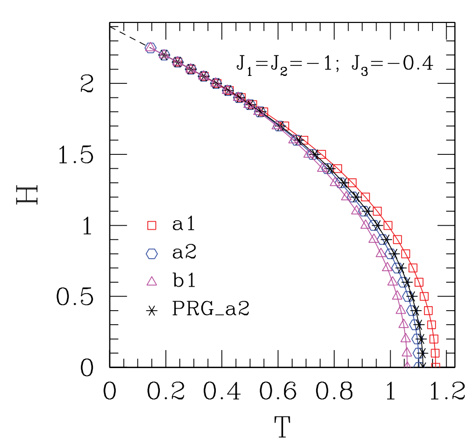

FIG. 5. (Color online) For $J_1 = J_2 = -1$, $J_3 = -0.4$, examples of approximate critical boundaries from solutions of Eq. (2) (all for $N = 8$) and Eq. (3) (with $N = 10$, $N' = 8$).

TABLE I. Adjusted values of initial slope S at $T = 0$ (followed by predictions from Ref. [14]) and quadratic term a in parabolic fit at $H = 0$, for phase diagrams in cases I–III [see, respectively, Eqs. (4) and (5)].

Case	S	S (Ref. [14])	a
I	$-0.321(7)$	0	0.205(3)
II	$\in [-0.03, +6 \times 10^{-4}]$	$(1/4)\ln 2$	0.504(2)
III	$-0.995(5)$	$(3/2)\ln 2$	0.158(1)

Taken together, our results for all cases I–III indicate that the phase transition remains second order everywhere along the phase boundary [justifying the use of Eq. (3)] and that it is in the Ising universality class [which supports Eq. (2)]. Near $T = 0$ our curves leave the H axis with (negative) slope S:

$$H_c(T) = H_c(0) + S\,T. \tag{4}$$

For $H \to 0$ their shape is well fitted by a parabolic form:

$$T_c(H) = T_c(0) - a\,H^2. \tag{5}$$

Our estimates of S and a are given in Table I. For each set of couplings, the error bars reflect the scatter among fits of large-N approximate curves, each corresponding to one of the eight combinations of calculational procedure and geometry. In the comparable problem of isotropic AFs (on both square and HC lattices), although the critical lines $H_c(T)$ of Ref. [9] do not exhibit reentrances, they are always above those found in Refs. [7,8] (except at the $T = 0$ and $H = 0$ ends, where the lines coincide in both cases). Thus the results presented here are consistent with previous ones, indicating that the methods employed in Refs. [9,14] tend to overestimate the extent of the ordered region in parameter space. We recall that the results given in Refs. [9,14] depend crucially on an unknown function $f(H)$ which is used, together with the smoothness postulate, to provide an extension of lemmas known to hold in zero field to the case $H \neq 0$. There appear to be no constraints on such function, apart from the condition $f(0) = 0$. In Ref. [9], a linear form $f(H) = AH$ gave the overestimates referred to above, for isotropic systems; it was also shown that, in order to produce a critical boundary in agreement with extant TM and other predictions, one needed to extend the Taylor expansion of $f(H)$ at least to third order, adjusting the corresponding coefficients to fit the TM or otherwise-obtained results. By contrast, in all anisotropic systems studied in Ref. [14], only the linear form was used for $f(H)$. One may conjecture whether such truncation is responsible for the apparently systematic overestimation of the extent of the ordered phase in the present case as well.

In conclusion, we have found no evidence of re-entrances, bulges, or horizontal sections in the numerically calculated phase diagrams here presented, except possibly for the low-temperature region in case II. There, our results strongly suggest that the critical line approaches the $T = 0$ axis at a very low angle, possibly even horizontally or (though less likely) at a very slight re-entrance. Similar behavior occurs in the square-lattice metamagnet studied in Ref. [13], where a sizable extent of the low-temperature phase boundary is found to be horizontal to within 0.1% (the same fractional deviation as the PRG curves here).

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[1] W. Kinzel and M. Schick, Phys. Rev. B **23**, 3435 (1981).
[2] Z. Rácz and T. Vicsek, Phys. Rev. B **27**, 2992 (1983).
[3] J. D. Noh and D. Kim, Int. J. Mod. Phys. B **6**, 2913 (1992).
[4] S. L. A. de Queiroz, T. Paiva, J. S. de Sá Martins, and R. R. dos Santos, Phys. Rev. E **59**, 2772 (1999).
[5] H. W. J. Blöte and M. P. Nightingale, Phys. Rev. B **47**, 15046 (1993).
[6] H. W. J. Blöte and M. P. M. den Nijs, Phys. Rev. B **37**, 1766 (1988).
[7] X.-N. Wu and F. Y. Wu, Phys. Lett. A **144**, 123 (1990).
[8] H. W. J. Blöte and X.-N. Wu, J. Phys. A **23**, L627 (1990).
[9] X.-Z. Wang and J. S. Kim, Phys. Rev. Lett. **78**, 413 (1997).
[10] F. Y. Wu, X. N. Wu, and H. W. J. Blöte, Phys. Rev. Lett. **62**, 2773 (1989).
[11] H. W. J. Blöte, F. Y. Wu, and X. N. Wu, Int. J. Mod. Phys. B **4**, 619 (1990).
[12] C. Rottman, Phys. Rev. B **41**, 2547 (1990).
[13] S. L. A. de Queiroz, Phys. Rev. E **80**, 041125 (2009).
[14] X.-Z. Wang and J. S. Kim, Phys. Rev. E **56**, 2793 (1997).
[15] V. Privman and M. E. Fisher, Phys. Rev. B **30**, 322 (1984).
[16] P. Nightingale and H. Blöte, J. Phys. A **16**, L657 (1983).
[17] A. Hucht, J. Phys. A **35**, L481 (2002).
[18] J. L. Cardy, in *Phase Transitions and Critical Phenomena*, Vol. 11, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1987).
[19] M. P. Nightingale, in *Finite Size Scaling and Numerical Simulations of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).