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Complex-temperature singularities of the susceptibility in the $d = 2$ Ising model: I. Square lattice

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Abstract. We investigate the complex-temperature singularities of the susceptibility of the 2D Ising model on a square lattice. From an analysis of low-temperature series expansions, we find evidence that, as one approaches the point $u = u_s = -1$ (where $u = e^{-4K}$) from within the complex extensions of the FM or AFM phases, the susceptibility has a divergent singularity of the form $\chi \sim A'_s(1+u)^{-\gamma'_s}$ with exponent $\gamma'_s = \frac{3}{2}$. The critical amplitude A'_s is calculated. Other critical exponents are found to be $\alpha'_s = \alpha_s = 0$ and $\beta_s = \frac{1}{4}$, so that the scaling relation $\alpha'_s + 2\beta_s + \gamma'_s = 2$ is satisfied. However, using exact results for β_s on the square, triangular, and honeycomb lattices, we show that universality is violated at this singularity: β_s is lattice-dependent. Finally, from an analysis of spin–spin correlation functions, we demonstrate that the correlation length and hence susceptibility are finite as one approaches the point $u = -1$ from within the symmetric phase. This is confirmed by an explicit study of high-temperature series expansions.

1. Introduction

Although exact closed-form expressions for the (zero-field) free energy and spontaneous magnetization of the two-dimensional Ising model were calculated long ago, no such expression has ever been found for the susceptibility, and this remains one of the classic unsolved problems in statistical mechanics. Any new piece of information on the susceptibility is thus of value, especially insofar as it specifies properties which an exact solution must satisfy. In particular, it is of interest to better understand the properties of the susceptibility as an analytic function of complex temperature. Several years ago, some results on complex-temperature singularities of the susceptibility for the Ising model were reported [1]. Here we continue the study of complex-temperature singularities of the susceptibility of the 2D Ising model.

2. Generalities and discussion of complex extensions of physical phases

We consider the Ising model on a lattice Λ at a temperature T and external magnetic field H defined in standard notation by the partition function

$$Z = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}} \tag{2.1}$$

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with the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i \tag{2.2}$$

where $\sigma_i = \pm 1$ are the Z_2 variables on each site i of the lattice, $\beta = (k_B T)^{-1}$, J is the exchange constant, $\langle ij \rangle$ denote nearest-neighbour pairs, and the magnetic moment $\mu \equiv 1$. Here we shall concentrate on the square (sq) lattice, but also make some comments for the triangular (t) and honeycomb (hc) lattices. We use the standard notation $K = \beta J$ and $h = \beta H$,

$$v = \tanh K \tag{2.3}$$

$$z = e^{-2K} = \frac{1 - v}{1 + v} \tag{2.4}$$

and

$$u = z^2 = e^{-4K} . \tag{2.5}$$

It will also be useful to express certain quantities in terms of the elliptic moduli $k_<$ and $k_> \equiv 1/k_<$. For the square lattice these are given by

$$k_< = \frac{1}{\sinh(2K)^2} = \frac{4u}{(1 - u)^2} \tag{2.6}$$

and

$$k_> = \frac{4v^2}{(1 - v^2)^2} . \tag{2.7}$$

We note the symmetries

$$K \to -K \Rightarrow \{v \to -v,\ z \to 1/z,\ u \to 1/u,\ k_x \to k_x\} \tag{2.8}$$

where $k_x = k_<$ or $k_>$. The reduced free energy per site is $f = -\beta F = \lim_{N\to\infty} N^{-1} \ln Z$ (where N denotes the number of sites on the lattice), and the zero-field susceptibility is $\chi_0 = \partial M(H)/\partial H|_{H=0}$, where $M(H)$ denotes the magnetization. Henceforth, unless otherwise stated, we only consider the case of zero external field and drop the subscript on χ_0. It is convenient to define the related quantity

$$\bar{\chi} \equiv \beta^{-1} \chi . \tag{2.9}$$

For the square (sq) lattice, $f(K, h = 0)$ was originally calculated by Onsager [2], and the expression for the spontaneous magnetization M was first reported by Onsager and calculated by Yang [3]. Solutions for $f(K, h = 0)$ and M were subsequently given for the triangular (t) and honeycomb or hexagonal (hc) lattices; for reviews, see [4–6]. We denote the critical coupling separating the symmetric, paramagnetic (PM) high-temperature phase from the phase with spontaneously broken Z_2 symmetry and ferromagnetic (FM) long-range order as K_c and recall that for the square lattice, $v_c = z_c = \sqrt{2} - 1$.

Here we shall study the susceptibility as a function of complex (inverse) temperature, K. For our purposes, it is important to discuss generalized notions of phases and thermodynamic quantities. *We define a complex extension of a phase as an extension, to complex K, of the physical phase which exists on a given segment of the real K-axis.* As noted, for example, in [1], for zero external field, there is an infinite periodicity in complex K under certain shifts along the imaginary K-axis, as a consequence of the fact that the spin–spin interaction on each link $\langle ij \rangle$ is $\sigma_i \sigma_j = \pm 1$. In particular, there is an infinite repetition of phases as functions of complex K; this infinitely repeated set of phases is reduced to a single set by using the variables v, z and/or u, since these latter variables have very simple properties under complex shifts in K:

$$K \to K + ni\pi \Rightarrow \{v \to v, \quad z \to z, \quad u \to u, \quad k_x \to k_x\} \tag{2.10}$$

$$K \to K + (2n+1)\frac{i\pi}{2} \Rightarrow \{v \to 1/v, \quad z \to -z, \quad u \to u, \quad k_x \to k_x\} \tag{2.11}$$

where n is an integer and, as before, $k_x = k_<$ or $k_>$. On a lattice with an even coordination number q, it is easily seen that these symmetries imply that the magnetization and susceptibility are functions of u only. Because the shift (2.11) leaves u invariant while mapping v to $1/v$, it maps a point in the FM phase (and its complex extension) to itself but maps a point in the (complex extension of the) PM phase out of this phase. Consequently, when studying complex-temperature properties of the model, it is more convenient to start within the FM phase, where the various quantities of interest can be expressed as Taylor series in the low-temperature expansion variable u. After this study, we shall proceed to investigate the properties of the susceptibility in the interior and boundary of the PM phase. It is useful to note that a given point v_0 or z_0 corresponds, in the complex K plane, to the set

$$K = K_0 + ni\pi \tag{2.12}$$

where $n \in Z$ and

$$K_0 = -\tfrac{1}{2}\ln z_0 \tag{2.13}$$

while a given point u_0 corresponds to the set

$$K = K_0 + \tfrac{1}{2}ni\pi \tag{2.14}$$

reflecting the structure of Riemann sheets of the logarithm.

The requisite complex extensions of the physical phases can be seen by using the known results on the locus of points on which the free energy is non-analytic. For the square lattice, these are given by the circles [7]

$$v_\pm(\theta) = \pm 1 + 2^{1/2}\,e^{i\theta} \qquad \text{i.e.} \quad z_\pm(\omega) = \pm 1 + 2^{1/2}\,e^{i\omega} \tag{2.15}$$

for $0 \leqslant \theta$ and $\omega < 2\pi$. Recall that the property that this locus of points are circles in both the high- and low-temperature variables v and z follows because these variables are related by the bilinear conformal transformation (2.4) which maps circles to circles. For later reference, these circles are shown in figures 1(*a*) and (*b*), respectively.

The circles in v or z constitute natural boundaries, within which the free energy is analytic but across which it cannot be analytically continued. They thus define the complex extensions of the physical phases which occur on the real v or z axes in the intervals $-v_c < v < v_c$ or $z_c < z < 1/z_c$ (PM), $v_c < v \leqslant 1$ or $0 \leqslant z < z_c$ (FM), and $-1 < v < -v_c$ or $1/z_c < z < \infty$ (AFM).

Using the general fact that the high-temperature expansions and (for discrete spin models such as the Ising model) the low-temperature expansions both have finite radii of convergence, we can use standard analytic continuation arguments to establish that not just the free energy, but also the magnetization and susceptibility are analytic functions within each of the complex-extended phases. This defines these functions as analytic functions of the respective complex variable (K, v, z, u, or others obtained from these). Of course, these functions are, in general, complex away from the physical line $-\infty < K < \infty$.

We shall also need a definition of singularity exponents of a function at a complex singular point. In the case of real K, one distinguishes, *a priori*, the critical exponent

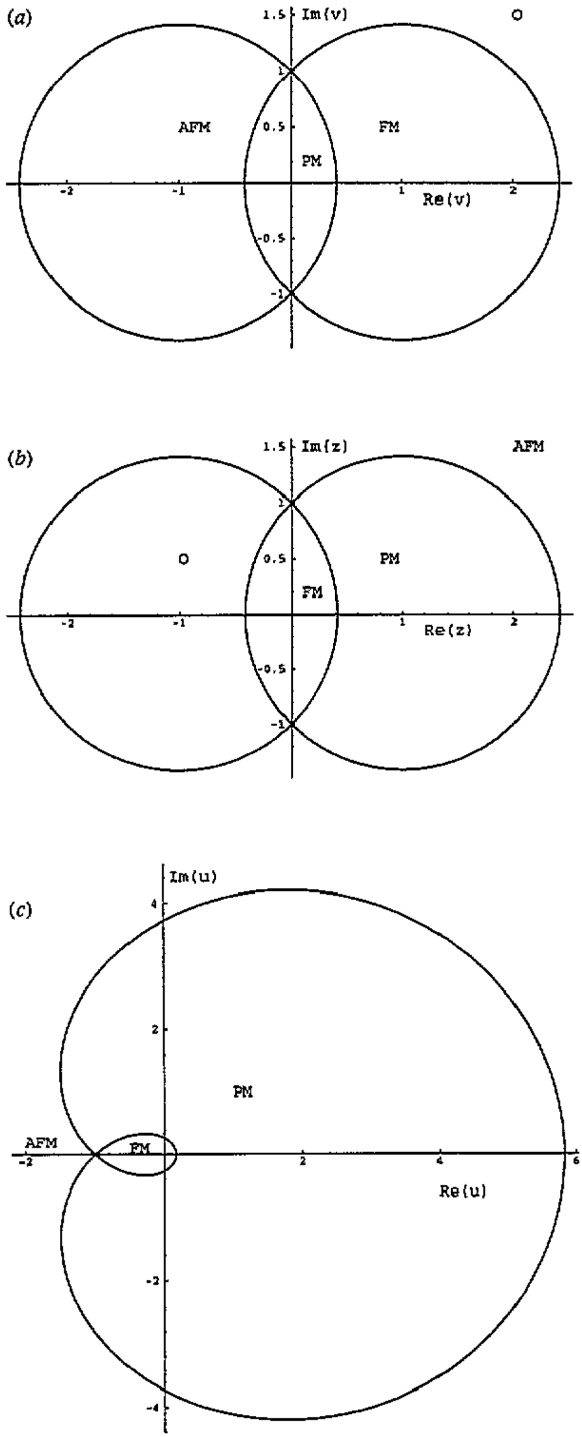

Figure 1. Phases and associated boundaries in the complex variables (*a*) v, (*b*) z, and (*c*) u, as defined in (2.3)–(2.5). In the variable $k_<$ defined in (2.6), the complex FM and AFM phases are mapped into the interior of the unit circle, and the PM phase to the exterior of this circle.

which describes the singular behaviour at a critical point approached from the symmetric, high-temperature phase from the corresponding exponent for the approach from the broken-symmetry, low-temperature phase. For a singular point in the complex plane, we shall again distinguish the critical exponents describing the singularity as approached from different phases. Thus, for the susceptibility $\bar{\chi}(\zeta)$ (where ζ refers to one of the complex variables listed before) which fails to be analytic at one or more singular point(s) $\{\zeta_s\}$, if the leading singularity in $\bar{\chi}(\zeta)$ can be represented in the power-law form

$$\bar{\chi}(\zeta)_{\text{sing.}} \sim (1 - \zeta/\zeta_s)^{-\gamma_{s,p}} \tag{2.16}$$

as ζ approaches ζ_s from within the the phase p, we shall refer to ζ_s as a complex singular point and $\gamma_{s,p}$ as the corresponding critical or singularity exponent for the approach to ζ_s from this phase. By analogy to standard usage for physical temperature, we shall set $\gamma_{s,\text{FM}} = \gamma_s'$ and $\gamma_{s,\text{PM}} = \gamma_s$ to refer to the critical exponents at ζ_s as approached from within the complex extensions of the FM and PM phases, respectively. We shall show that for the specific point $u_s = -1$, $\gamma_{s,\text{AFM}} = \gamma_{s,\text{FM}}$. Critical exponents for other quantities at complex-temperature singular points are defined in an analogous manner. The locus of points ζ_s where a given function is singular in the complex ζ plane will not, in general, be a discrete set, in contrast to the case for the Ising model on the physical, real K axis. This is illustrated by the locus of points (2.15) where the free energy is singular. Even for a function like the magnetization, which, in the complex FM phase where it is non-vanishing, is an algebraic function in $\zeta = k_<$ or $\zeta = z$ of the form $M = \prod_{j=1}^{n_s}(\zeta - \zeta_s)^{\beta_s}$, the discrete points ζ_s also in general involve associated branch cuts, since the exponents β_s are not integers.

It should be noted that a phase may exist for complex v or z which is not the complex extension of any physical phase. An example of this phenomenon occurs in the present case; the fourth region, denoted O in figures 1(a) and (b) constitutes such a phase.

In contrast to the usual ferromagnetic critical point of the Ising model, which can be approached only within the PM phase or FM phase (and similarly, the AFM critical point of this model, which can be approached only from within the PM or AFM phase), a general complex singularity may be approached from within more than two phases. For example, in figure 1 the singularities at $v = \pm i$, or equivalently, $z = \pm i$, can be approached from within the PM, FM, or AFM complex-extended phases, or, indeed, from the region O which is not analytically connected to any physical phase.

Since for the square lattice $\bar{\chi}(z)$ has the symmetry noted above, $\bar{\chi}(z) = \bar{\chi}(-z)$, it is useful to display the complex-extended phases as functions of u. Under the conformal transformation $u = z^2$, the circles in figure 1(b) are mapped to a single curve, which is a type of limaçon of Pascal, defined by

$$\text{Re}(u) = 1 + 2^{3/2}\cos\omega + 2\cos 2\omega \tag{2.17}$$

$$\text{Im}(u) = 2^{3/2}\sin\omega + 2\sin 2\omega \tag{2.18}$$

traced out completely for $0 \leqslant \omega < 2\pi$. In this variable, there are three complex-extended phases, as shown in figure 1(c): PM, FM, and AFM. The mapping from z to u reduced the number of complex-extended phases from the four which are present in the variable z or v to three; since the points in the O phase are related to those in the complex-extended PM phase by $z \to -z$, these two phases are mapped to a single phase in the u plane. The points $z = \pm i$, at which the PM, FM, AFM, and O phases are all contiguous, are mapped to the single point $u = u_s = -1$ in the u plane. In the terminology of algebraic geometry, the point $u_s = -1$ is a singular point, specifically a multiple point of index 2, of the limaçon (2.18) forming the natural boundary between the complex phases, whereas all other points on this curve, including the PM–FM critical point u_c and the PM–AFM critical point at $u = 1/u_c$, are regular (ordinary) points of the curve. Here, a multiple point of index n of a curve C is a point through which n arcs of C pass (see, for example, [8]). For later reference, the physical critical points are $u_c = 3 - 2\sqrt{2} = 0.171\,572\,875\ldots$ separating the PM and FM phases and $u_c^{-1} = 3 + 2\sqrt{2} = 5.828\,427\,1\ldots$ separating the PM and AFM phases. In the complex K plane, these correspond to the infinite set of critical points $K_c = \pm\frac{1}{2}\ln(1+\sqrt{2}) + ni\pi/2$, where $n \in Z$. Under the transformation $u \to 1/u$, the complex-extended PM phase maps onto itself, while the complex-extended FM phase maps to the AFM phase, and vice versa.

Finally, in terms of the elliptic moduli, the natural boundaries have the very simple form of the unit circle in the complex $k_<$ or $k_>$ planes:

$$k_< = 1/k_> = e^{i\theta} \tag{2.19}$$

with $0 \leqslant \theta < 2\pi$. These incorporate the symmetries

$$u \to 1/u \;\Rightarrow\; k_x \to k_x \tag{2.20}$$

$$v \to 1/v \;\Rightarrow\; k_x \to k_x \tag{2.21}$$

where k_x denotes $k_<$, $k_>$, or κ. Given the inversion symmetry (2.20), it follows that the transformation (2.6) from u to $k_<$ maps both the complex-extended FM and AFM phases onto the same region, which is the interior of the unit circle in the complex $k_<$ plane. The complex-extended PM phase is mapped to the exterior of this circle. Under the mapping, the actual limaçon in the u plane wraps around the unit circle in the $k_<$ plane twice. In particular, both the PM–FM critical point $u_{c,sq}$ and the PM–AFM critical point $1/u_c$ are mapped to the single point, $k_< = k_> = 1$. The complex-temperature singular point $u_s = -1$ is mapped to $k_< = k_> = -1$.

Having discussed these preliminaries, we proceed to study the susceptibility.

3. Analysis of low-temperature series

3.1. Analysis of series for $\bar{\chi}_r$ in the variable u

The low-temperature series expansion for $\bar{\chi}$ for the Ising model on the square lattice is

$$\bar{\chi} = 4u^2\left(1 + \sum_{n=1}^{\infty} c_n u^n\right). \tag{3.1}$$

This expansion has a finite radius of convergence and, by analytic continuation from the physical low-temperature interval $0 \leqslant u < u_c$, applies throughout the complex extension of the FM phase. Since the factor $4u^2$ is known exactly, it is convenient to study the reduced (r) function

$$\bar{\chi}_r \equiv 2^{-2}u^{-2}\bar{\chi} = 1 + \sum_{n=1}^{\infty} c_n u^n . \tag{3.2}$$

The expansion coefficients c_n were calculated to order $n = 9$ in 1971 by the King's College group [9] and were extended to order $n = 21$ by Baxter and Enting in 1978 [10] (with exact coefficients up to $n = 19$ and nearly exact $n = 20$ and 21 terms). Very recently, the c_n's have been calculated to order $n = 26$ (i.e. $\bar{\chi}$ to $O(u^{28})$) by Briggs *et al* [11], as part of a general calculation of low-temperature series for q-state Potts models with $q = 2$–10 on the square lattice. We have carried out a dlog Padé analysis of this series to investigate the singular behaviour of the susceptibility in the complex u plane. (For reviews of this method, see [14].) As one approaches a complex singular point denoted by 's' on the boundary of

Table 1. Values of u_s from Padé approximants to low-temperature series for $\bar{\chi}_r$ starting with the series to $O(u^{12})$. The superscript $*$ indicates that the approximant has one or more nearly coincident pole-zero pair(s) closer to the origin than u_s. Our criterion for near coincidence is that $|u_{pole} - u_{zero}| < 10^{-4}$.

N	$[(N-2)/N]$	$[(N-1)/N]$	$[N/N]$	$[(N+1)/N]$	$[(N+2)/N]$
6	—	−1.050 26	−1.076 08*	−0.992 720	−0.990 763
7	−1.090 18*	−1.036 35	−0.990 673	−0.992 677*	−1.007 52*
8	−1.000 60	−1.022 16	−1.003 63*	−0.997 028	−0.988 543
9	−1.007 62*	−1.186 78	−0.981 169	−0.995 418 5*	−0.996 322 5*
10	−0.983 770	−1.138 76*	−0.996 264*	−0.995 312*	−0.998 649*
11	−0.999 211	−1.003 98	−0.998 086*	−0.997 751 5*	−0.998 400*
12	−0.999 976*	−0.997 679*	−0.998 044*	−0.997 225*	—
13	−0.999 073*	−0.996 210*	—	—	—

Table 2. Values of γ_s' from Padé approximants to low-temperature series for $\bar{\chi}_r$ starting with the series to $O(u^{12})$.

N	$[(N-2)/N]$	$[(N-1)/N]$	$[N/N]$	$[(N+1)/N]$	$[(N+2)/N]$
6	—	1.975	2.174*	1.474	1.455
7	2.297*	1.879	1.454	1.474*	1.631*
8	1.563	1.771	1.583*	1.513	1.419
9	1.628*	1.533	1.321	1.497*	1.508*
10	1.358	1.732*	1.507*	1.496*	1.536*
11	1.545	1.605	1.528*	1.524*	1.533*
12	1.554*	1.523*	1.528*	1.517*	—
13	1.543*	1.503*	—	—	—

the complex-extended FM phase from within this phase, $\bar{\chi}$ is assumed to have the leading singularity (s)

$$\bar{\chi}(u) \sim A_s'(1 - u/u_s)^{-\gamma_s'}\big(1 + a_{1,s}(1 - u/u_s) + \cdots\big) \tag{3.3}$$

where A_s' and γ_s' denote, respectively, the critical amplitude and the corresponding critical exponent, and the dots ... represent analytic confluent corrections. One may observe that we have not included non-analytic confluent corrections to the scaling form in (3.3). The reason is that, although such terms are generally present at critical points in statistical mechanical models, previous studies have indicated that they are very weak or absent for the usual critical point of the 2D Ising model [12, 13]. The dlog Padé study then directly gives u_s and γ_s'. As noted above, the prefactor $4u^2$ is known and is analytic, so we actually carry out the dlog Padé study on $\bar{\chi}_r$. This study yields evidence for a divergent branch point singularity at a particular complex-temperature point, which we denote by u_s. (The use of u_s above referred to generic complex-temperature point(s), of which there might, *a priori*, be more than one; henceforth, we use this symbol to refer to the specific point found from the Padé study.) The results for u_s and γ_s' from the diagonal and near-diagonal approximants are listed in tables 1 and 2, starting with series for $\bar{\chi}_r$ to $O(u^{12})$ and going up to $O(u^{26})$. We do not find evidence for any other complex-temperature singularities within the range described by the small-u expansion. From this Padé analysis of the low-temperature series, we infer the values

$$u_s = -0.998 \pm 0.002 \tag{3.4}$$

$$\gamma_s' = 1.52 \pm 0.06 \tag{3.5}$$

where the uncertainties are estimates. These results suggest the conclusion that as u approaches the point

$$u_s = -1 \tag{3.6}$$

from within the FM phase, $\bar{\chi}$ has a divergent singularity with exponent

$$\gamma_s' = \tfrac{3}{2}. \tag{3.7}$$

This inference was also reached by Enting, Guttmann and Jensen; see note added in proof. As noted above, this point $u_s = -1$ corresponds to the two points $z_s = -v_s = \pm\mathrm{i}$; in the complex K plane it corresponds to the infinite set of points given by

$$K_s = -\tfrac{1}{4}\mathrm{i}\pi + \tfrac{1}{2}n\mathrm{i}\pi \tag{3.8}$$

with $n \in Z$.

In the following we shall show that the critical exponent for the inverse correlation length (mass gap) describing row or column connected spin–spin correlation functions at this singular point is $\nu_{s,\mathrm{row}}' = 1$. A naive complex-temperature analogue of the usual argument for the scaling relation $\nu'(2-\eta) = \gamma'$, in conjunction with our inferred value of γ_s' in (3.7), would lead to the further inference that the exponent describing the asymptotic decay of the row or column connected 2-spin correlation function at the singular point $u_s = -1$ is $\eta_{s,\mathrm{row}}' = \frac{1}{2}$ (where we append the prime to indicate that the calculation of the spin–spin correlation function involves a limit from the complex FM phase). However, we shall show that the situation near the complex-temperature singular point $u = -1$ is considerably more complicated than the case at the physical critical point with its simple scaling relations $\nu'(2-\eta) = \gamma'$ and $\nu(2-\eta) = \gamma$. Among other things, we shall show that the correlation length and $\bar{\chi}$ are finite when one approaches $u = -1$ from the complex PM phase.

The dlog Padé study did not yield any evidence for other complex singularities, i.e. it did not give poles whose positions were highly stable as one varied the orders of the approximants. As usual, the values of the position of the singular point vary less among the Padé entries than the values of the exponent. Also, as expected, the values of γ_s' show less scatter in the higher-order Padé entries than in the lower-order entries. It is true, however, that these values of γ_s' do exhibit more scatter than the values of the usual susceptibility exponent γ' for the PM–FM critical point u_c. To make this comparison quantitative, it is sufficient to show the values of u_c and γ' extracted from just the diagonal Padé entries; these are given in table 3.

Table 3. Values of $u_{c,\mathrm{ser}}$ and γ' from diagonal Padé approximants to low-temperature series for $\bar{\chi}_r$ starting with the series to $O(u^{13})$.

$[N/N]$	$u_{c,\mathrm{ser}}$	$\lvert u_{c,\mathrm{ser}} - u_c\rvert / u_c$	γ'
[6/6]	0.171 540 17	1.9×10^{-4}	1.740
[7/7]	0.171 560 38	0.73×10^{-4}	1.745
[8/8]	0.171 465 27*	6.3×10^{-4}	1.791*
[9/9]	0.171 568 58*	2.5×10^{-5}	1.747*
[10/10]	0.171 570 13	1.6×10^{-5}	1.748
[11/11]	0.171 572 32	3.2×10^{-6}	1.749
[12/12]	0.171 574 23*	7.9×10^{-6}	1.751*
Exact	0.171 572 875 ...	0	1.750

Table 4. Values of u_s from Padé approximants to $g(u) = (1 - 6u + u^2)^{7/4}\bar{\chi}_r$, starting with the series for $g(u)$ to order $O(u^{12})$.

N	$[(N-2)/N]$	$[(N-1)/N]$	$[N/N]$	$[(N+1)/N]$	$[(N+2)/N]$
6	—	−1.052 79	−1.078 22*	−0.991 486	−1.001 045
7	−1.090 02*	−1.045 02	−0.999 217	−0.989 684*	−1.008 33*
8	−1.010 665	−1.021 41	−1.003 84*	−0.996 939	−0.989 857
9	−1.011 88*	−1.343 02	−0.985 198	−0.995 437	−0.996 976
10	−0.988 462	−1.264 78*	−0.996 803	−0.995 048*	−0.998 644*
11	−1.001 56	−1.003 54	−0.998 084	−0.997 731	−0.998 407*
12	−1.001 685*	−0.997 653	−0.998 042*	−0.996 954*	—
13	−0.999 656*	−0.994 374*	—	—	—

Table 5. Values of γ_s' from Padé approximants to $g(u) = (1 - 6u + u^2)^{7/4}\bar{\chi}_r$, starting with the series for $g(u)$ to order $O(u^{12})$.

N	$[(N-2)/N]$	$[(N-1)/N]$	$[N/N]$	$[(N+1)/N]$	$[(N+2)/N]$
6	—	1.998	2.179*	1.464	1.561
7	2.278*	1.950	1.540	1.449*	1.640*
8	1.664	1.769	1.585*	1.512	1.434
9	1.674*	1.356	1.372	1.497	1.516
10	1.418	1.490*	1.513	1.493*	1.536*
11	1.575	1.600	1.528	1.524	1.533*
12	1.576*	1.523	1.528*	1.514*	—
13	1.551*	1.481*	—	—	—

3.2. Analysis of series for g(u)

Clearly, a property of Padé approximants which is crucial for our study is their sensitivity to singularities which are not the closest to the origin of the Taylor series expansion. In order to explore the possibility of obtaining a more sensitive probe of the complex singular point, we have also carried out a similar study of a series with the physical singularity removed. In order to keep the coefficients rational, we actually multiply $\bar{\chi}$ by the factor $[(u - u_c)(u - 1/u_c)]^{7/4} = (1 - 6u + u^2)^{7/4}$ and thus study

$$g(u) \equiv \left(1 - 6u + u^2\right)^{7/4} \bar{\chi}_r(u) . \tag{3.9}$$

This is an old technique (see, for example, [5]). Note that the spurious finite branch-point singularity introduced at the PM–AFM critical point has no effect on our analysis, since the small-$|u|$ series for $\bar{\chi}$ and g only apply in the FM region, which is not contiguous with the region of the PM–AFM critical point in the u plane. The results of our Padé analysis of the series for $g(u)$ are given in tables 4 and 5.

As one can see from these tables, the resultant values for u_s and γ_s' are in very good agreement with those from our analysis of the series for $\bar{\chi}_r$. One improvement that occurs is a slight reduction of the number of entries with nearly coincident pole-zero pairs, which should increase the accuracy of the results somewhat.

3.3. Analysis of series for $\bar{\chi}$ in the variable $k_<$

Finally, it is useful to transform the series for the susceptibility from the usual low-temperature variable u to the elliptic modulus $k_<$ and to study the resultant series. An

Table 6. Values of $(k_<)_{s,ser}$ and γ_s' from diagonal Padé approximants to low-temperature series for $\bar{\chi}_r$ starting with the series to $O(k_<^{13})$. CP denotes a complex pair of poles close to -1. The superscript $*$ indicates that the approximant has one or more nearly coincident pole-zero pair(s) closer to the origin than $(k_<)_s = -1$. As before, our criterion for near-coincidence is that $|(k_<)_{pole} - (k_<)_{zero}| < 10^{-4}$.

$[N/N]$	$(k_<)_{s,ser}$	$\|(k_<)_{s,ser} + 1\|$	γ_s'
[6/6]	−0.998 766	1.2×10^{-3}	1.513
[7/7]	−0.999 940	0.60×10^{-4}	1.552
[8/8]	−1.000 012	1.2×10^{-5}	1.555
[9/9]	−0.999 734	2.7×10^{-4}	1.543
[10/10]	−0.999 819*	1.8×10^{-4}	1.546*
[11/11]	−0.999 873	1.3×10^{-4}	1.549
[12/12]	CP	—	—

important motivation for this is that $\bar{\chi}$ is given formally by a sum over all connected correlation functions, and these correlation functions, which can be computed exactly in terms of certain Toeplitz determinants [16, 17], have explicit forms which are polynomials in the complete elliptic integrals $K(k_x)$ and $E(k_x)$ [18], where $k_x = k_<$ in the FM and AFM phases and $k_x = k_>$ in the PM phase. The variables $k_<$ and $k_>$ are thus natural ones for low- and high-temperature series expansions of $\bar{\chi}$, respectively. We therefore have transformed the known small-$|u|$ series to one in $k_<$, which takes the form

$$\bar{\chi} = 2^{-2}k_<^2\left(1 + \sum_{n=1}^{\infty} c_n' k_<^n\right). \tag{3.10}$$

The series in parentheses defines a reduced function $\bar{\chi}_r = 4k_<^{-2}\bar{\chi}$ as before. Since as a function of u, $k_<$ has the expansion near $u = u_s = -1$,

$$k_< = -1 + \tfrac{1}{4}(u+1)^2 + O\big((u+1)^3\big) \tag{3.11}$$

with no linear term, it follows that in the variable $k_<$, the singular form of $\bar{\chi}$ corresponding to (3.3), as $k_<$ approaches the point $k_< = -1$ from within the FM or AFM phase (i.e. from within the interior of the unit circle in the complex $k_<$ plane) is

$$\bar{\chi}(k_<) \sim B_s'(1+k_<)^{-\gamma_s'/2}(1 + b_1(1+k_<) + \cdots) \tag{3.12}$$

where B_s' is the critical amplitude for this expression of the singularity in terms of the variable $k_<$. We have performed a dlog Padé analysis of the series in $k_<$ for $\bar{\chi}_r$, i.e. an analysis of the function $d\ln\bar{\chi}_r/dk_<$. Our results for the diagonal entries are given in table 6. The results from the series in $k_<$ agree very well with those which we obtained from the other series. The analysis of the series in $k_<$ also gives results for the regular PM–FM critical point at $k_< = 1$ and the associated exponent γ' of comparable accuracy to that of the series in u. We have also carried out an analysis of the series for $\bar{\chi}_r$ in the variable u using differential approximants (for further details on this method, see section 7 below). This yields results close to those in table 6.

One important new piece of information can be obtained from our analysis of the series for $\bar{\chi}$ in the variable $k_<$ near the singular point $k_< = (k_<)_s = u_s = -1$: this is an answer to the question of whether the critical exponent is the same when one approaches this point from within the interior of the complex-extended FM phase and from within the complex-extended AFM phase. Recall from figure 1(c) that in the u plane these approaches are distinct, since the complex FM and AFM phases lie on opposite sides of u_s. Since the complex FM phase is the one which contains the origin in the u plane, our analysis of the small-$|u|$ series could only determine the singular behaviour as u approached u_s from within the complex FM phase. However, since the complex FM and AFM phases are mapped onto each other in the $k_<$ plane, our analysis of the series in this variable shows that the exponent γ_s' is the same for the approach to $u_s = (k_<)_s = -1$ from within both the FM and AFM phases (as has been implicit in our notation).

Since the low-temperature series for $\bar{\chi}$ is not usually given in terms of the variable $k_<$, we note that it has an interesting feature. The first few terms are

$$\bar{\chi}_r = 1 + k_< + \frac{13}{2^3}k_<^2 + \frac{13}{2^3}k_<^3 + \frac{139}{2^6}k_<^4 + \frac{139}{2^6}k_<^5 + \frac{685}{2^8}k_<^6 + \frac{2739}{2^9}k_<^7 + \frac{51603}{2^{14}}k_<^8 + O(k_<^9). \tag{3.13}$$

Near the point $u_s = (k_<)_s = -1$, the terms up to order $O(k_<^5)$ of the series exactly cancel amongst each other in a successive pairwise fashion, so that the first non-zero terms in the series for $\bar{\chi}_r$ start at order $O(k_<^6)$ (i.e. for $\bar{\chi}$ at $O(k_<^8)$). To say it differently, these first six terms can be expressed as $(1+k_<)(1+(13/2^3)k_<^2+(139/2^6)k_<^4)$. One can interpret this as being a hint of a structure which persists to all orders in the exact susceptibility; with this motivation, one can add and subtract terms in higher orders so as to put $\bar{\chi}_r$ in the form

$$\bar{\chi} = (1 + k_<)f_1 - 2^{-12}k_<^7 f_2 . \tag{3.14}$$

Computing the functions $f(k_<)_j$, $j = 1, 2$ and defining the convenient variable

$$y \equiv 2^{-4}k_<^2 \tag{3.15}$$

we find

$$f_1 = 1 + 26y + 556y^2 + 10\,960y^3 + 206\,412y^4 + 3\,775\,480y^5 + 67\,668\,304y^6 + 1\,194\,824\,896y^7 + 20\,856\,575\,980y^8 + 360\,778\,731\,928y^9 + 6\,195\,017\,443\,856y^{10} + 105\,730\,294\,168\,640y^{11} + 1\,795\,278\,082\,108\,368y^{12} + O(y^{13}) \tag{3.16}$$

and

$$f_2 = 1 + 33y + 770y^2 + 15\,650y^3 + 296\,006y^4 + 5\,363\,335y^5 + 94\,504\,364y^6 + 1\,633\,461\,856y^7 + 27\,844\,153\,964y^8 + 469\,735\,545\,258y^9 + O(y^{10}) . \tag{3.17}$$

We have performed a Padé analysis of the functions $d\ln f_j/dy$. We find strong evidence of a singularity in f_1 of the form $f_1 \sim |1 - k_<^2|^{-7/4}$ as $k_<^2$ increases toward 1 from below. Combining this with the $(1 - k_<)$ prefactor, it follows that the singularity in $\bar{\chi}$ arising from the f_1 term can be written as

$$(1 + k_<)f_1 \sim |1 - k_<|^{-7/4}|1 + k_<|^{-3/4} \tag{3.18}$$

as $k_<^2$ approaches 1 from below. For example, the [6/6] Padé approximant gives $16y = k_<^2 = 0.999\,844$ as the position of the singularity, and 1.745 as the exponent. The results from the study of f_2 are also consistent with this conclusion for the singularity in $\bar{\chi}$. Recalling that $|1 + k_<|^{-3/4} = \text{constant} \times |1 + u|^{-3/2}$ as $k_< \to -1$ or equivalently, as $u \to -1$, one sees that the singular form (3.18) agrees very nicely with our determination of the complex-temperature singularity by analyses of the small-$|u|$ series for $\bar{\chi}_r(u)$, $g(u)$, and $\bar{\chi}_r(k_<)$ given above.

3.4. Critical amplitude at u_s

In order to calculate the critical amplitude A'_s in the susceptibility as one approaches $u=-1$ from within the FM phase, we compute the series for $(\bar\chi_r)^{1/\gamma'_s}$. Since the exact function $(\bar\chi_r)^{1/\gamma'_s}$ has a simple pole at u_s, one performs the Padé analysis on the series itself instead of its logarithmic derivative. The residue at this pole is $-u_s(A'_{r,s})^{1/\gamma'_s}$, where $A'_{r,s}$ denotes the critical amplitude for $\bar\chi_r$. Using our inferred value $\gamma_s=\frac{3}{2}$ to calculate the series and the value $u_s=-1$ to extract $A'_{r,s}$, we finally multiply by the prefactor to obtain $A'_s=4u_s^2A'_{r,s}=4A'_{r,s}$. (Alternatively, one could extract $(A'_{r,s})^{1/\gamma'_s}$ from the residue by dividing by the measured pole position, $u_{s,ser}$ from the given Padé rather than the inferred exact position, and could use the prefactor $4u^2_{s,ser}$ to get A'_s; the differences between the two methods are quite small and vanish asymptotically; these differences are incorporated in the final uncertainty which is quoted for the critical amplitude.) Our results from the diagonal Padé entries are listed in table 7. From this analysis, we calculate

$$A'_s=0.186\pm0.001 \tag{3.19}$$

where the quoted uncertainty is an estimate.

Table 7. Values of $(A'_s)^{2/3}$ from Padé approximants to small-$|u|$ series for $(\bar\chi_r)^{1/\gamma}$. CP indicates a complex pair of poles near to $u_s=-1$.

$[N/N]$	u_s	$R_s=-u_s(A'_{r,s})^{2/3}$
[6/6]	−0.993 282	0.128 915
[7/7]	−0.994 2585	0.129 496
[8/8]	−0.994 204	0.129 460
[9/9]	−0.994 088	0.129 3865
[10/10]	−0.995 080	0.130 178
[11/11]	−0.993 497	0.129 294
[12/12]	CP	CP

This value may be compared with the low-temperature critical amplitude in this model at the usual PM–FM critical point, u_c, defined by $\bar\chi(u)\sim A'_c|1-u/u_c|^{-7/4}$ as $u\to u_c$ from below. A'_c was determined first by analysis of low-temperature series expansions [5] and subsequently to higher accuracy by analytic methods [13]† to be $A'_c=0.068\,865\,538\ldots$. Using our determination of A'_s, it follows that $A'_s/A'_c=2.701\pm0.015$. We note that this is consistent, to within the numerical accuracy, with the analytic relation $A'_s/A'_c=(-\ln u_c)^{7/4}=2.696\,699\,5\ldots$.

4. Singular behaviour of other quantities at $u_s=-1$

4.1. Specific heat

In this section we extract the singular behaviour of the exactly known thermodynamic quantities at the complex-temperature singular point $u_s=-1$. We begin with the specific heat. It is convenient to consider $K^{-2}C$, which (in units with $k_B\equiv 1$) is given by [2]

$$K^{-2}C=\frac{4}{\pi}\left(\frac{1-\kappa'}{\kappa^2}\right)\left[2\big(K(\kappa)-E(\kappa)\big)-(1-\kappa')\big(\tfrac{1}{2}\pi+\kappa'K(\kappa)\big)\right] \tag{4.1}$$

† Reference [13] actually gives the critical amplitude $A'_{c,T}$ defined by $\bar\chi(T)\sim A'_{c,T}|1-T_c/T|^{-7/4}$; we have converted this to A'_c here.

where the elliptic modulus is

$$\kappa = \frac{2}{(k_>^{1/2} + k_>^{-1/2})} = \frac{2}{(k_<^{1/2} + k_<^{-1/2})} = \frac{4u^{1/2}(1-u)}{(1+u)^2} \tag{4.2}$$

and its complementary modulus is $\kappa' = (1-\kappa^2)^{1/2}$. We use the standard convention that the branch cut for the complete elliptic integrals runs from $m \equiv \kappa^2 = 1$ to $m = \infty$ along the positive real axis in the complex m-plane. From equation (4.2), it follows that as u approaches -1 with $\mathrm{Im}(u)$ small and positive, $\kappa \to \mathrm{i}\infty$ (and if $\mathrm{Im}(u)$ is small and negative, then $\kappa \to -\mathrm{i}\infty$, taking the usual convention for the branch cut for the square root), and thus $\kappa' \to \infty$. From inspection of (4.1), it is clear that as $u \to -1$, C diverges, with the leading divergence arising from the last term, $-\frac{4}{\pi}(\kappa'^3/\kappa^2)K(\kappa) \to \frac{4}{\pi}\kappa' K(\kappa)$. Using the identity (see for example [20]) $\kappa' K(\kappa) = K(\mathrm{i}\kappa/\kappa')$ and the fact that as $\lambda \to 1$, $K(\lambda) \to \frac{1}{2}\ln(16/(1-\lambda^2))$, we can express the most singular term as $\frac{4}{\pi}\ln(4|\kappa|)$ as $u \to -1$. Next, using the fact that near $u = -1$, $1/\kappa = -\frac{\mathrm{i}}{8}(1+u)^2 + \mathrm{O}((1+u)^3)$, we find, finally, that the leading divergence in C as $u \to -1$ is

$$C \sim \frac{8}{\pi} K_{\mathrm{s}}^2 \ln\left(\frac{1}{(1+u)}\right). \tag{4.3}$$

Taking the value of K_{s} on the first Reimann sheet in (3.8), i.e. $K_{\mathrm{s}} = -\mathrm{i}\pi/4$, this becomes

$$C \sim -\frac{\pi}{2} \ln\left(\frac{1}{(1+u)}\right). \tag{4.4}$$

Since the elliptic integrals and also the factor κ' only depend on κ^2, the leading singularity is of the same type whether u approaches $u_{\mathrm{s}} = -1$ with $\mathrm{Im}(u)$ positive, negative, or zero, and also whether the approach occurs from within the complex FM, AFM, or PM phases. The logarithmic divergence in C at u_{s} is evidently of the same type as the divergence at the physical PM–FM and PM–AFM critical points. Note, however, that at these latter points, $\kappa \to 1$ ($\kappa' \to 0$) so that the $\kappa' K(\kappa)$ term (which gives the leading divergence at $u = -1$) vanishes, and the divergence arises instead from the first term in the square brackets of (4.1), $2K(\kappa)$. Another obvious difference is that, while the specific heat is required to be positive at physical temperatures, it is, in general, complex at complex-temperature points, and the critical amplitude at u_{s} is real but negative. The critical exponents corresponding to this logarithmic divergence in C at u_{s} are

$$\alpha_{\mathrm{s}} = \alpha'_{\mathrm{s}} = 0\,. \tag{4.5}$$

As one crosses the complex-temperature phase boundaries at points other than $u = u_{\mathrm{c}}$, $u = 1/u_{\mathrm{c}}$, and $u = -1$, the specific heat C has singularities associated with the fact that the image point in the κ^2 plane crosses the image of these boundaries, namely, the line segment extending from $\kappa^2 = 1$ to $\kappa^2 = \infty$, which is the natural branch cut of the complete elliptic integrals $K(\kappa)$ and $E(\kappa)$ in (4.1.1).

From the thermodynamic relation $C_H - C_M = \chi^{-1} T((\partial M/\partial T)_H)^2$, and the fact that the term on the right-hand side is finite as $u \to -1$ from within the complex-temperature FM phase, one may infer that the specific heat at constant magnetization, C_M, has the same logarithmic singularity as the specific heat (at constant field) $C(H = 0)$ in this limit.

4.2. Magnetization

Next, we make use of the exactly known expressions for the spontaneous magnetization M to analyse the behaviour as a function of complex temperature. In particular, we shall extract the critical exponent β_{s} at the complex-temperature singular point $u = u_{\mathrm{s}} = -1$.

For the square lattice, for real temperature, M vanishes for $K < K_{c,sq}$ (where for clarity we restore here the subscript indicating the lattice type) and, for $K_{c,sq} < K < \infty$ is given by [3] $M = M_{sq} = (1 - k_<^2)^{1/8}$, or, in terms of u,

$$M_{sq} = \frac{(1+u)^{1/4}(1-6u+u^2)^{1/8}}{(1-u)^{1/2}} . \tag{4.6}$$

What is normally discussed is the vanishing of M at the usual PM–FM critical point, $u_c = 3 - 2\sqrt{2}$, with exponent $\beta = \frac{1}{8}$. However, as we discussed in section 2, the function describing the magnetization for positive temperature can be analytically continued throughout the complex extension of the FM phase, up to the boundaries of this phase, which for the square lattice are specified by the limaçon (2.18). Carrying out this analytic continuation, one sees two important results.

(i) The only point, other than the physical PM–FM critical point, where M vanishes continuously is at $u = u_s = -1$. Defining an associated critical exponent as

$$|M| \sim \text{constant} \times |1 - u/u_s|^{\beta_s} \tag{4.7}$$

as u approaches u_s from within the complex-extended FM phase, we find the value

$$\beta_{s,sq} = \frac{1}{4} . \tag{4.8}$$

(ii) At all other points (i.e. all points except u_c and u_s) along the boundary of the complex extension of the FM phase, M vanishes discontinuously.

Result (ii) follows because if one starts in the physical PM phase, a similar analytic continuation argument shows that M vanishes identically all throughout the complex extension of this phase. Inspection of (4.6) shows that the (real and imaginary parts of the) analytic continuation of M are non-zero as one approaches the boundary of the complex-extended FM phase from within that phase at points other than $u = u_c$ and $u = -1$. Therefore, M must vanish discontinuously as one crosses this boundary from the complex FM to the complex PM phase, as claimed.

For the complex-extended AFM phase, we use the well known symmetry which holds on loose-packed lattices: under the transformations $K \to -K$ and $\sigma_i \to \eta_i \sigma_i$, where $\eta_i = 1$ (-1) for σ_i on the even (odd) sublattice, the Hamiltonian is invariant, while the uniform magnetization M and the staggered magnetization M_{st} interchange their roles. The above transformation takes $k_< \to k_<$, $z \to 1/z$, $u \to 1/u$. The expression (4.6) is invariant and thus describes the staggered magnetization in the physical AFM phase as well as the uniform magnetization in the physical FM phase. As before, one generalizes this to a definition of the staggered magnetization in the complex-extended AFM phase by analytic continuation from the physical region $-\infty \leqslant K \leqslant -K_c$ throughout the complex AFM phase, as indicated in figure 1. One sees that analogues of the two results which we obtained for M can also be derived for M_{st}:

(i) M_{st} vanishes continuously at two points on the border of the complex-extended AFM phase, namely, $u = 1/u_c = 3+2\sqrt{2}$, the usual PM–AFM critical point, and $u = u_s = -1$, the complex-temperature singular point where M also vanishes.

(ii) At all other points on the border of the complex-extended AFM phase, M_{st} vanishes discontinuously as one crosses this border into the PM phase. Note that, as is clear from figure 1, the only point where the complex FM and AFM phases are contiguous is the single point $u = u_s = -1$, or equivalently, the two points $z = \pm i = -v$.

In passing, we note that for both the uniform and staggered magnetizations, the apparent divergence at $u = 1$ plays no role since this point is outside the two respective regions (complex FM and AFM phases) where the expression (4.6) for these quantities applies.

4.3. The behaviour of the inverse correlation length as $u \to -1$.

4.3.1. Approach from within complex (A)FM phase. For the Ising model on the square lattice, in the physical low-temperature phase with real K in the interval $K_c < K \leqslant \infty$, the asymptotic decay of the row (or equivalently, column) connected correlation functions is given by [19]

$$\langle \sigma_{(0,0)} \sigma_{(0,n)} \rangle_{\rm conn} \sim n^{-2}\, {\rm e}^{-|n|/\xi_{\rm FM,row}} \tag{4.9}$$

where the inverse correlation length (mass gap) is

$$\xi^{-1}_{\rm FM,row} = \ln((v/z)^2) = \ln\left[z^{-2}\left(\frac{1-z}{1+z}\right)^2\right]. \tag{4.10}$$

We now analytically continue this result into the complex extension of the FM phase and inquire where the mass gap vanishes. We find that for points within, and on the border of, the complex-extended FM phase, the mass gap vanishes for the following set:

$$\xi^{-1}_{\rm FM,row} = 0 \qquad \text{for} \quad z = \{z_c,\ \pm{\rm i}\} \tag{4.11}$$

i.e. the usual PM–FM critical point $z_c = \sqrt{2} - 1$ and at the two points $z_s = \pm{\rm i}$ ($u_s = -1$). The additional apparent zero at the PM–AFM critical point $z = -1/z_c$ is not relevant for the complex FM phase because this point lies outside this phase and thus outside the region which can be reached by analytic continuation of the original formula (4.9); however, it will be relevant for the inverse correlation length defined within the complex-extended AFM phase (see below). We note the somewhat subtle point that the correct analytic continuation of the physical, real-K theory to complex K requires that one use $\xi^{-1}_{\rm FM,row} = \ln((v/z)^2)$ as given in (4.10) and not $\xi^{-1}_{\rm FM,row} = 2\ln(v/z)$; although these are identical expressions for physical K, the latter form would miss the zero in $\xi^{-1}_{\rm FM,row}$ at $u = -1$.

We now extract the critical exponent(s) for this inverse correlation length (mass gap) at $z = \pm{\rm i}$ as these points are approached from within the complex-extended FM phase. These exponents (which will turn out to be equal) are defined by

$$\xi^{-1}_{\rm FM,row} \sim \text{constant} \times |z \mp {\rm i}|^{\nu'_{\pm {\rm i},row}} \quad \text{for} \quad z \to \pm{\rm i} \tag{4.12}$$

from within the FM phase. Expanding $\xi^{-1}_{\rm FM,row}$ about these points gives

$$\xi^{-1}_{\rm FM,row} = 0 + 2(\pm{\rm i} - 1)(z \mp {\rm i}) + O((z \mp {\rm i})^2) \tag{4.13}$$

from which it follows that

$$\nu'_{{\rm i},row} = \nu'_{-{\rm i},row} = 1\,. \tag{4.14}$$

This motivates the use of a single exponent to describe the singularity at the single point $u_s = -1$ corresponding to $z = \pm{\rm i}$, as approached from within the complex-extended FM phase:

$$\nu'_{s,row} = 1\,. \tag{4.15}$$

By the standard argument noted above which shows that on a loose-packed lattice such as the square lattice

$$\eta_i \eta_j \langle \sigma_i \sigma_j \rangle(-K)_{\rm conn} = \langle \sigma_i \sigma_j \rangle(K)_{\rm conn} \tag{4.16}$$

it follows that the same inverse correlation length (4.10) describes the asymptotic decay of the connected 2-spin correlation functions along a row or column in the AFM phase, i.e. formally, $\xi^{-1}_{\rm FM,row} = \xi^{-1}_{\rm AFM,row}$, although the same expression is used in different phases. Now $\xi^{-1}_{\rm AFM,row}$ vanishes at the physical PM–AFM critical point $z = -1/z_c$, i.e. $u = 1/u_c$, and at the complex-temperature singular points $z = \pm i$. It follows that the expansion (4.13) also controls the critical exponent as one approaches the points $u = -1$ from the AFM phase (i.e. from the left in figure 1(*b*)).

The value of $\nu'_{s,\mathrm{row}}$ is evidently the same as the value $\nu' = 1$ for the physical PM–FM critical point, as approached from within the FM phase. However, one encounters several new features at the complex-temperature singular point, which we now discuss.

One may also extract a correlation length critical exponent from the asymptotic decay of the diagonal (d) correlation function,

$$\langle \sigma_{(0,0)}\sigma_{(n,n)}\rangle_{\mathrm{conn}} \sim n^{-2}\,\mathrm{e}^{-r/\xi_{\mathrm{FM,d}}} \tag{4.17}$$

where the distance $r = 2^{1/2}|n|$. In the physical FM phase,

$$\xi^{-1}_{\mathrm{FM,d}} = -2^{-1/2}\ln(k_<^2) \tag{4.18}$$

$$= -2^{-1/2}\ln\left(\left[\frac{4u}{(1-u)^2}\right]^2\right). \tag{4.19}$$

As with the row (column) spin–spin correlation functions, we may analytically continue (4.17)–(4.19) to apply throughout the complex extension of the FM phase. Although the detailed form of $\xi^{-1}_{\mathrm{FM,d}}$ is different from that of $\xi^{-1}_{\mathrm{FM,row}}$, they both have the same complex zeros within the range of this analytic continuation, i.e. the complex FM phase and its boundary. It may be recalled that near the physical PM–FM critical point,

$$k_<^2 = 1 + 2(4+3\sqrt{2})(u-u_c) + O\big((u-u_c)^2\big) \tag{4.20}$$

so that the exponent which describes the vanishing of the inverse correlation length characterizing the diagonal correlation function is the same as that for the row or column correlation functions. However, the situation is different at $u = -1$: using the expansion near $u = -1$ (see also (3.11))

$$k_<^2 = 1 - \tfrac{1}{2}(1+u)^2 + O\big((1+u)^3\big) \tag{4.21}$$

it follows that near $u = -1$,

$$\xi^{-1}_{\mathrm{FM,d}} = 2^{-3/2}(1+u)^2 + O\big((1+u)^3\big)\,. \tag{4.22}$$

Hence, the correlation length exponent describing the vanishing of the inverse correlation length for diagonal correlation functions, at $u = u_s = -1$, as approached from within the complex FM phase, is

$$\nu'_{s,\mathrm{diag}} = 2 \tag{4.23}$$

i.e. twice the value of the mass gap exponent extracted from the row/column correlation functions. This situation is unprecedented for critical exponents at physical critical points.

4.3.2. Approach from complex PM *phase.* From an analysis of the asymptotic decays of both the row/column and diagonal correlation functions in the complex extension of the symmetric, PM phase, we find that the correlation length does *not* diverge as one approaches the points $v = \pm i$ corresponding to the point $u = -1$ from within this phase. This finding is very important, since it implies that the susceptibility is finite at $u = -1$ when this point is approached from within the complex PM phase.

In the physical PM phase, the row (or column) correlation function has the asymptotic decay [19]

$$\langle \sigma_{(0,0)}\sigma_{(0,n)}\rangle \sim |n|^{-1/2}\,\mathrm{e}^{-|n|/\xi_{\mathrm{PM,row}}} \tag{4.24}$$

where

$$\xi_{\mathrm{PM,row}}^{-1} = \ln(z/v) = \ln\left[v^{-1}\left(\frac{1-v}{1+v}\right)\right]. \tag{4.25}$$

As before, we may analytically continue this throughout the complex-extended PM phase. The mass gap $\xi_{\mathrm{PM,row}}^{-1}$ vanishes only at the physical PM–FM critical point $v_c = \sqrt{2}-1$. (The apparent zero at $-1/v_c = -(\sqrt{2}+1)$ is not relevant because this point lies outside the complex-extended PM phase where the above analytic continuation is valid.) In particular, as one approaches the points $v = \pm \mathrm{i}$ from within the complex PM phase, $\xi_{\mathrm{PM,row}} \to \ln(-1)$, so that $\langle \sigma_{(0,0)}\sigma_{(0,n)}\rangle \sim (-1)^n |n|^{-1/2}$ as $|n| \to \infty$.

We find the same result for the diagonal correlation function, which, in this complex PM phase, has the asymptotic decay

$$\langle \sigma_{(0,0)}\sigma_{(n,n)}\rangle \sim |n|^{-1/2}\,\mathrm{e}^{-r/\xi_{\mathrm{PM,d}}} \tag{4.26}$$

where $r = 2^{1/2}|n|$ and

$$\xi_{\mathrm{PM,d}}^{-1} = -2^{-1/2}\ln(k_>) \tag{4.27}$$

$$= -2^{-1/2}\ln\left(\frac{4v^2}{(1-v^2)^2}\right). \tag{4.28}$$

Now near $v = \pm \mathrm{i}$,

$$k_> = -1 - (v \mp \mathrm{i})^2 + O\left((v \mp \mathrm{i})^3\right). \tag{4.29}$$

Hence, although $\xi_{\mathrm{PM,d}}^{-1}$ vanishes at the physical critical point v_c, it is finite at the points $v = \pm \mathrm{i}$, where $\xi_{\mathrm{PM,d}}^{-1} = 2^{-1/2}\ln(-1)$, so that $\langle \sigma_{(0,0)}\sigma_{(n,n)}\rangle \sim |n|^{-1/2}(-1)^n$ at these points, just as was true of the row and column correlation functions. One thus encounters precisely the type of situation that we discussed before in [1], where $\mathrm{Re}(\xi^{-1}) = 0$ but $\mathrm{Im}(\xi^{-1})$ is non-zero. Note that the sum $\sum_{n_0}^{\infty}(-1)^{-n}n^{-1/2}$ (where n_0 is an unimportant lower cut-off) is finite. Of course, although the correlation length is finite at $v = \pm \mathrm{i}$, as approached from within the PM phase, it is singular at these points since it is unequal to the value obtained as the points are approached from a different direction in the complex v, z, or u planes. The asymptotic decay of the general 2-spin correlation function $\langle \sigma_{(0,0)}\sigma_{(m,n)}\rangle$ has been calculated (using Toeplitz determinant methods) [19]; carrying out an analytic continuation of this result from the physical PM phase into its complex extension, we again find that the correlation length is finite at $v = \pm \mathrm{i}$. Since a divergence in $\bar{\chi}$ on the border of the (complex extension of the) PM phase can only arise from a divergence in the sum over 2-spin correlation functions contributing to $\bar{\chi}$, the above results constitute an analytic demonstration that the susceptibility is finite at the points $v = \pm \mathrm{i}$, as approached from within the complex PM phase. This is in sharp contrast to the approach from within the complex FM or AFM phases, where we have shown that $\bar{\chi}$ is divergent. This type of phenomenon is, again, to our knowledge, unprecedented in the study of singularities in thermodynamic functions at physical critical points.

4.3.3. A theorem on $\bar{\chi}$. From our results in the previous two subsections, using the same reasoning as in [1], we can infer the following theorem.

Theorem. The susceptibility $\bar{\chi}$ has at most finite non-analyticities on the natural boundary curve (circles in v or z, limaçon in u) separating the complex-extended PM, FM, and AFM phases, apart from the divergent singularities as one approaches the point $u_c = 3 - 2\sqrt{2}$ from within either the complex PM or FM phase and the point $u_s = -1$ from within the complex FM or AFM phase.

5. Scaling relations and other critical exponents at $u_s = -1$

5.1. $\alpha_s' + 2\beta_s + \gamma_s' = 2$

Using our result (3.7) for γ_s', together with the exponents α_s' and β_s extracted from the known exact expressions for C and M in (4.5) and (4.8), we find that the complex analogue of the scaling relation (from the low-temperature side) $\alpha' + 2\beta + \gamma' = 2$ is satisfied:

$$\alpha_s' + 2\beta_s + \gamma_s' = 2 \tag{5.1}$$

where the subscript 's' indicates that this refers to the point $u_s = -1$ and the primes indicate that the approach to this point is from the complex-extended broken-symmetry phases, FM or AFM. To be precise, this relation is satisfied to within the numerical accuracy of our determination of γ_s' in (3.5) and is satisfied exactly if one uses our inference in (3.7) of the exact value of γ_s'. However, our results in the previous section, in particular, the demonstration that $\bar{\chi}$ is finite at $v = \pm i$ ($u = -1$) as approached from within the complex PM phase, and hence that $\gamma_s < 0$, already shows that

$$\alpha_s + 2\beta_s + \gamma_s \neq 2 \tag{5.2}$$

i.e. the scaling relation for the approach from within the PM phase, is *not* valid at u_s. We do not know of any extension of the arguments for usual exponent relations to complex temperature, so it should not be considered a surprise that such relations do not hold at a complex-temperature singularity.

5.2. *Hyperscaling relations*

Since we have shown above that the inverse correlation length is finite at the points $v = \pm i$ when approached from within the complex PM phase, the corresponding exponent $\nu_s < 0$. Hence, the hyperscaling relation $d\nu = 2 - \alpha$ does not hold at these points, as approached from within the complex PM phase. Concerning the hyperscaling relation for the approach to $u_s = -1$ from within the complex FM or AFM phases, namely, $d\nu' = 2 - \alpha'$, if one used the correlation length exponent $\nu_{s,\mathrm{row}} = 1$ extracted from the row or column correlation functions, then this relation would be satisfied. However, the situation is more complicated, since, in particular, $\nu'_{s,\mathrm{diag}} = 2 \neq \nu'_{s,\mathrm{row}}$.

6. Violation of universality at $u_s = -1$

Evidently, complex-temperature singularities clearly have different properties from physical, real-temperature critical points. Among other things, quantities which are real for physical T in general become complex for complex T. Furthermore, various positivity relations, such as the property that the specific heat $C > 0$ is not true even when C is real. One should therefore be cautious concerning the question of whether a given property associated with a physical critical point will apply at a complex-temperature singular point. Indeed, we shall now demonstrate a violation of universality at the complex-temperature singular point u_s.

We recall the meaning of universality as applied to statistical mechanical models not involving frustration or competing interactions: the universality class, as specified by the critical exponents, depends on (i) the symmetry group G of the Hamiltonian and the related space of the order parameter; (ii) the dimensionality of the lattice, but (iii) not on the details of the Hamiltonian, such as additional spin–spin couplings (provided that these are invariant under G and do not introduce frustration or competing interactions), and (iv) not on the lattice type (again, provided that this does not cause frustration).

We shall now demonstrate, using exact results, that property (iv) is violated at the point $u_s = -1$. In order to do this, we use the expressions for the spontaneous magnetization on the triangular and honeycomb lattices. These can be written in the same general form (4.6) for the square lattice, but with elliptic moduli which are different functions of z:

$$M = \left(1 - (k_{<,\Lambda})^2\right)^{1/8} \tag{6.1}$$

where instead of the relation (2.6) for $k_{<,\mathrm{sq}}$, one has

$$k_{<,\mathrm{t}} = \frac{4z^3}{(1+3z^2)^{1/2}(1-z^2)^{3/2}} \tag{6.2}$$

and

$$k_{<,\mathrm{hc}} = \frac{4z^{3/2}(1-z+z^2)^{1/2}}{(1-z)^3(1+z)}\,. \tag{6.3}$$

These apply to the physical FM phases for each lattice, i.e. where $0 \leqslant k_< < 1$. The explicit forms in terms of the usual low-temperature variable u for the triangular and honeycomb lattices are thus [21]

$$M_\mathrm{t} = \left(\frac{1+u}{1-u}\right)^{3/8}\left(\frac{1-3u}{1+3u}\right)^{1/8} \tag{6.4}$$

and [22]

$$M_\mathrm{hc} = \frac{(1+z^2)^{3/8}(1-4z+z^2)^{1/8}}{(1-z)^{3/4}(1+z)^{1/4}} \tag{6.5}$$

which apply within the respective FM phases on these lattices and vanish elsewhere. (Recall that since the honeycomb lattice has an odd coordination number, $q = 3$, M and $\bar{\chi}$ are not invariant under $z \to -z$ as they are for lattices of even q.) We first note a similar feature of the spontaneous magnetization on all three lattices: M vanishes continuously at the same generic set of points, namely the respective PM–FM critical points on each lattice, and the point $u = -1$, or equivalently the two points $z = \pm\mathrm{i}$. As is well known, the critical exponent $\beta = \frac{1}{8}$ is the same at the respective physical PM–FM critical points. However, this is *not* true at $u = -1$: for the square lattice, the critical exponent was extracted above as $\beta_{s,\mathrm{sq}} = \frac{1}{4}$, but for the other lattices

$$\beta_{s,\mathrm{t}} = \beta_{s,\mathrm{hc}} = \tfrac{3}{8} \neq \beta_{s,\mathrm{sq}}\,. \tag{6.6}$$

Given the fact that M has the same form (6.1) in terms of the (different) elliptic moduli $k_{<,\Lambda}$ for the three lattices, and given that $u_s = -1$ maps to $k_{<,\Lambda} = -1$ for each of these lattices, it follows that $M \sim |1 + k_{<,\Lambda}|^p$ as $k_{<,\Lambda}$ approaches -1 from with the FM phase for each case, with the same value $p = \frac{1}{8}$. However, this is not the same as the usual meaning of universality, since the $k_{<,\Lambda}$ differ as functions of z for each of the three lattices.

Since early studies of low-temperature series expansions, it has been known that different lattice types have different numbers of complex-temperature singular points (see, for example, [25] and references therein). However, to our knowledge, the obvious violation of universality noted above has not been explicitly discussed in the literature. Indeed, in an early study of complex-temperature (and complex-activity) properties of the 3D Ising model [23], from analyses of low-temperature series expansions on the simple cubic (sc), body-centred cubic (bcc), and face-centred cubic (fcc) lattices, it was found that the numerical evidence was consistent with the equality of critical exponents on these three lattices. The critical exponents at the complex-temperature singular point $u \simeq -0.285$ in the Ising model on the simple cubic lattice were recently determined to higher precision in [24]. It would be useful to calculate longer low-temperature series for C, M and $\bar{\chi}$ on the bcc and fcc lattices to compare with the higher-accuracy critical exponents obtained in [24] for the sc lattice. However, our exact results on β_s already show that universality does *not, in general, hold at complex-temperature critical points.*

Some possible insight into this violation may be gained by remembering that even at physical critical points, universality does not, in general, hold when there is frustration. One of the earliest examples is the (isotropic) antiferromagnetic Ising model on the triangular lattice, for which there is no PM–AFM phase transition at finite K. Accordingly, when examining a given singular point to see if one could expect universality to hold, one of the first things which one would necessarily check would be the presence or absence of frustration, which, in turn, would involve checking whether various spin configurations only partially minimize the internal energy. But this initial check cannot be performed in the usual way at a complex-temperature singular point, since at such a point the Hamiltonian and internal energy are not, in general, real numbers.

7. Analysis of high-temperature series expansion for the susceptibility

In section 4, as a consequence of our study of the complex-temperature behaviour of correlation lengths, we showed analytically that the susceptibility is finite at the points $v = \pm\mathrm{i}$ (i.e. $u = -1$) as approached from within the complex extension of the PM phase. In this section we shall carry out a study of high-temperature series expansions for the susceptibility. The results confirm our analytic demonstration and give further information about $\bar{\chi}$ at these points. To our knowledge, this is the first time that a comparison has been made of the behaviour at a complex-temperature singularity as approached from both the complex-extended FM (AFM) and PM phases. For technical reasons, the study of the high-temperature series in the vicinity of $v = \pm\mathrm{i}$ turns out to be considerably more difficult than was the case with the low-temperature series in the vicinity of the equivalent single point $u = -1$. We begin with a simple dlog Padé study, which is adequate to confirm the absence of a divergent singularity; we then proceed to a study with differential approximants.

Recall that the high-temperature series expansion for the susceptibility is given by

$$\bar{\chi} = 1 + \sum_{n=1}^{\infty} a_n v^n \tag{7.1}$$

in terms of the usual high-temperature expansion variable. We have also transformed the series to one in the elliptic modulus variable $(k_>)^{1/2}$,

$$\bar{\chi} = 1 + \sum_{n=1}^{\infty} a'_n (k_>)^{n/2} \tag{7.2}$$

via the relation

$$(k_>)^{1/2} = 2v/(1-v^2). \tag{7.3}$$

Note the symmetry

$$v \to -1/v \Rightarrow (k_>)^{1/2} \to (k_>)^{1/2}. \tag{7.4}$$

The motivation for using the variable $(k_>)^{1/2}$ is the same as was discussed in reference to the low-temperature series, namely that the exact expressions for the spin–spin correlation functions which actually contribute to the susceptibility are polynomials in the complete elliptic integrals of modulus $k_>$ in the PM phase (multiplied by algebraic functions of $(k_>)^{1/2}$) [16–18]. Under the mapping from v to $(k_>)^{1/2}$, the boundaries between the phases transform as follows: the circle $v = -1+2^{1/2}\,e^{i\theta}$ is mapped to the right-hand unit semicircle in the $(k_>)^{1/2}$ plane, i.e. $(k_>)^{1/2} = e^{i\phi}$ with $-\pi/2 \leqslant \phi \leqslant \pi/2$. Given the symmetry (7.4), this is a two-fold covering; in particular, the image of the the PM–FM critical point v_c and the point $-1/v_c$ is the single point $(k_>)^{1/2} = 1$. Similarly, the circle $v = 1+2^{1/2}\,e^{i\theta}$ is mapped by a two-fold covering to the left-hand unit semicircle, $(k_>)^{1/2} = e^{i\phi}$ with $\frac{3}{2}\pi \geqslant \phi \geqslant \pi/2$. The points $-v_c$ (the PM–AFM critical point) and $1/v_c$, are taken to the point $(k_>)^{1/2} = -1$. Finally, the points $v = \pm i$ which lie on the intersections of the two circles are mapped to $(k_>)^{1/2} = \pm i$, respectively.

For the square lattice, the a_n have been calculated to the very high order v^{54} by Nickel [26]. We have performed a dlog Padé analysis on this series and have found evidence against a divergence in $\bar{\chi}$ as v approaches $\pm i$ from within the PM phase. Since $\bar{\chi}$ is real for real v, it follows that if the Padé approximant for $d\ln(\bar{\chi})/dv$ has a pole at $v = v_0$ with residue R_0 at some complex point v_0, then it also has a pole at $v = v_0^*$ with residue R_0^*. Writing the singular part of $\bar{\chi}$ as $(1 - v/v_0)^{-\gamma_0}$ near $v = v_0$ and recalling that $R_0 = -\gamma_0$, it follows that at the two complex-conjugate poles, the real parts of the exponents are equal, while the imaginary parts (if non-zero) are reversed in sign. Thus, without loss of generality, it suffices to consider only the singularity at $v = i$.

We find that the Padé approximants to $d\ln(\bar{\chi})/dv$ yield a reasonably stable pole near to $v = i$, with $\mathrm{Re}(\gamma_{v=i}) < 0$. However, even for rather high-order $[N/N]$ Padé entries with $15 \leqslant N \leqslant 23$, the pole position is not as close to the singular point as one would require for accurate results; typically, $|v_{i,\mathrm{ser}} - i| \simeq 0.08$, much larger than the usual level of $O(10^{-3})$ (or better) which one would expect for reasonable accuracy.

We have therefore studied the equivalent series (7.2) in the elliptic modulus variable, $(k_>)^{1/2}$. In terms of the latter variable, the leading form of the singularities at $(k_>)^{1/2} = \pm i$ is given by

$$\bar{\chi}_{\mathrm{sing}} \sim C_{\pm i}|1 \pm i(k_>)^{1/2}|^{-\gamma_{\pm i}/2} \tag{7.5}$$

since the Taylor series expansion of $(k_>)^{1/2} \mp i$ as a function of v, near the points $v = \pm i$, starts with the quadratic term:

$$(k_>)^{1/2} = \pm i \pm \tfrac{1}{2} i(v \mp i)^2 + O\big((v \mp i)^3\big)\,. \tag{7.6}$$

Of course, the Padé approximants exhibit the well known pole at $(k_>)^{1/2} = 1$ due to the usual PM–FM critical singularity and the sequence of poles and zeroes starting near to $(k_>)^{1/2} = -1$ and continuing outward along the negative real axis attributed to the finite $(1+x)\ln|1+x|$ PM–AFM singularity, where $x = (k_>)^{1/2}$. For reference, the high-order dlog Padé entries for the pole position near the physical PM–FM critical point get this accurate to order $O(10^{-7})$. They also yield extremely precise determinations of the exponent, γ; indeed, among the $[N/N]$ entries with N around 20, the values of γ only differ from 1.75 by amounts of order 10^{-4}–10^{-5}. As regards complex-temperature singularities, the approximants exhibit two poles which converge to $(k_>)^{1/2} = \pm i$. These, together with the values of $\mathrm{Re}(\gamma_i)$, are shown in table 8. The values of $\mathrm{Re}(\gamma_i)$ are stable and are negative, indicating that $\bar{\chi}$ has finite singularities at $v = \pm i$ as these points are approached from within the complex PM phase. (The values of $\mathrm{Im}(\gamma_i)$ will be discussed below.) This confirms the conclusion of our analytic study in section 4, namely that $\bar{\chi}$ is finite at $v = \pm i$ as approached from within the complex PM phase. (That it is singular is obvious since it has different values when approached from different directions in the complex v, z, or u plane.)

Table 8. Values of $(k_>)_i^{1/2}$ and $\mathrm{Re}(\gamma_i)$ from diagonal dlog Padé approximants to high-temperature series for $\bar{\chi}$ starting with the series to $O((k_>^{1/2})^{15}) = O(v^{15})$.

$[N/N]$	$(k_>)_i^{1/2}$	$\lvert(k_>)_i^{1/2} - \mathrm{i}\rvert$	$\mathrm{Re}(\gamma_i)$
[7/7]	0.972 846i + 0.032 631	4.2×10^{-2}	−0.4297
[8/8]	1.003 43i + 0.034 469	3.5×10^{-2}	−0.5749
[9/9]	1.006 32i + 0.015 344	1.7×10^{-2}	−0.7720
[10/10]	1.007 29i + 0.003 183	0.8×10^{-2}	−0.832 35
[11/11]	0.997 106i + 0.001 684	3.3×10^{-3}	−0.6024
[12/12]	0.999 979i + 0.000 388	3.9×10^{-4}	−0.6432
[13/13]	0.999 715i + 0.000 650*	7.1×10^{-4}	−0.6404*
[14/14]	1.000 53i + 0.006 735	6.8×10^{-3}	−0.7166
[15/15]	1.000 26i + 0.006 752*	6.8×10^{-3}	−0.7101*
[16/16]	0.998 362i + 0.003 564	3.9×10^{-3}	−0.6380
[17/17]	0.998 506i + 0.003 520*	3.8×10^{-3}	−0.6409*
[18/18]	0.999 870i + 0.003 009	3.0×10^{-3}	−0.6727
[19/19]	0.998 932i + 0.002 885	3.1×10^{-3}	−0.6442
[20/20]	0.999 033i + 0.002 739*	2.9×10^{-3}	−0.6449*
[21/21]	0.999 021i + 0.002 416	2.6×10^{-3}	−0.6391
[22/22]	0.999 472i + 0.002 638	2.7×10^{-3}	−0.6567
[23/23]	0.999 487i + 0.002 646	2.7×10^{-3}	−0.6573
[24/24]	0.999 162i + 0.002 051	2.2×10^{-3}	−0.6374

To check the sensitivity of the dlog Padé analysis to possible divergent singularities, we have studied the test function

$$\bar{\chi}(x)_{\mathrm{test}} = A_{c,x}(1-x)^{-7/4} - A_{\mathrm{AFM},x}(1+x)\ln(1+x) + A_{s,x}(1+x^2)^{-\gamma_s/2} + B \tag{7.7}$$

where $x = (k_>)^{1/2}$. This function incorporates the known PM–FM and PM–AFM singularities, a hypothetical divergent singularity at $(k_>)^{1/2} = v = \pm\mathrm{i}$ with exponent corresponding to $(1+v^2)^{-\gamma_s}$, and an additional background term B. We have used the known critical amplitudes $A_{c,x} = 2^{7/8}A_{c,v} = 1.4153665\ldots$, where $A_{c,v}$ is defined by $\bar{\chi}_{\mathrm{sing}} \sim A_{c,v}(1 - v/v_c)^{-7/4}$ for $v \nearrow v_c$ and is given by $A_{c,v} = 0.77173406\ldots$ [12, 27]; and $A_{\mathrm{AFM},x} = 2^{1/2}A_{v,\mathrm{AFM}} = 0.28$, where $A_{v,\mathrm{AFM}}$ is defined by $\bar{\chi}_{\mathrm{sing}} \sim -A_{v,\mathrm{AFM}}(1+v/v_c)\ln|1+v/v_c|$ for $-v \nearrow -v_c$ and is given by $A_{v,\mathrm{AFM}} \simeq 0.20$ [27]. We have varied $A_{s,x}$ and B over a range of values and γ_s over the range $\frac{1}{4} < \gamma_s \leqslant \frac{3}{2}$, and have found that if these quantities have values such that the dlog Padé approximants locate the singularities at $v = (k_>)^{1/2} = \pm\mathrm{i}$ with an accuracy comparable to that which we observe in table 8, then the approximants also yield reasonably accurate values for γ_s. In particular, if we make the values of $A_{s,x}$, γ_s and/or B so small that the Padé fails to yield an accurate value for γ_s, then it also fails to locate the singularities at $(k_>)^{1/2} = \pm\mathrm{i}$ in the test function with the accuracy that it does successfully locate them for the actual $\bar{\chi}$. Hence, the dlog Padé would not miss divergent singularities at $v = (k_>)^{1/2} = \pm\mathrm{i}$ if they were really present in $\bar{\chi}$.

However, the dlog Padé method is not, in general, satisfactory for a finite singularity, and hence, given that $\mathrm{Re}(\gamma_i) < 0$, one cannot, *a priori*, trust the actual values of γ_i which it yields. The appropriate technique to investigate such finite singularities in the presence of background terms is provided by differential approximants (DA) [15, 28–32]. To be precise, if a function of a generic variable ζ is of the product form $f(\zeta) = \prod_{j=1}^{N}(1-\zeta/\zeta_j)^{-p_j}$, then *the dlog Padé method is, in principle, adequate to obtain the positions and exponents for the* singularities even if some $p_j < 0$. If f has an additive background term near a singularity, i.e. if $f_{\mathrm{sing}} \sim A(1-\zeta/\zeta_j)^{-p_j} + B(\zeta)$ with $B(\zeta)$ analytic near ζ_j, then, if a given $p_j > 0$, the first Darboux theorem [14] shows that for sufficiently high orders, this will dominate over $B(\zeta)$ so that the dlog Padé method can still be satisfactory, but if the given $p_j < 0$, then one should use differential approximants.

We recall that in the differential approximant method the function $f = \bar{\chi}$ being approximated satisfies a linear ordinary differential equation (ODE) of Kth order, $\mathcal{L}_{M,L} f_K(\zeta) = \sum_{j=0}^{K} Q_j(\zeta) D^j f_K(\zeta) = R(\zeta)$, where $Q_j(\zeta) = \sum_{\ell=0}^{M_j} Q_{j,\ell}\zeta^\ell$ and $R(\zeta) = \sum_{\ell=0}^{L} R_\ell \zeta^\ell$ [15, 30–32]. In one implementation of the method [30, 31], $D \equiv d/d\zeta$, while in another [30, 31], $D \equiv \zeta d/d\zeta$. We adopt the choice for D used in [32, 15]; these authors have found that both choices give comparable results. The solution to this ODE, with the initial condition $f(0) = 1$, is the resultant approximant, labelled as $[L/M_0; \ldots; M_K]$. The general solution of the ODE has the form $f_j(\zeta) \sim A_j(\zeta)|\zeta - \zeta_j|^{-p_j} + B(\zeta)$ for $\zeta \to \zeta_j$. The singular points ζ_j are determined as the zeros of $Q_K(\zeta)$ and are regular singular points of the ODE, and the exponents are given by $-p_j = K - 1 - Q_{K-1}(\zeta_j)/(\zeta_j Q_K'(\zeta_j))$. Further details on the method can be found in [15, 30–32]. For an extrapolation procedure to be discussed below, we shall use a number of poles at different positions close to the singularity; for this reason, we use unbiased differential approximants. Studying the susceptibility series in the variable v, we find that the differential approximants do not yield singularities sufficiently close to $\pm$i to be accurate, just as was true of the dlog Padé method (which is a special case of DA). As before, we have obtained considerably better results with the series in the elliptic modulus variable $(k_>)^{1/2}$. We have calculated the $K = 1$ differential approximants $[L/M_0; M_1]$ for $4 \leqslant L \leqslant 24$ and $10 \leqslant M_0 \leqslant 20$ with $M_1 = M_0$, $M_0 \pm 1$ subject to the constraint $L + M_0 + M_1 + 2 \leqslant 49$ (terms up to $O(v^{49}) = O((k_>^{1/2})^{49})$ were used). Many of the poles may reflect finite singularities along the arcs of the circles bounding the complex PM phase, as discussed previously [1]. To consider a pole to represent the singularity at $(k_>)^{1/2} = \mathrm{i}$, we require that its distance from this point satisfy $|(k_>)^{1/2} - \mathrm{i}| < 1 \times 10^{-2}$. Secondly, we shall show the poles which lie within the circle $|k_>| = 1$ which forms the boundary of the complex PM phase; these exhibit less scatter than a set including poles outside this circle and allow us to make at least a crude inference for the value of γ_i (consistent with the theorem of [1] which guarantees that $\mathrm{Re}(\gamma_\mathrm{i}) < 0$). In table 9 we display the $K = 1$ differential approximants with L even which satisfy these conditions. (The approximants with odd L are not listed to save space; they yield conclusions in agreement with those obtained from the approximants with even L.) Evidently, there is a large scatter of values of γ_i. Also, the distances from the singularity are usually larger than the $O(10^{-3})$ level which one would normally consider necessary for accurate results. However, we can still draw useful information from this table. First, all of the values of γ_i satisfying the two conditions above have the property that $\mathrm{Re}(\gamma_\mathrm{i}) < 0$. Second, the approximants in table 9 which yield poles closest to $(k_>)^{1/2} = \mathrm{i}$, namely $\left[\frac{10}{16}; 18\right]$, $\left[\frac{20}{12}; 12\right]$, $\left[\frac{22}{10}; 12\right]$, and $\left[\frac{24}{10}; 11\right]$, do give roughly consistent values of $\mathrm{Re}(\gamma_\mathrm{i})$. If we plot the values of $\mathrm{Re}(\gamma_\mathrm{i})$ as a function of the distance $|(k_>)^{1/2} - \mathrm{i}|$ and extrapolate to zero distance from the singularity, we obtain $\mathrm{Re}(\gamma_\mathrm{i}) \simeq -0.65$. This is consistent with the values obtained for this quantity from the dlog Padé study.

We can make further progress by noticing an important correlation: the sign of $\mathrm{Im}(\gamma_\mathrm{i})$ is opposite to the sign of the deviation $\mathrm{Re}((k_>)_\mathrm{i}^{1/2})$ from zero. Indeed, when we plot the values of $\mathrm{Im}(\gamma_\mathrm{i})$ as a function of $\mathrm{Re}((k_>)_\mathrm{i})$, they can be roughly fit to a line going through zero when $\mathrm{Re}((k_>)_\mathrm{i}^{1/2}) = 0$. But the singularity which we are studying is at $(k_>)^{1/2} = \mathrm{i}$, so we are led to the tentative conclusion that for this singularity, $\mathrm{Im}(\gamma_\mathrm{i}) = 0$. It follows also that for the conjugate singularity at $(k_>)^{1/2} = -\mathrm{i}$, $\mathrm{Im}(\gamma_{-\mathrm{i}}) = 0$, whence $\gamma_\mathrm{i} = \gamma_{-\mathrm{i}} = \gamma_\mathrm{s}$. As regards the values of $\mathrm{Im}(\gamma_\mathrm{i})$ from the dlog Padé study, one can see that all of the high-order diagonal approximants are characterized by the same (positive) sign for $\mathrm{Re}((k_>)^{1/2}$,

Table 9. Values of $(k_>)_{\rm i}^{1/2}$ and $\gamma_{\rm i}$ from $K = 1$ differential approximants to high-temperature series for $\bar{\chi}$. See the text for a definition of the $[L/M_0; M_1]$ approximant.

$[L/M_0; M_1]$	$(k_>)_{\rm i}^{1/2}$	$\lvert(k_>)_{\rm i}^{1/2} - {\rm i}\rvert$	$\gamma_{\rm i}$
[4/18; 19]	0.993 373i + 0.004 293	0.79×10^{-2}	−1.420 − 1.079i
[4/18; 20]	0.991 349i + 0.002 545	0.90×10^{-2}	−1.820 − 0.8796i
[8/18; 16]	0.990 874i + 0.003 398	0.97×10^{-2}	−1.950 − 0.3293i
[8/18; 17]	0.988 550i − 0.006 664	1.3×10^{-2}	−1.944 + 1.741i
[8/18; 18]	0.990 839i + 0.004 293	1.0×10^{-2}	−2.164 − 0.3726i
[10/16; 18]	0.999 122i − 0.001 421	1.7×10^{-3}	−0.8568 + 0.4512i
[12/10; 10]	0.998 7905i − 0.005 881	0.60×10^{-2}	−1.243 + 0.4854i
[14/10; 10]	0.990 038i + 0.007 285	1.2×10^{-2}	−2.294 − 1.181i
[14/12; 14]	0.990 566i − 0.001 845	0.96×10^{-2}	−1.611 + 0.3934i
[18/10; 10]	0.990 270i + 0.002 944	1.0×10^{-2}	−1.907 − 0.3510i
[18/12; 12]	0.998 597i + 0.011 27	1.1×10^{-2}	−0.7024 − 1.417i
[20/10; 11]	0.994 749i − 0.001 108	0.54×10^{-2}	−1.267 + 0.3876i
[20/10; 12]	0.995 176i − 0.002 265	0.53×10^{-2}	−1.214 + 0.5585i
[20/12; 10]	0.998 042i + 0.008 232	0.85×10^{-2}	−0.1837 − 1.433i
[20/12; 11]	0.995 593i − 0.003 949	0.59×10^{-2}	−1.105 + 0.9183i
[20/12; 12]	0.998 991i − 0.000 353	1.1×10^{-3}	−0.6833 + 0.3278i
[22/10; 11]	0.997 787i − 0.002 213	3.1×10^{-3}	−0.8149 + 0.6317i
[22/10; 12]	0.998 212i − 0.001 353	2.2×10^{-3}	−0.7283 + 0.5223i
[24/10; 9]	0.993 917i − 0.006 415	0.88×10^{-2}	−1.850 + 0.9510i
[24/10; 10]	0.997 266i − 0.001 653	3.2×10^{-3}	−0.9898 + 0.4162i
[24/10; 11]	0.997 902i + 0.000 488 2	2.2×10^{-3}	−0.5841 − 0.0597i
[24/10; 12]	0.997 133i − 0.008 122	0.86×10^{-2}	−1.120 + 1.803i

i.e. the pole positions are slightly to the right of $(k_>)^{1/2} = {\rm i}$. This correlates with the observed feature that these Padé approximants have the stable non-zero negative values ${\rm Im}(\gamma_{\rm i}) \simeq -0.25$. Indeed, when we examine other poles in the dlog Padé approximants reasonably close to the point $(k_>)^{1/2} = {\rm i}$, we observe the same correlation that ${\rm Im}(\gamma_{\rm i})$ has a sign opposite to that of ${\rm Re}((k_>)^{1/2})$. This suggests that if we had a reasonably large set of such nearby poles, then we could carry out an extrapolation similar to the one that we performed with the differential approximants. There are not enough close poles with ${\rm Re}((k_>)^{1/2}) < 0$ to do this accurately, but one can say that such an extrapolation is crudely consistent with ${\rm Im}(\gamma_{\rm i}) = 0$.

Summarizing, then, the results of our analysis with differential approximants, like those of the simple dlog Padé study, confirm our analytic demonstration that $\bar{\chi}$ is finite (although, of course, singular) at the points $v = (k_>)^{1/2} = \pm{\rm i}$ (i.e. $u = -1$) when approached from within the complex PM phase. Furthermore, if we restrict to the four poles closest to $v = (k_>)^{1/2} = {\rm i}$, the DAs yield values for ${\rm Re}(\gamma_{\rm i})$ which are roughly mutually consistent. Note that for these four poles, the distance from the singularity, $2\text{–}3 \times 10^{-3}$, is comparable to that for the poles produced by the high-order dlog Padé approximants in table 8. Moreover, when we extrapolate the values of ${\rm Re}(\gamma_{\rm i})$ to apply precisely at the location of the singularity, we obtain a value consistent with that from the dlog Padé approximants. Using a similar extrapolation procedure with the differential approximants, we infer that ${\rm Im}(\gamma_{\rm i}) = 0$.

We recall that, in principle, $\bar{\chi}$ may have singularities elsewhere on the arcs forming the natural boundary of the complex PM phase, as discussed in [1]. It was proved there that if such singularities exist, they must be finite. Indeed, from a simple dlog Padé study, it was observed in that paper that the poles lay close to these arcs. The differential approximants presumably give some information about these possible finite singularities along the arcs.

We shall leave the more detailed investigation of the behaviour on these arcs to future work. However, from our present results, we may make some interesting observations. To the extent that the poles in the differential approximants away from $(k_>)^{1/2} = \pm\mathrm{i}$ lie near to the arcs bounding the complex PM region, they might reflect finite singularities in $\bar{\chi}$ along these arcs. The results of our study then suggest that the associated exponents would have non-zero imaginary parts, at points along the arcs in v or circle in $(k_>)^{1/2}$ apart from the points $(k_>)^{1/2} = \pm 1$ ($v = \pm v_c$) and $(k_>)^{1/2} = \pm\mathrm{i}$ ($v = \pm\mathrm{i}$). In assessing this possibility, it is, of course, incumbent upon one to first check whether there are any rigorous theorems forbidding this. We have not been able to derive any such theorem. Of course, the usual rigorous theorems governing the behaviour of thermodynamic quantities and, in particular, their critical exponents, assume physical values of the temperature. Two properties which must be satisfied are that $\bar{\chi}$ must be real and positive for physical temperature. These two properties do not exclude the existence of a complex exponent at a complex-temperature singularity in $\bar{\chi}$. To demonstrate this, we consider a generic form for the singular part of $\bar{\chi}$ with such singularities:

$$\bar{\chi}_{\mathrm{sing}}(\zeta) = A_j(1 - \zeta/\zeta_0)^{-\gamma_0} + A_0^*(1 - \zeta/\zeta_0^*)^{-\gamma_0^*} \tag{7.8}$$

where ζ denotes a generic variable (v, $(k_>)^{1/2}$ z, etc), $\mathrm{Im}(\gamma_0) \neq 0$, and the form (7.8) applies, say, for $|\zeta| < |\zeta_0|$. Evidently, this has the property that

$$\bar{\chi}_{\mathrm{sing}}(\zeta^*) = \bar{\chi}_{\mathrm{sing}}(\zeta)^* \tag{7.9}$$

which implies that if ζ is real, then $\bar{\chi}(\zeta)$ is also real†. We have also checked that one can write down examples of $\bar{\chi}_{\mathrm{sing}}$ of the form in (7.8) which yield not just real but positive $\bar{\chi}$ for physical temperature. If $\bar{\chi}$ has a singularity at the point $\zeta = \zeta_0$ of the leading form in (7.8) where the real and imaginary parts of γ_0 are given by

$$\gamma_0 = \gamma_{\mathrm{R}} + \mathrm{i}\gamma_{\mathrm{I}} \tag{7.10}$$

then for $\zeta = \zeta_0(1 + \epsilon\, \mathrm{e}^{\mathrm{i}\theta})$, as $\epsilon \to 0$,

$$\bar{\chi} \sim |\epsilon|^{-\gamma_{\mathrm{R}}}[\cos(\gamma_{\mathrm{I}} \ln(|\epsilon|)) - \mathrm{i}\sin(\gamma_{\mathrm{I}} \ln(|\epsilon|))]\,. \tag{7.11}$$

Given our theorem above that $\bar{\chi}$ must be finite on the arcs away from $v = v_c$ and $v = \pm\mathrm{i}$ (approached from within the FM or AFM phases), it follows that γ_{R} must be negative away from these points. The effect of the non-zero γ_{I} is to produce an infinitely rapid oscillation in $\bar{\chi}$ as $\zeta \to \zeta_0$ with $|\zeta| < |\zeta_0|$. Although the points on the arcs are not isolated singularities, but instead, points on the natural boundaries between the complex-extended PM, FM and AFM phases, this behaviour is quite analogous to the infinitely rapid oscillations at isolated essential singularities such as in the functions $\zeta \sin(1/\zeta)$ or $\zeta \cos(1/\zeta)$ at $\zeta = 0$. Given our result that $\bar{\chi}$ diverges at $u = -1$ as one approaches this point from the complex FM or AFM phases, but has a finite singularity as one approaches the point from the complex PM phase, one may observe that this behaviour is somewhat reminiscent of the function $\exp(1/\zeta)$, which has an (isolated) essential singularity at $\zeta = 0$ and diverges (vanishes) when this point is approached from the positive (negative) real axis.

A physical argument for the divergence in the susceptibility at a second-order phase transition, such as the PM–FM critical point, is to note that the magnetization vanishes continuously as one approaches this point from within the FM phase, so that, in the limit, an arbitrarily small external field H has an arbitrarily large relative effect on the resultant

† Actually, real ζ may still correspond to complex temperature, for example, as (2.10) shows, $K = r + n\mathrm{i}\pi$ with r real corresponds to real u and hence real $\bar{\chi}$. The symmetries (2.10) and (2.11) imply that for the indicated infinite sets of complex values of K, quantities such as $\bar{\chi}$ are still real.

magnetization $M(H)$. This argument also agrees with the divergence in the susceptibility that we found at the complex-temperature point $u = -1$, as approached from within the complex-extended FM phase, since this is the only other point at which M vanishes continuously, starting from within the complex FM phase. For the physical PM–FM critical point the same argument motivates the divergence in $\bar{\chi}$ as one approaches this point from within the PM phase. However, our analytic demonstration (and confirmation via high-temperature series analysis) that $\bar{\chi}$ has a finite singularity when one approaches $u = -1$ from within the complex PM phase shows that, for complex-temperature singularities, this reasoning for physical temperatures is not applicable in a naive manner.

8. Conclusions

In summary, we have carried out a study of the complex-temperature singularities of the susceptibility of the 2D Ising model on a square lattice. From an analysis of low-temperature series expansions, we have found evidence that, as one approaches the point $u = u_s = -1$ from within the complex extensions of the physical ferromagnetic or antiferromagnetic phases, $\bar{\chi}$ has a divergent singularity. Our results are consistent with the conclusion that the critical exponent for this singularity is $\gamma_s' = \frac{3}{2}$. We have also calculated the critical amplitude. However, from an analysis of the asymptotic decays of spin–spin correlation functions, we have shown that the correlation length is finite, and hence the susceptibility is finite (although both are singular) at the points $v = \pm i$ corresponding to $u = -1$ when approached from within the complex-extended symmetric, paramagnetic phase. This is confirmed by a study of high-temperature series expansions.

Our results are of interest because they elucidate the behaviour of the susceptibility as an analytic function. The goal of calculating the susceptibility of the 2D Ising model (or even making a conjecture for this function which agrees with available series expansions) has remained elusive for half a century since Onsager's calculation of the free energy. Our results should be useful for this quest because they provide new properties which must be satisfied by such a conjecture or calculation.

One can think of a number of further related studies to perform. In one direction, using low- and high-temperature expansions, we have carried out analyses with dlog Padé and differential approximants to investigate complex-temperature singularities of $\bar{\chi}$ in the Ising model on the triangular and honeycomb lattices. Our results will be reported in a sequel paper. One could also examine other models like the $d = 2$, $q = 3$ Potts model. Yet another topic is how ideas of conformal field theory, which have greatly illuminated the critical behaviour at the physical critical points of various 2D models, can be applied to this complex-temperature singularity. Clearly, there is much work for the future.

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Note added in proof. After the submission of this manuscript, we were informed by Professor Tony Guttmann that he, I Enting, and I Jensen had previously concluded that for the spin-$\frac{1}{2}$ Ising model on the square lattice, $\bar{\chi}$ has a divergent singularity at $u = -1$ with exponent $\gamma_s = \frac{3}{2}$, from an analysis of the low-temperature series expansion for $\bar{\chi}$, in the paper 'Low-temperature series expansions for the spin 1 Ising model' (1994), published as [33]. This paper also reports an extended calculation of this low-temperature series to $O(u^{38})$, i.e. c_n to $n = 36$ in the notation of our (3.1), as well as new low-temperature series and analyses for the spin-1 Ising model on the square lattice. We thank Professor Guttmann for kindly informing us of this work and for interesting discussions.

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