Critical Behavior of the Two-Dimensional Ising Susceptibility

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We report computations of the short- and long-distance (scaling) contributions to the square-lattice Ising susceptibility. Both computations rely on summation of correlation functions, obtained using nonlinear partial difference equations. In terms of a temperature variable τ, linear in $T/T_c - 1$, the short-distance terms have the form $\tau^p(\ln|\tau|)^q$ with $p \geq q^2$. A high- and low-temperature series of $N = 323$ terms, generated using an algorithm of complexity $O(N^6)$, are analyzed to obtain the scaling part, which when divided by the leading $|\tau|^{-7/4}$ singularity contains only integer powers of τ. Contributions of distinct irrelevant variables are identified and quantified at leading orders $|\tau|^{9/4}$ and $|\tau|^{17/4}$.

I. Introduction.— The two-dimensional Ising model has been extremely useful as a testing ground for new theoretical ideas and methods in the study of phase transitions and critical phenomena. Our present understanding is the result of a series of dramatic developments spanning more than half a century, starting with Onsager's exact computation of the free energy [1], followed by Yang's derivation of the spontaneous magnetization [2] and by the work of many researchers on the correlation functions, including Toeplitz determinantal formulas [3], exact expressions for their behavior at large separation [4], and nonlinear partial difference equations for their efficient computation [5–7], to mention only those results which are used in the present work. All results above apply to the zero-field case. While an exact expression for the susceptibility as the sum of two-point correlation functions over all separations [4] exists, a useful closed form expression does not. Moreover, as we discuss, there are strong indications that the susceptibility has a natural boundary in the complex plane [8,9], a feature which rules out any expression in terms of the "standard" functions of mathematical physics.

Nevertheless, it is desirable to obtain as detailed information about the susceptibility as possible, not only because of its physical importance, but also because of the significant role it plays in ideas about scaling and the renormalization group. In the vicinity of the ferromagnetic critical point at temperature $T = T_c$, the susceptibility exhibits a singularity of the form

$$\beta^{-1}\chi_\pm = C_{0_\pm}(2K_c\sqrt{2})^{7/4}|\tau|^{-7/4}F_\pm(\tau) + B(\tau). \quad (1)$$

Here $\beta = (k_BT)^{-1}$, $\tau = \frac{1}{2}(s^{-1} - s)$, $s = \sinh 2K$, and $\sinh 2K_c = 1$ with $K = \beta J$ the conventional Ising model coupling constant. The scaling-amplitude functions $F_\pm(\tau)$ are normalized to unity at $\tau = 0$. As a consequence of the exact knowledge of the long-range correlations, the coefficients $C_{0_\pm}$ were calculated exactly [10] in terms of the

solution of a Painlevé III equation. Additionally, the leading behavior of both $F_\pm(\tau)$ was computed to be $1 + \frac{1}{2}\tau$. The antiferromagnetic susceptibility, on the other hand, is dominated by the short-distance correlation functions and has leading singularity (const $\times \tau \ln|\tau|$). Such short-distance "background" terms are present as well in the ferromagnetic susceptibility and are denoted by $B(\tau)$ in (1). The leading amplitudes of the analytic and singular parts of $B(\tau)$ were computed for a general wave vector dependent susceptibility in [11,12].

An analysis [13] of a 51 term high-temperature series by means of differential approximants yielded two further correction terms in the scaling-amplitude function F_+, with numerical amplitudes close to rational values, $\frac{5}{8}\tau^2 + \frac{3}{16}\tau^3$, and confirmed that the same scaling-amplitude function is numerically consistent with the first 11 terms in the low-temperature expansion. These results agreed with the prediction [14] that the corrections to scaling are entirely due to the nonlinearity of the scaling fields and not to the presence of irrelevant operators [14]. However, a recent analysis of 115 term high- and low-temperature series [15] showed that this prediction appears to break down in the amplitude of τ^4.

The study reported in this Letter substantially improves on all the above results. We extend the methods of [11,12] to compute both antiferromagnetic and ferromagnetic background amplitudes on the isotropic lattice to $O(\tau^{14})$. All such terms are seen to be of the form $\tau^p(\ln|\tau|)^q$ with $p \geq q^2$. We simultaneously compute high-temperature series to order 323 and low-temperature series to order 646 in 123 h on a 500 MHz DEC Alpha with 21164 processor running MAPLE™ V version 5.1.

We analyze these series by two independent methods, making use of the computed background amplitudes and the known complex singularity structure [9,15] to obtain the scaling-amplitude functions $F_\pm$ to $O(\tau^{14})$.

Several important conclusions can be drawn from our results. First, only pure integer powers of τ enter the

scaling-amplitude functions and no logarithmic terms are present. Second, the high- and low-temperature scaling-amplitude functions are not equal to each other. The amplitudes start to differ at $O(\tau^6)$. Third, the coefficients of τ^4 and τ^5, which are clearly rational, are not those predicted by simple two-variable scaling [14]. We surmise that at least two irrelevant operators must be invoked to account for the above results—one entering at τ^4, the other at τ^6.

Further remarks on the scaling implications of our work can be found in section V, while the remainder of the Letter will outline the methods by which the ferromagnetic results were obtained. A fuller account, including details of the antiferromagnetic singularity, will appear elsewhere.

II. Singularity structure and natural boundary.—It was argued in [8] that on the anisotropic lattice, the contribution to the susceptibility of the high-temperature graphs with $2N$ vertical bonds contains more and more poles as N increases, and that in the limit $N \to \infty$ these poles form a dense set in the complex plane. In [9] it was shown that in the expansion of the susceptibility in j-particle contributions [4]

$$\beta^{-1}\chi = \begin{cases} \sum_{j \text{ odd}} \chi^{(j)} & T > T_c, \\ \sum_{j \text{ even}} \chi^{(j)} & T < T_c, \end{cases} \qquad (2)$$

the higher-particle components give rise to an ever increasing number of singularities that appear to form a dense set on the circle $|s| = 1$. In fact, the two phenomena are precisely correlated, with the former being the highly anisotropic limit, and the latter the isotropic limit, of the set of singularities for the generic anisotropic model. These occur at

$$\cosh(2K)\cosh(2K') - \sinh(2K)\cos\frac{2\pi m}{j} -$$
$$\sinh(2K')\cos\frac{2\pi m'}{j} = 0, \quad (3)$$

with $m, m' = 1, 2, \ldots j$, and $K, K' = \beta J_x, \beta J_y$. It will be noted that the left-hand side of (3) is the denominator in the Onsager integral for the free energy and thus we find the (to us) surprising result that the singularity structure of $\chi^{(j)}$, a property of the Ising model in a magnetic field, is intimately connected with a property in zero field. Barring unexpected cancellation in the $j \to \infty$ limit (and we have evidence against this) we believe that this set forms a natural boundary.

Since the critical point lies on this natural boundary the expansion (1) cannot be convergent; that (1) defines an asymptotic expansion is suggested by the following argument: In the τ plane, the singularities defined by (3) lie on the imaginary τ axis and each singularity is a branch point [9,15]. With the branch cuts chosen to point away from $\tau = 0$ one can show the cumulative discontinuity of either χ_+ or χ_- across the cut at $\tau = i\mathcal{T}$, $\mathcal{T} \to 0$, scales as $\exp(-a/\mathcal{T}^2)$ with $a = 39.76$. The contribution of a cut discontinuity of this form to the coefficient of τ^p in (1) is proportional to $\Gamma(p/2)/a^{p/2}$ as $p \to \infty$. Because $a \, (= 39.76)$ is large this contribution is numerically tiny

in all of the series terms we can generate and in particular we cannot tell whether the divergence with p applies to the long-distance or the short-distance part in (1), or some combination of the two. In a practical (numerical) sense the natural boundary is of no consequence and its very existence is ignored for the remaining analysis discussed below.

III. Computation of short-distance amplitudes and high- and low-temperature series.—The essential tool for the computation of both the background amplitudes and the high- and low-temperature series coefficients is the set of nonlinear partial difference equations for the two-point correlation functions $C(m, n) = \langle \sigma_{00}\sigma_{mn} \rangle$, given in [6]. These completely determine all the off-diagonal two-point functions once the diagonal ones ($m = n$) are given. The latter can be computed either by means of an independent set of difference equations [7] or, as we have done here, directly from the Toeplitz determinant expressions. The susceptibility, $\beta^{-1}\chi = \sum [C(m, n) - \langle \sigma_{00} \rangle^2]$, is computed by successively adding the contributions of pairs of square shells $C_N = \sum C(m, n)$ with $|m| + |n| = 2N$ and $|m| + |n| = 2N + 1$.

The implementation of the difference equations to obtain high- and low-temperature expansions is straightforward using the multiple precision integer arithmetic capabilities of MAPLE™ or MATHEMATICA™, and the time complexity is no worse than $O(N^6)$.

The key to computing the short-distance background amplitudes is to obtain expansions of the partial sums $S_N = \sum_{n=0}^{N} C_n$ in τ directly and to identify which terms in the series contribute to the short-distance part and which to the long-distance part. A combination of analytic work and numerical fitting leads us to a conjecture for the short-distance expansion of the shell sums, namely

$$\sqrt{s}\, C_N = N^{3/4} \sum_{p=0}^{\infty} (\ln|N\tau|)^p (N\tau)^{p^2} A_N^{(p)}, \qquad (4)$$

where the $A_N^{(p)}$ are Taylor series in τ with coefficients that are asymptotic Laurent series in N^{-1}; the highest power of N multiplying τ^q in $A_N^{(p)}$ is N^q. The partial sums S_N are

$$\sqrt{s}\, S_N = \sqrt{s} \sum_{n=0}^{N} C_n = \sum_{q=0}^{\infty} \sum_{p=q^2} R_N^{(p,q)} \tau^p (\ln|\tau|)^q \quad (5)$$

with $R_N^{(p,q)}$ functions of N only. Asymptotically, for large N, $R_N^{(p,q)}$ is a sum of powers $N^{7/4+p'}$, with possible multiplicative $\ln(N)$ corrections, plus a constant $b^{(p,q)}$ which arises from the small n terms in the sum (5) where the asymptotic expressions are not valid and sum and integral are not synonymous. The p' are integers $p' \leq p$.

We must assume that (5) remains valid up to N of the order $1/\tau$ where it can, in principle, be matched term by term to a large distance expansion that properly describes the roughly exponential $\exp(-N\tau)$ decay of correlations as $N \to \infty$. Explicit matching formed the basis of the previous calculations of terms in the short-distance χ (cf. [11,12]) but this becomes extremely cumbersome at higher order. Here we argue that the exponential decay

implies a cutoff on N that is proportional to $1/\tau$ and that we can identify the temperature behavior of terms in S_N in Eq. (5) by the replacement $N \to 1/\tau$. All terms whose variation is as a fractional power of τ, with possibly logarithmic multipliers, are discarded as assumed contributions to the long-distance part of χ. Clearly all that remains is the constant part of $R_N^{(p,q)}$, namely $b^{(p,q)}$, and this is extracted by numerical fitting to give

$$\sqrt{s}\, B = \sum_{q=0} \sum_{p=q^2} b^{(p,q)} \tau^p (\ln|\tau|)^q \qquad (6)$$

for the short-distance part of χ in Eq. (1). The coefficients $b^{(p,q)}$ must be determined to very high accuracy to be useful for the subtraction procedure described in the next section; the complete list for $p < 15$ will be given elsewhere. The result $p \geq q^2$ we call the fermionic constraint since it can be traced back to the Toeplitz determinant that led to the correlations of the form in Eq. (4).

IV. Scaling amplitudes.—The contribution of the short-distance terms may now be subtracted from the high- and low-temperature series, leaving the long-distance part, from which the scaling amplitudes may be computed using any of a variety of series analysis techniques. Such analysis is vastly simplified by the observation that there are no logarithmic or noninteger power contributions to the scaling-amplitude functions $F_\pm$.

To show this, independently of any fitting procedure, we have noted that any contribution to $F_\pm$ which is not a positive integer power of τ would manifest itself in the high order series coefficients of the scaled susceptibility, $(1 - s^{\pm 4})^{-1/4} \chi_\pm$. The $1 + \tau/2$ terms in $F_\pm$, as poles in the scaled susceptibility, also contribute but as their residues proportional to $C_{0_\pm}$ are known to high precision, they can be subtracted. The residual coefficients are comparable in magnitude to those expected from the first ne-

glected short-distance term which enters at τ^{15}. We may place limits on the size of the amplitudes of any putative nonanalytic terms in the scaling-amplitude functions. For example, for terms of the form $A_p \tau^p \ln|\tau|$, the bounds,

$$|A_p| < 10^{-35} 300^p / \Gamma(p-1), \qquad T > T_c, \quad (7)$$

$$|A_p| < 10^{-37} 600^p / \Gamma(p-1), \qquad T < T_c, \quad (8)$$

reasonably exclude all p less than about 15.

On purely numerical grounds, the absence of logarithmic corrections is surprising since it implies the cancellation of the many logarithmic multipliers in the scaling terms we discarded in the previous section. On the other hand, the absence of logarithms appears to be a requirement of the combination of the fermionic constraint $p \geq q^2$ in (5) and renormalization group scaling as discussed in the next section.

To compute the coefficients of the integer powers of τ in the scaling-amplitude functions $F_\pm$, we have carried out two independent analyses, one in the s plane, the other in the v plane, where $v = \tanh K$ is the conventional high-temperature variable. The natural boundary singularities at $|s| = 1$ are mapped to two circles, $|v \pm 1| = \sqrt{2}$. As they are farther from the origin than the ferromagnetic and antiferromagnetic singularities at $v = \pm(\sqrt{2} - 1)$ their amplitudes are exponentially damped and may be neglected in the analysis. The s-plane analysis must take account of these singularities explicitly. The two analyses are in complete agreement.

We find numerically that the scaling-amplitude functions multiplied by $\sqrt{s}$ appear to be even functions of τ, the coefficients of the odd terms being comparable in magnitude to the uncertainties in the even coefficients. The rational coefficients of τ^2 and τ^4 below we conjecture to be exact, and these values were fixed in the final fitting. The results, with uncertainty only in the final digits, are

$$\sqrt{s}\, F_+ = 1 + \tau^2/2 - \tau^4/12 - 0.123\,529\,228\,575\,208\,666\,3\tau^6 + 0.136\,610\,949\,809\,095\tau^8$$
$$- 0.130\,438\,972\,13\tau^{10} + 0.121\,512\,9\tau^{12} - 0.113\tau^{14} + O(\tau^{15}),$$

$$\sqrt{s}\, F_- = 1 + \tau^2/2 - \tau^4/12 - 6.321\,306\,840\,495\,936\,623\,067\tau^6 + 6.251\,997\,470\,460\,243\,29\tau^8$$
$$- 5.689\,659\,975\,618\,0\tau^{10} + 5.142\,218\,271\tau^{12} - 4.674\,72\tau^{14} + O(\tau^{15}). \qquad (9)$$

V. Comparison with scaling predictions.—Prior to the analysis of [15], all known amplitudes were in agreement with the hypothesis that corrections to scaling were due to scaling-field nonlinearity, and not to the presence of irrelevant variables. Here for the first time, we quantify the error in this "simple" scaling theory. Ignoring irrelevant operators, the expressions for the free energy, magnetization, and susceptibility in zero magnetic field are [14]

$$f(\tau) = -A[a_0(\tau)]^2 \ln|a_0(\tau)| + A_0(\tau),$$
$$M(\tau < 0) = B b_1(\tau) |a_0(\tau)|^{1/8},$$
$$\beta^{-1} \chi_\pm(\tau) = C_\pm [b_1(\tau)]^2 |a_0(\tau)|^{-7/4}$$
$$\qquad\qquad - E a_2(\tau) a_0(\tau) \ln|a_0(\tau)| + D(\tau),$$

$$(10)$$

where A, B, $C_\pm$, and E are constants and $A_0(\tau)$ and $D(\tau)$ are analytic functions of τ. The functions $a_0(\tau)$ and $b_1(\tau)$ are the leading terms in the expansion of the scaling fields, and can be determined from the free energy and magnetization. The result for $\chi_\pm$ is of the form (1) but with F replacing $F_\pm$ where

$$\sqrt{s}\, F = 1 + \frac{\tau^2}{2} - \frac{31\tau^4}{384} + \frac{125\tau^6}{3072} + O(\tau^8). \quad (11)$$

Note that this expression should hold in both temperature regimes.

The difference between (9) and (11) we believe to be due to the effects of one or more irrelevant operators, confluent with the simple scaling terms. As there is no free parameter to vary in the model, we cannot identify these operators from the information we have. However, it is likely that there are at least two mechanisms at work, one entering at $O(\tau^4)$ which preserves the equality of F_+ and F_-, and a second entering at $O(\tau^6)$ which breaks this symmetry. In order to probe these effects further, we hope to study the model with anisotropy, and on other periodic lattices.

The corrections to scaling we have found are confluent with expected analytic terms and in the renormalization group picture of scaling this leads to the possibility of logarithmic terms as well (cf. [16]). Logarithmic corrections are not demanded—the issue is whether the scaling fields are coupled and this depends on microscopic details. Barma and Fisher [17] have investigated a model renormalization group flow in detail and conclude that in the case of a confluence, here labeled by integer index m, one must expect either no coupling between fields or corrections of the form $(\tau^m \log|\tau|)^k$ to all order k. Since the latter violates the fermionic constraint $mk \geq k^2$ we conclude there cannot be *any* logarithmic terms in the scaling-amplitude function $F_\pm$ as we have verified to $O(\tau^{15})$.

In conclusion we would like to emphasize the power and utility of the nonlinear recursion relations [6] in numerical studies such as we have described. Our results could not have been obtained without them and since they generalize to many-point functions [18] one can begin to consider analyzing other models such as the "double Gaussian" [17] to further clarify the nature of corrections to scaling and test various renormalization group and conformal field theory assumptions.

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