Field-induced ordering in critical antiferromagnets

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Transfer-matrix scaling methods have been used to study critical properties of field-induced phase transitions of two distinct two-dimensional antiferromagnets with discrete-symmetry order parameters: triangular-lattice Ising systems (TIAF) and the square-lattice three-state Potts model (SPAF-3). Our main findings are summarized as follows. For TIAF, we have shown that the critical line leaves the zero-temperature, zero-field fixed point at a finite angle. Our best estimate of the slope at the origin is\( \left( (d T_i / d H)\right)_{H=0}=4.74\pm 0.15 \). For SPAF-3 we provided evidence that the zero-field correlation length diverges as\( \xi(T\to 0, H=0)=\exp(a T^{\eta}) \), with\( \eta=1.08\pm0.13 \), through analysis of the critical curve at\( H\neq 0 \) plus crossover arguments. For SPAF-3 we have also ascertained that the conformal anomaly and decay-of-correlations exponent behave as\( (a) H=0; c=1, \eta=1/3 \). (b)\( H\neq 0; c=1/2, \eta=1/4 \).

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I. INTRODUCTION

Frustrated systems with macroscopically degenerate ground states still pose intriguing theoretical challenges. For pure Ising and \( q \)-state Potts antiferromagnets (AF’s), in particular, this degeneracy results solely from the interplay between “dynamics” (i.e., the number of states per lattice site) and geometry (lattice topology). In this paper we shall deal exclusively with Ising and three-state Potts AF’s, respectively, on the triangular and square lattices. It is well established that, in the absence of an external magnetic field, both systems display a critical ground state (in the sense that spin-spin correlations decay algebraically with distance), and are paramagnetic for all temperatures \( T>0 \) [1–5]. In both cases, a uniform field \( H \) removes the residual entropy per spin, and long-range order can set in at finite temperatures, below a field-dependent phase boundary \( T_c(H) \) [6,7].

For the Ising antiferromagnet on the triangular lattice (TIAF), the phase transition at \( T_c(H) \) has been determined to be in the 3-state ferromagnetic Potts model universality class [6,8]; subsequent analysis in the context of conformal invariance [9] led to a conformal anomaly (or central charge) \( c=4/5 \), which is also consistent with the value for the three-state Potts ferromagnet [10]. Further, it has been found that the critical phase at \( T=H=0 \) extends into a small region \( T=0, H=H_{KT}=0.27 \) [11–13]; that is, \( H \) is not a relevant scaling field at \( T=0 \), as initially thought [6]. At \( H_{KT} \) the system undergoes a Kosterlitz-Thouless (KT) transition to a long-range ordered state [13]. Within the zero-temperature critical phase, one has continuously-varying critical exponents and, accordingly [14], the conformal anomaly is \( c=1 \) [13]. Much less is known about field effects on the three-state Potts antiferromagnet on the square lattice (SPAF-3), apart from indications that, for \( H \neq 0 \) the transition at the corresponding \( T_c(H) \) belongs to the two-dimensional Ising model universality class [7].

Since the scaling behavior (i.e., relevance or marginality) of the uniform field at \( T=0 \) influences the shape of the critical curve near \( T=H=0 \) in a fundamental way, an accurate evaluation of \( T_c(H) \) is clearly of interest. With this in mind, here we investigate the finite-temperature field-induced transition in both the TIAF and the SPAF-3, by means of transfer-matrix scaling methods [15,16]. For TIAF we concentrate on the shape of the critical curve close to \( T=H=0 \), for reasons to be stated in the corresponding section. For SPAF-3 we determine the critical curve, as well as the conformal anomaly and the decay-of-correlations exponent \( \eta \) along it. The layout of the paper is as follows. In Sec. II we outline our calculational procedure for the free energy and the correlation length, from which we determine the conformal anomaly and the critical curve, respectively. Results for the TIAF and SPAF-3 are presented in Secs. III and IV, respectively. Section V summarizes our findings.

II. MODELS AND TRANSFER MATRIX SCALING

We consider infinitely long strips of width \( L \), with periodic boundary conditions in both directions. Ising or Potts spins sit on lattice sites and interact with each other, as well as with a uniform field, according to the Hamiltonian (including the multiplicative factor \( -\beta=-1/k_B T \)),

\[
\mathcal{H} = -K \sum_{\langle i,j \rangle} \delta \sigma_i \sigma_j + H \sum_i \delta \sigma_i 0, \tag{1}
\]

where the first sum runs over nearest-neighbor sites of either a triangular or a square lattice, depending, respectively, on whether \( \sigma_i \) is taken to be 0 or 1 (Ising), or 0, 1, or 2 (three-state Potts); a convenient strip geometry for a triangular lattice corresponds to the usual square strip with additional bonds along a fixed diagonal direction. \( K \) is the exchange coupling constant and the field \( H \) has been taken along the 0 direction.

We shall use units in which, for the triangular Ising ferromagnet, \( T_c^{-1} \equiv K_c = \frac{1}{2} \ln \sqrt{3} \), and for TIAF the upper critical field [such that \( T_c(H=H_c)=0 \) is \( H_c=6 \) [6,9]. For SPAF-3, the corresponding quantities are \( T_c^{-1} = \ln(\sqrt{3}+1) \) (ferromagnet), \( H_c=4 \) [7].

As usual [15,16], the free energy per spin \( f_i(T,H) \) and the correlation length \( \xi_L(T,H) \) are given by
\[ f_L(T, H) = -\frac{\xi}{\beta} \ln \lambda_1; \quad \xi_L^{-1}(T, H) = -\frac{\xi}{\ln(\lambda_2/\lambda_1)} \quad (2) \]

where \( \lambda_1 \) (\( \lambda_2 \)) is the largest (second-largest) eigenvalue of the transfer matrix between two successive columns; the geometric factor \( \xi = 2/\sqrt{3} \) for triangular, and 1 for square lattices.

We have obtained finite-size estimates of the critical line by standard phenomenological renormalization group (PRG) procedures [15,16]: for fixed \( H \) we consider pairs of strips of respective widths \( L \) and \( L' \) and solve the implicit equation

\[ L \xi_L^{-1}(T^*, H) = L' \xi_L^{-1}(T^*, H) \quad (3) \]

for the fixed-point temperature \( T^* \). This approach is rather safe because the only underlying assumption is that a second-order phase transition occurs without any further hypothesis on its universality class. As explained in detail below, we will be particularly concerned with the proximity of \( T = 0 \) and \( H = 0 \), where crossover between different sorts of critical behavior is expected. Owing to sublattice symmetries, \( L \) and \( L' \) must be both multiples of 3 for TIAF (where we use \( L' = L - 3 \), \( L = 6, \ldots, 18 \)), and 2 for SPAF-3 (respectively \( L' = L - 2 \), \( L = 4, \ldots, 12 \)). At some special points, such as \( (T = 0, H = 0) \), we went up to \( L = 14 \) for SPAF-3.

For each fixed \( H \) the sequence of finite-\( L \)-estimates of \( T^* \) was extrapolated against suitable inverse powers of \( L \), so that a set of temperatures \( T^*_c(H) \) was produced, which represents our best approximation to the true critical curve. We then calculated the free energy and the correlation length for finite \( L \), as in Eq. (2), at \( T^*_c(H) \). From these we produced finite-size estimates of the conformal anomaly \( c \) and the decay-of-correlations exponent \( \eta \), respectively, via

\[ L^2[f_L(T_c) - f_{S}(T_c)] = -\frac{\pi c}{6}, \quad (4) \]

and

\[ \eta = \frac{L \pi}{\xi(T_c)}, \quad (5) \]

as given by conformal invariance [10,17], where the \( H \) dependence of \( T_c \) (and thus, of \( c \) and \( \eta \)) is implicitly understood. The sequences of finite-\( L \) estimates \( c_L \) and \( \eta_L \) were again extrapolated to \( L \to \infty \) to give the final values \( c(H) \) and \( \eta(H) \).

The extrapolated phase boundaries were usually obtained under the simplifying assumption of single-power corrections to scaling: for given \( H \) we assumed

\[ T^*(L, H) - T_c(H) \sim L^{-\theta}. \quad (6) \]

It is expected [18,19] that \( \psi = \omega + 1/\nu \), where \( \omega \) is the leading correction-to-scaling exponent:

\[ \xi_L(T_c) = A_0 L (1 + A_1 L^{-\omega} + \cdots) \quad (7) \]

and \( \nu \) is the correlation-length critical exponent, known to be \( 5/6 \) (1) for three-state Potts (Ising) ferromagnets [relevant for TIAF (SPAF-3) in nonzero field]. However, \( \omega \) is not known in advance; though in several cases [20] numerical evidence has been given in support of \( \omega = 2 \), this is, in principle, a nonuniversal quantity that depends on the pertinent operator algebra, and probably on lattice effects as well; e.g., for Ising ferromagnets on triangular and honeycomb lattices, it has been found [21] that \( \omega = 4 \) fits Eq. (7) extremely well. Attempts to keep \( \omega \) fixed at 2 in Eq. (6) for the present case resulted in fits of widely varying quality. Thus we took a pragmatic view, and for each \( H \) varied \( \psi \) within reasonable limits (to be spelt out below) until a good fit turned out. More often than not, the smallest-\( L \) term \([L = 6(4)\) for TIAF (SPAF-3)] was discarded. Typical uncertainties for \( T^*_c(H) \) were one part in \( 10^4 \), which means that the dominant contributions to final spreads in \( \eta(H) \) and \( c(H) \) are attributable to the respective extrapolations of \( c_L \) and \( \eta_L \) to \( L \to \infty \).

From Eq. (7), the corrections to \( \eta_L \) of Eq. (5) are expected to behave as \( L^{-\omega} \). Surprisingly, a fixed \( \omega = 2 \) gave reasonably good fits throughout the range of fields investigated, for both models. For the conformal anomaly the additional unknown \( f_S(T_c) \) arises; assuming corrections to scaling to Eq. (4) also with \( \omega = 2 \) (in this case, such corrections have been shown to work well for Potts [22] and Ising [23] ferromagnets) we performed least-squares fits of our data to a parabolic form in \( L^{-2} \).

Further, the field dependence of \( c \) and \( \eta \) can be analyzed within a finite-size scaling (FSS) theory of crossover effects [24]. We first assume the existence of two bulk correlation lengths, \( \xi^0 \) and \( \xi^T \): the former is only divergent at \( T \to 0, H = 0 \); the latter diverges both at \( T \to 0, H = 0 \) (i.e., \( \xi^0 - \xi^T \) in this case), as well as at \( T_c(H) > 0 \), with different asymptotic forms. The two scaling variables are then \( L/\xi^0 \) and \( L/\xi^T \), which allows us to cast the finite-size correlation length and free energy in the forms

\[ \xi_L^{-1}(T, H) = L Q(L/\xi^0, L/\xi^T) \quad (8) \]

and

\[ f_L(T, H) = L^{-d R(L/\xi^0, L/\xi^T)}, \quad (9) \]

respectively, where \( Q \) and \( R \) are extended scaling functions. The crucial difference between the scaling of these and of any other quantity (e.g., susceptibility, specific heat, magnetization) is that the leading power in the \( L \) dependence is fixed, instead of a ratio of critical exponents, \( x/\nu \), which may change from \( x_0/\nu_0 \) to \( x_T/\nu_T \). Indeed, the main \( H \) dependence in the crossover function is expected to arise as \([f(H)]^\epsilon \), with \( \epsilon = x_T/\nu_T - x_0/\nu_0 \) [24]. Thus, low-order corrections to the asymptotic behavior must be wiped out; the field-dependent crossovers in both \( \eta \) and \( c \) are therefore expected to be quite fast. We shall see that these predictions are borne out rather well by numerical data for SPAF-3. For TIAF, technical difficulties (to be described) connected to extrapolation of the critical boundary translate into a more mixed picture.

### III. TRIANGULAR ISING ANTIFERROMAGNET

For TIAF in the range \( 1 \leq H \leq 5.5 \), best fits to Eq. (6) were attained with \( \psi = 3.5–5.5 \) (higher values for lower fields). In that region our PRG estimates extrapolate to values virtually identical to those found in Ref. [9]. Those authors started...
from the assumption that, for all \( H \neq 0 \), the TIAF is in the same universality class as the three-state two-dimensional Potts ferromagnet \([6,8]\), and located the points \((T, H)\) where \( \xi_4(T, H) = 15L/4\pi \), corresponding to \( \eta = 4/15 \) as given by conformal invariance \([17]\). Procedures of this sort were put forward by Blöte and den Nijs \([20]\), and are expected to be less vulnerable than PRG to numerical inaccuracies, provided the universality class of the transition is not in doubt. However, near a multicritical point (such as \( T = H = 0 \) here) crossover effects may also take their toll. Indeed, even though there is no \textit{a priori} reason to question universality in the present case, convergence of the data of Ref. \([9]\) deteriorates rapidly close to the origin, to such an extent that the authors quote no extrapolations for the critical line for \( H \approx 0.5 \). In our investigation, we found that for \( 0.15 \leq H \leq 0.5 \) the PRG curves crossed each other, thus making the extrapolation procedure unworkable. An example can be seen near the right edge of Fig. 1 above, which also shows that closer to the origin the curves again behave monotonically against \( L \).

Before giving details of extrapolation in that region, we recall that the shape of the low-\( T \), low-\( H \) phase boundary was discussed in Ref. \([6]\). At the time it was believed that \( H \) was a relevant scaling field along \( T = 0 \), from which it was concluded that, since the correlation length diverges as \( \exp(\alpha T) \) \([25]\) at \( H = 0 \), \( T \to 0 \), the critical line should approach the origin tangentially to the \( T \) axis. On the other hand, PRG with \( L = 6 \) and 9, in the notation of our Eq. (3), yielded a finite slope at the origin. This was interpreted as a deficiency of the calculational method \([6]\). Here we have reexamined the matter by extending PRG to \( L = 18 \), extrapolating our data and making contact with the more recent results \([12,13]\) that point to the existence of a Kosterlitz-Thouless phase at \( T = 0 \), \( H \neq 0 \).

In Fig. 1 the fixed-point solutions of Eq. (3) are displayed. Though convergence becomes prohibitively slow for \( H \leq 8 \times 10^{-3} \), there is plenty of leeway to establish that, as \( H \to 0 \), all our finite-\( L \) curves become straight lines which (to within one part in \( 10^3\)–\(10^7\)) cross the origin. The straight sections become shorter with growing \( L \), thus one must be careful before predicting a finite slope at the origin for the actual phase diagram. In Table I we show the slopes \( S_L \) of the straight sections of finite-\( L \) curves, as well as the values

![FIG. 1. PRG estimates of the critical line of TIAF near the origin, obtained by solving Eq. (3). \( L \) values given on figure (\( L' = L - 3 \)).](image)

<table>
<thead>
<tr>
<th>( L )</th>
<th>( S_L \</th>
<th>( H_{\text{max}}(L) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>1.4979±0.0001</td>
<td>—</td>
</tr>
<tr>
<td>9</td>
<td>2.0414±0.0002</td>
<td>0.170±0.010</td>
</tr>
<tr>
<td>15</td>
<td>2.4564±0.0002</td>
<td>0.130±0.010</td>
</tr>
<tr>
<td>18</td>
<td>2.8078±0.0002</td>
<td>0.105±0.010</td>
</tr>
<tr>
<td>Extr.</td>
<td>4.74±0.15</td>
<td>0.01±0.02</td>
</tr>
</tbody>
</table>

\( H_{\text{max}}(L) \) above which said curves begin to deviate from linear behavior. Error bars for \( H_{\text{max}}(L) \) are somewhat subjective, but certainly quite conservative, as can be seen from visual inspection. Should \( L \to \infty \) extrapolation produce a definitely negative value of \( H_{\text{max}} \), one could be sure that the finite slope is a finite-size artifact. However, we have found \( H_{\text{max}}(\infty) = 0.01±0.02 \) from a rather good scaling of our data against \( L^{-1} \).

Bearing in mind that the only \textit{“small”} typical field naturally arising in the problem, \( H_{KT} \), is one order of magnitude larger than this \([\text{thus a strictly positive} \ H_{max}(\infty) \ \text{of order} \ 10^{-2} \ \text{would have no clear physical origin}]\), we interpret the above result as signaling that \( H_{\text{max}}(\infty) \) is \textit{exactly} zero. So, (i) the critical line does leave the origin at a finite slope (for which our best estimate, 4.74±0.15, comes from extrapolation of the \( S_L \) against \( L^{-2} \)); but (ii) the straight-line part of the critical curve is of zero extent: one only has \( d^2T_c/dH^2 \neq 0 \) at the origin. This latter quantity must be negative for all \( H > 0 \), as no inflection points are expected.

These conclusions are consistent with the presence of a critical phase on the \( H \) axis near the origin. The exponentially diverging correlation length \([25] \) at \( H = 0, T = 0 \) is roughly in balance with the (already infinite) \( \xi_4(T) \) along the zero-temperature axis. This way the critical line, where crossover between temperature- and field-dominated behavior takes place, starts at finite angles with both axes.

Going back to extrapolation of the critical line for \( 0 < H \approx 0.15 \), we first note that, by construction, our procedure of fixed-\( H \) extrapolation automatically yields a straight line with slope 4.74±0.15 for all \( H \leq H_{\text{max}}(18) \approx 0.09 \). From the preceding arguments on the extent of the straight-line part, and concavity, of the critical curve, this is an upper limit: \( T_{\text{crit}}^r(H) \approx T_{\text{crit}}^l(H) \). Also, for \( 0.09 \leq H \leq 0.15 \) we have not managed to produce good fits with single powers; instead, we were forced to resort to two-power fits using \( L^{-1} \) and \( L^{-2} \). These facts have strong effects on the evaluation of \( c \) and \( \eta \) near \( H = 0 \), which we now turn to discuss.

Recall that at \( T = H = 0 \) one has \([25,13] \) \( c = 1 \) and \( \eta = 1/2 \), while for \( H 
eq 0 \) the three-state Potts values \( c = 4/5 \), \( \eta = 4/15 \) are believed to hold \([9]\). Our results for \( c \) and \( \eta \) along the extrapolated critical line, near the origin, are shown in Fig. 2. From the discussion in Sec. II one might assume that, apart from higher-order crossover effects, both quantities should behave in a step-function fashion. On the contrary, we see that they hover around their zero-field values for a significant range of \( H \), which coincides with that

\[ \begin{align*}
H_{\text{max}}(L) & \approx \frac{1}{\pi} \ln \left( \frac{L}{L_0} \right) + \text{constant} \\
S_L & \approx \\
\end{align*} \]
where our extrapolation gives a straight line. Further on along the \( H \) axis, convergence begins to deteriorate. Taking into account (i) the conclusion that straight-line sections of PRG curves are finite-size effects; (ii) the inescapable distortion imposed by them on our constant-\( H \) extrapolations; plus (iii) the fact that the true critical line is only expected to be straight at the origin, where it is joined by the KT line, we tentatively interpret the plateau-like behavior of \( c \) and \( \eta \) as a manifestation of the KT phase in an artificial, finite-size-induced fashion. We have not yet managed to propose a numerical test of this idea; however, as shown in the next section, a measure of self-consistency of the argument is numerical test of this idea; however, as shown in the next section, a measure of self-consistency of the argument is

\[ \text{estimated resulting from a three-point fit, were then extrapolated by a Bulirsch-Stoer algorithm [26], which essentially amounts to assuming a single-power correction to scaling. Our best fit corresponded to that power being around 2.} \]

\[ \text{The unitary value of } c \text{ has been predicted for the case [28,29] and is consistent with continuously-varying critical exponents [14], thus one might expect, e.g., a KT phase on the } T=0 \text{ axis, by analogy with TIAF. We shall return to this point below. Our result for } \eta \text{ apparently contradicts the direct evaluation of correlation functions of Ref. [30], which yields } \eta=1.33\pm0.02. \text{ To explain this, we recall the prediction of Ref. [4] which, for SPAF-3 with only first-neighbor interactions (in their language: } \nu=1, \mu=2\pi/3, \gamma_K=1/2), \text{ reads} \]

\[ G(r) \approx \frac{A}{r^{4/3}} + \frac{B}{r^{1/3}}, \quad (11) \]

\( G(r) \) is the critical \( (T=0) \) spin-spin correlation function at distance \( r \); the sign of the second term depends on whether the two sites are on the same sublattice [4], that is, it is associated to the staggered magnetization. The result of Ref. [30] is for correlations between spins on opposite corners of \( N \times N \) finite lattices with \( N \ll 15 \), thus it gives the decay of the uniform magnetization, dominated at short distances by the first term of Eq. (11). Indeed, a plot of their data in the form \( r^{4/3} G(r) \) against \( r \) appears to approach a straight line for large \( r \), with \( A=1.4 \) and \( B=5 \times 10^{-3} \). On the other hand, by relying on the amplitude-exponent relation given by conformal invariance [17], our approach automatically picks up the behavior of the smallest gap (or longest correlation length) of the transfer matrix, which indeed couples to the staggered magnetization. These considerations were very recently rederived via a height representation of the model [31] and confirmed by numerical work [32]. In the present case, our estimate is entirely consistent with the second term of Eq. (11), and also with Monte Carlo work [32,33].

We have paid special attention to the shape of the critical curve near the origin. Throughout the range \( 0.002 \ll H < 0.011 \), we managed good fits to Eq. (6) with \( \psi \) in the range 4.9–6.7. For now, we concentrate on the analysis of that region.

We recall that, although it is agreed that in zero field the system is critical only at \( T=0 \), there seems to be no consensus about how the correlation length diverges, except in that an exponential singularity \( \xi(T \to 0, H = 0) = \text{exp}(\alpha/T^\nu) \) is present. The value of \( \nu \) has been variously estimated as \( 1.3 \) (by analysis of the Roomany-Wyld approximant [34] in a transfer-matrix calculation [3], and Monte Carlo (MC) work [33]); \( 1 \) (further Monte Carlo work [35] and 3/4 (conformal invariance arguments coupled with an analysis of the eigenvalue spectrum of the transfer matrix [28]).

If we assume that, along the \( T=0 \) axis, \( H \) is a relevant variable with scaling index \( y_H \), a standard crossover argument [6] implies that on the critical curve \( T_{\text{c,ext}} \sim |\ln H|^{1/y_H} \). If, on the other hand, an extended critical phase is present as in TIAF, the results of Sec. III indicate that such shape is unlikely to be found. To be fair, we must point out that there is no compelling symmetry-based argument (such as vortex unpinning for TIAF [12,13]) that leads one to infer the possible existence of a soft phase here.

In Fig. 3 we show our results for \( T_{\text{c,ext}} |\ln H|^{1/y_H} \) against \( H \) for \( x = 3/4, 1, 4/3 \) as well as our best fit for an asymptotically
ties behave close to step-functions, converging to the respec-
tive Ising values \( c = 1/2, \eta = 1/4 \). At \( H = 0.5 \) the curve for \( c \) has a minimum. We used strips of width \( L \leq 14 \) to produce an accurate estimate both of \( T_c \) and \( c \), which turned out as \( c = 0.47 \pm 0.002 \). Thus we conclude that the (unaccounted for) residual crossover effects produce deviations of order at most \( \sim 6\% \).

V. CONCLUSIONS

We have studied critical properties of field-induced phase transitions of selected two-dimensional antiferromagnets with discrete-symmetry order parameters. Throughout our work, we attempted to minimize numerical effects originating from crossover between different universality classes, by applying carefully selected procedures both for finite-size calculations and for extrapolation of finite-size data to the infinite-lattice limit. For TIAF we did not entirely succeed, owing mainly to residual effects ascribed to a Kosterlitz-Thouless phase along the zero-temperature axis. For SPAF-3, where our evidence shows that such phase is not present, we present results which are clean and unambiguous, for all quantities investigated.

Our main findings are summarized as follows. For TIAF, we have shown that the critical line leaves the zero-temperature, zero-field fixed point at a finite angle. Our best estimate of the slope at the origin is \( (dT_c/dH)_{T-0} = 4.74 \pm 0.15 \). For SPAF-3 we provided evidence that the zero-field correlation length diverges as \( \xi(T \to 0, H = 0) = \exp(\alpha T^{-1}) \), with \( x = 1.08 \pm 0.13 \), through analysis of the critical curve at \( H \neq 0 \) plus crossover arguments. For SPAF-3 we have also ascertained that the conformal anomaly and decay-of-correlations exponent behave as \( (a) \ H = 0: c = 1, \eta = 1/3; (b) H \neq 0: c = 1/2, \eta = 1/4 \).

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