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LETTER TO THE EDITOR

Zeros of the partition function for higher-spin 2D Ising models

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Abstract. We present calculations of the complex-temperature zeros of the partition functions for 2D Ising models on the square lattice with spin $s = 1, \frac{3}{2}$ and 2. These give an insight into complex-temperature phase diagrams of these models in the thermodynamic limit. Support is adduced for a conjecture that all divergences of the magnetization occur at endpoints of arcs of zeros protruding into the FM phase. We conjecture that there are $4[x^2] - 2$ such arcs for $s \geq 1$, where $[x]$ denotes the integral part of x .

The Ising model has long served as a simple prototype of a statistical mechanical system which (for spatial dimensionality $d > 1$) undergoes a phase transition with associated spontaneous symmetry breaking and long-range order. The zero-field $d = 2$ spin- $\frac{1}{2}$ Ising model is exactly solvable; the free energy f and spontaneous magnetization M were first derived by Onsager and Yang, respectively [1, 2] (both for the square lattice). However, no exact closed-form expressions have ever been found for f or any other thermodynamic quantity for any higher-spin Ising model in $d = 2$ (or higher d). It is therefore of considerable value to establish further properties of higher-spin Ising models, since these help one to make progress toward an exact solution. In this letter we present calculations of the complex-temperature zeros of the partition functions of the 2D Ising model on the square lattice for the higher spin values $s = 1, \frac{3}{2}$ and 2. These results enable one to infer information about the complex-temperature (T) phase diagrams in the thermodynamic limit for these models. Combining our results with analyses of low-temperature series by Guttman *et al* [3, 4], we adduce support for our conjecture on complex-temperature divergences in M . We also infer a new conjecture on arcs of zeros.

There are several reasons for interest in complex- T properties of spin models: (i) one can understand more deeply the behaviour of various thermodynamic quantities by seeing how they behave as analytic functions of complex T (e.g. complex- T singularities can affect behaviour for physical temperature); (ii) one can see how the physical phases of a given model generalize to regions for complex T ; (iii) as noted, a knowledge of complex- T properties helps in the search for exact solutions. The earliest papers on complex- T properties in the Ising model include [5–10] for $s = \frac{1}{2}$; such properties for higher-spin (2D and 3D) Ising models were first studied in [11, 12] (see also [13, 14]). Later papers for $s = \frac{1}{2}$ include [15–20].

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The spin- s (nearest-neighbour) Ising model on the square lattice is defined, in standard notation, by the partition function $Z = \sum_{\{S_n\}} e^{-\beta \mathcal{H}}$, with

$$\mathcal{H} = -(J/s^2) \sum_{\langle nn' \rangle} S_n S_{n'} - (H/s) \sum_n S_n \quad (1)$$

where $S_n \in \{-s, -s+1, \dots, s-1, s\}$ and $\beta = (k_B T)^{-1}$. $H = 0$ unless otherwise indicated. We define $K = \beta J$, $v = \tanh K$ and $u_s = e^{-K/s^2}$. Z is then a generalized (i.e. with negative as well as positive powers) polynomial in u_s . We denote the physical critical point as K_c for a given s , and $(u_s)_c = \exp(-K_c/s^2)$. The (reduced) free energy is $f = -\beta F = \lim_{N_s \rightarrow \infty} N_s^{-1} \ln Z$ in the thermodynamic limit.

Early series studies (mainly for 3D) gave evidence that the critical exponents of the phase transition between the Z_2 -symmetric, paramagnetic (PM) phase and the phase with spontaneous symmetry breaking and long-range ferromagnetic (FM) order are independent of s [13, 21]. This is in agreement with expectations from renormalization-group arguments, since changing s does not change the Z_2 symmetry group of \mathcal{H} . However, for complex temperature, the value of s does have interesting effects.

Since there is no closed-form expression for f for $s \geq 1$, one cannot directly determine the locus of complex- T points where f is non-analytic (aside from the points $K = \pm\infty$ where it is trivially non-analytic). However, from calculations of zeros for the 2D spin- $\frac{1}{2}$ Ising model and comparison with exact results, one knows that as the lattice size increases, the zeros of Z occur on, or progressively closer to, the above locus of points where, in the thermodynamic limit, f is non-analytic. By studying the zeros of Z on finite lattices with varying boundary conditions, one can thus make reasonable inferences about this locus of points and the corresponding complex- T phase diagram.

For the $d = 2$, $s = \frac{1}{2}$ Ising model with isotropic couplings J on the square lattice (as well as on the triangular and honeycomb lattices, and also certain heteropolygonal lattices [20]), as $N_s \rightarrow \infty$, these zeros of the partition function in z merge to form continuous curves, including possible line segments. The complex- T phase diagram is comprised of phases bounded by such curves where leading and next-to-leading eigenvalues of the transfer matrix \mathcal{T} (which are, in general, complex here) become degenerate in magnitude and hence there is a non-analytic change in f . We now show that (for isotropic J) the zeros of Z again merge to form a one-dimensional variety (i.e. curves including possible line segments, instead of areas) in the complex u_s plane for arbitrary s . Using the discrete translation invariance of the square lattice, one can, by Fourier transformation methods, write

$$f = \ln(2s+1) + \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\theta_1 d\theta_2}{(2\pi)^2} g(A + B(\cos\theta_1 + \cos\theta_2)) \quad (2)$$

where A and B are functions of u_s . The locus of points where g and hence f are non-analytic is given by an equation involving only the argument of g , namely, $A + B(\cos\theta_1 + \cos\theta_2)$. Now since the two independent (periodic) variables θ_1 and θ_2 only enter in the combination $\cos\theta_1 + \cos\theta_2 \equiv x$, the argument of g can be written as $A(u_s) + B(u_s)x$, so that the equation involves a single independent real variable ($-2 \leq x \leq 2$). Hence, the continuous locus of points where f is non-analytic (i.e. excluding the trivial isolated points $K = \pm\infty$) is a one-dimensional variety in the u_s plane. The zeros of Z and corresponding curves where f is non-analytic are invariant under $u_s \rightarrow u_s^*$ and also, for a bipartite lattice, under the mapping $u_s \rightarrow 1/u_s$.

In order to compute the zeros, we calculate Z for finite lattices with specified boundary conditions. We have done this by means of a transfer matrix method [22], and have used both periodic and helical boundary conditions. We have also used a type of helical boundary

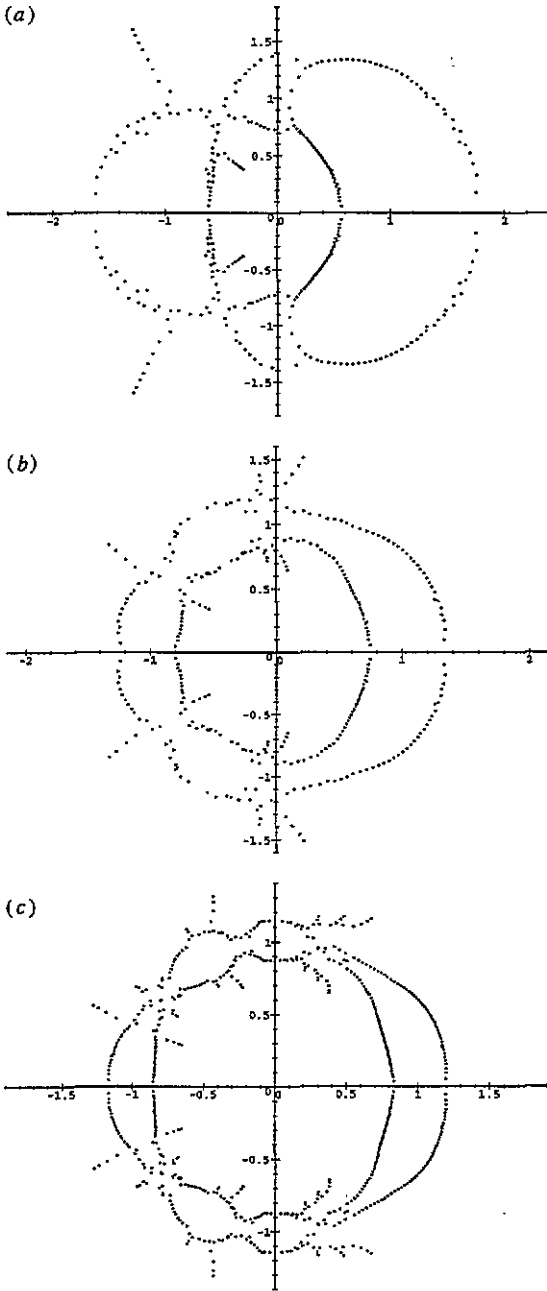


Figure 1. Plots of zeros of Z for the Ising model on the square lattice, as functions of $u_s = e^{-K/s^2}$, for (a) $s = 1$, lattice size 8×10 ; (b) $s = \frac{3}{2}$, lattice size 6×6 ; (c) $s = 2$, lattice $5 \times (\frac{38}{5})$. See text for notation. (a), (b) use periodic boundary conditions, while (c) uses Creutz helical boundary conditions.

condition introduced by Creutz [23] which reduces finite-size effects. We follow the notation of [23] to label the lattice in this case: $N_1 \times (N_s/N_1)$, where N_s denotes the total number of sites and N_1 denotes the number of sites in all the rows except the last.

In figure 1 we show the zeros of Z for the Ising model on a square lattice with (i) $s = 1$, lattice size 8×10 ; (ii) $s = \frac{3}{2}$, lattice size 6×6 ; (iii) $s = 2$, lattice $5 \times (\frac{38}{5})$. The horizontal and vertical axes are $\text{Re}(u_s)$ and $\text{Im}(u_s)$ for each s . We have calculated zeros for a number of different lattices. Although we only show one plot for each s here, the features which we

point out were observed on all of the lattices used, with all types of boundary conditions. The actual plots shown in figures 1(a) and (b) used periodic boundary conditions, while that in figure 1(c) used Creutz helical boundary conditions. We note that an early calculation of the zeros for $s = 1$ on smaller lattices (up to 4×4) was given in [11].

First, up to some slight scatter, the zeros can be connected by curves, in agreement with our general argument above. Second, for each s , the model has physical PM, FM and AFM phases, and these have analytic continuations to form phases in the u_s plane; we denote these as (complex- T) PM, FM and AFM phases. The symmetry of the phases about the unit circle $|u_s| = 1$ follows from the $u_s \rightarrow 1/u_s$ symmetry of the model.

Third, the phase diagram also includes phases (labelled 'O') which have no overlap with any physical phase. For $s = 1, 2$ there is an O_1 phase to the left of the FM phase separating it from the AFM phase. We conjecture that this is true for arbitrary integral s . We restrict this conjecture to integral s since we already know that it does not hold in the exactly solved $s = \frac{1}{2}$ model; in that case, there is no O phase (in the $u_{1/2} \equiv e^{-4K}$ variable), and the FM and AFM (and PM) phases are directly contiguous at $u_{1/2} = -1$ (see figure 1(c) of [17]). The number of O phases increases as a function of s . For $s = 1$, our results suggest that in addition to O_1 , there is also an O_2 above, and its complex-conjugate (CC) O_2^* phase below, the FM phase. There is no definite indication of any other O phases. For $s = \frac{3}{2}$, there is an O_1 phase or a CC pair of O_1 and O_1^* phases to the left of the FM phase, and CC O_2 and O_2^* phases to the upper and lower left of the FM phase. There may be other O phases also. For $s = 2$, there appear to be several CC pairs of O phases in addition to the definite O_1 phase.

Fourth, one may study special points separating complex- T phases. Because of the $u_s \rightarrow 1/u_s$ symmetry, and the consequent manner in which the phases group themselves around the unit circle $|u_s| = 1$, it follows that if two such phases are contiguous at a single point, then this point lies on this unit circle. An exactly known example is the case $u_{1/2} = -1$ for $s = \frac{1}{2}$. From our $s = 1$ zeros, it is likely that one such point $u_{1;12}$ separates the O_1 and O_2 phase (so that also $u_{1;12}^*$ separates the O_1 and O_2^* phases); if this is the case, then it is likely that $u_{1;12} = e^{2\pi i/3}$. For $s = \frac{3}{2}$, we infer likely intersection points of phase boundaries at $u_{3/2;a} = i$ and $u_{3/2;b} = e^{4\pi i/5} = \frac{1}{4}(-\sqrt{5} - 1 + i\sqrt{2}\sqrt{5 - \sqrt{5}}) \simeq -0.809 + 0.588i$ together with their CCs. For $s = 2$, we infer likely intersection points at $u_{2;a} = e^{\pi i/3}$, $u_{2;b} = e^{2\pi i/5} = (1/4)(-1 + \sqrt{5} + i\sqrt{2}\sqrt{5 + \sqrt{5}}) \simeq 0.309 + 0.951i$, and $u_{2;c} = e^{4\pi i/5}$, together with their CCs. There may be other such points for $s = 2$.

Fifth, in addition to the zeros that lie on boundaries which, in the thermodynamic limit, would separate complex- T phases, there are also zeros which lie on arcs which do not separate phases, but rather protrude into, and end in, the FM and AFM phases. As our exact solution of the complex- T phase diagram for the 1D spin- s Ising model [24] shows, such arcs can represent the degeneracy, on a finite curve, of the leading and next-to-leading eigenvalues of \mathcal{T} . For $s = \frac{1}{2}$, there are no such protruding arcs for the square lattice, although exact results show that they do occur for other 2D lattices (triangular (in FM), honeycomb (PM), kagomé (PM), 3-12 lattice (PM) [20]). We denote the number of arcs protruding into the phase ph (and terminating in endpoints (e)) as $N_{e,ph}$. If these arcs occur at complex values of u_s , then the $u_s \rightarrow u_s^*$ symmetry implies that they must occur as CC pairs, so $N_{e,FM}$ is even. For all of the s values that we have studied (on the square lattice), the arcs do occur at complex values of u_s , which leads one to infer that $N_{e,FM}$ is even on the square for all s (this will follow from our conjecture (3)†. Independent of this, for any

† This inference does not apply to other lattices; indeed, one knows of cases where $N_{e,FM}$ is odd, e.g. exact results show that $N_{e,FM} = 1$ for $s = \frac{1}{2}$ on the triangular lattice.

Table 1. Endpoints of arcs protruding into the FM phase. Entries in column denoted $(u_s)_{e,Z}$ are the positions of the last zeros on the arcs in figures 1(a)–(c).

s	$N_{e,FM}$	$(u_s)_{e,Z}$	$\frac{ (u_s)_{e,Z} }{(u_s)_c}$
1/2	0	—	—
1	2	$-0.305 \pm 0.381i$	0.874
3/2	6	$0.09 \pm 0.65i$	0.88
		$-0.07 \pm 0.72i$	0.98
		$-0.54 \pm 0.34i$	0.85
2	14	$0.38 \pm 0.65i$	0.90
		$0.30 \pm 0.73i$	0.95
		$0.21 \pm 0.80i$	1.0
		$-0.23 \pm 0.69i$	0.87
		$-0.40 \pm 0.69i$	0.965
		$-0.68 \pm 0.49i$	1.0
		$-0.655 \pm 0.29i$	0.86

bipartite lattice the $u_s \rightarrow 1/u_s$ symmetry implies that $N_{e,FM} = N_{e,AFM}$.

For $s = 1$ (figure 1(a)), we find an arc protruding in a 'NW–SE' direction into the FM phase and a corresponding arc protruding in a SE–NW direction into the AFM phase, together with their complex conjugates, so $N_{e,FM} = 2$ for $s = 1$. For $s = \frac{3}{2}$ (figure 1(b)), we find three CC pairs of arcs protruding into the FM phase, so $N_{e,FM} = 6$. For $s = 2$ (figure 1(c)), we infer seven such CC pairs of arcs, so $N_{e,FM} = 14$. Our results are summarized in table 1†. For $s \geq \frac{3}{2}$ we list the positions of the last zeros to an accuracy of 0.01 in real and imaginary parts because this is typical of the differences between the locations of these zeros for different lattice sizes and BCs. The values of $|(u_s)_{e,Z}|$ are calculated using these positions to their full accuracy for the lattices in figure 1. The values of $(u_s)_c$ used for the last column are from [3, 4].

From previous studies of the $s = \frac{1}{2}$ Ising model for lattices in $d = 2, 3$, we have been led to formulate several general conjectures for complex- T singularities in M and the susceptibility $\bar{\chi}$. One of these is:

Conjecture 1. For the zero-field $s = \frac{1}{2}$ Ising model on an arbitrary (regular) lattice with even coordination number q , M diverges at a point $z = e^{-2K}$ if and only if z is an endpoint of an arc (of non-analyticities of f , as discussed above) protruding into the FM phase.

A corollary of conjecture 1 is that on a bipartite lattice, for each such endpoint there is another with $K \rightarrow -K$ at which the staggered magnetization M_{st} diverges‡. In [19] we proved (as theorem 1 in the first paper) that if M diverges at a given point $z = e^{-2K}$, so does $\bar{\chi}$, and thus, for a bipartite lattice, if M_{st} diverges, so does the staggered susceptibility, $\chi^{(a)}§$. Since there is no obvious reason why this conjecture should be limited to $s = \frac{1}{2}$, it is natural to consider the following generalization:

Conjecture 1s. For the zero-field Ising model with arbitrary s on an arbitrary (regular) lattice with even q , M diverges at a point u_s if and only if u_s is an endpoint of an arc of

† We add the usual caution that analyses on finite lattices up to a given size can never rigorously exclude the possibility that there are changes in the arcs as one gets closer to the thermodynamic limit.

‡ We record a related conjecture here [20]: conjecture 2: For the $s = \frac{1}{2}$ Ising model on an arbitrary (regular) lattice with odd coordination number q , in addition to the divergences at arc endpoints specified by conjecture 1, M also diverges at the point $z = -1$ if and only if this point can be reached from within the FM phase.

§ Our study of the exactly solvable $s = \frac{1}{2}$ Ising model with $\beta H = i\pi/2$ in [18] suggests that it is possible to generalize conjecture 1 to a class of non-zero external fields.

non-analyticities of f protruding into the FM phase.

A corollary of conjecture 1s is that on a bipartite lattice, to each such point, there corresponds a point $1/u_s$ in the AFM phase, and M_{sr} diverges at a point $1/u_s$ in the AFM phase if and only if $1/u_s$ is the endpoint of an arc protruding into the AFM phase (the image, under $u_s \rightarrow 1/u_s$, of the arc in the FM phase).

Combining our determination of the positions of the endpoints of arcs protruding into the FM phase with the results of low-temperature series analyses in [3] ($s = 1$) and [4] $1 \leq s \leq 3$, we find that for the values $s = 1$, $\frac{3}{2}$ and 2 where the comparison can be made, there is excellent support for conjecture 1s. Of course, the position of the last zero on an arc calculated for a finite lattice will not, in general, be precisely the same as the endpoint in the thermodynamic limit, but we expect it to be close for the lattices of the sizes that we are using. For $s = 1$, [3] found divergences in M at the CC points $u_1 = -0.30196(3) \pm 0.37875(5)i$, which match nicely with the arc endpoints we have found for this case. As a consequence of our theorem 1 in [19], these divergences in M automatically imply divergences in $\bar{\chi}$, and these were also observed in [3]. For $s = \frac{3}{2}$ and 2, all of the divergences in M again match the locations of the arc endpoints which we have found [4]. For example, for $s = \frac{3}{2}$, preliminary results give [4] $u_{3/2} = 0.0948(1) \pm 0.6410(2)i$ and $-0.5291(2) \pm 0.3379(2)i$ for the two such singularities closest to the origin, in agreement with our values in table 1, with a similar match for the third. These comparisons indicate that the last zero on an arc for the finite lattices which we have used is a distance of about 0.01 farther away from the origin than the singularity positions from series analyses [4, 3], which presumably reflect the thermodynamic limit. (For $s = 1$, the difference in distances is less, about 0.004.) We infer that the last zeros on the arcs give values of $\rho = |u_s|/(u_s)_c$ which are larger than the exact values by roughly 1%.

These results differ with an old conjecture [12] that for the spin- s Ising model the number $N_{cs, \rho < 1}$ of complex-temperature singularities within the disc $\rho < 1$ is $N_{cs, \rho < 1} = qs - 2$, where q is the coordination number of the lattice. Here, this would yield $N_{cs, \rho < 1} = 4s - 2 = 2, 4$, and 6 for $s = 1, \frac{3}{2}$, and 2, rather than the respective values 2, 6, and ≥ 10 which we find with $\rho < 1$.

Combining our present calculation of partition function zeros with an exact determination of the complex- T phase structure of the 1D spin- s Ising model [24], we make the following conjecture: for the spin s Ising model on the square lattice, the number of endpoints of arcs protruding into the complex- T FM (equivalently, AFM phase) is

$$N_{e,FM} = N_{e,AFM} = 4[s^2] - 2 \quad (3)$$

for $s \geq 1$, where $[x]$ denotes the integral part of x . Combining this with the exactly known result for $s = \frac{1}{2}$, the general formula reads $N_{e,FM} = N_{e,AFM} = \max\{0, 4[s^2] - 2\}$.

We next discuss the s dependence of the PM phase. In general, for a fixed lattice and temperature, an increase in s has the effect of allowing more randomness, and hence increasing the disorder in the model. This is reflected in the well known fact that K_c is a monotonically increasing (e^{-K_c} is a monotonically decreasing) function of s [12, 13, 21, 4]. Thus, the disordered, PM phase increases in extent as s increases. However, although K_c increases as a function of s , the ratio K_c/s^2 which occurs in the variable u_s decreases, approaching zero as $s \rightarrow \infty$. Indeed, as $s \rightarrow \infty$, K_c approaches a finite limiting value, $K_c(s) \nearrow K_c(s = \infty)$. This follows since in this $s \rightarrow \infty$ limit (renormalizing Z so that each spin summation is normalized to measure 1 rather than $2s + 1$), one obtains the continuous-spin Ising model, with $Z = (\prod_n \int_{-1}^1 (d\bar{s}_n/2)) \exp(K \sum_{\langle nn' \rangle} \bar{s}_n \bar{s}_{n'})$. For $d > 1$

this model has a transition at a finite value of K [25], namely, $\lim_{s \rightarrow \infty} K_c(s)$. Since $K_c/s^2 \rightarrow \text{constant}/s^2 \rightarrow 0$ as $s \rightarrow \infty$, it follows that $(u_s)_c \nearrow 1$ as $s \rightarrow \infty$. Hence, in terms of u_s , the physical PM phase appears to decrease in size as s increases and, in the limit as $s \rightarrow \infty$, to contract to a set of measure zero. This has also been noted in [4], where it was suggested that as $s \rightarrow \infty$, both the physical critical point and the complex- T singularities in u_s will converge to the unit circle $|u_s| = 1$. In the case of the physical critical point, one should note, however, that this is really due to the definition of u_s ; in fact, in a fixed variable such as K or v , the physical PM phase actually increases in extent, reaching a limiting size, as $s \rightarrow \infty$. From our plots of zeros, we conclude more generally that not just the PM phase but the O phases also cluster more closely around the unit circle $|u_s| = 1$ as s increases. We can thus state a stronger form of the conjecture of [4]: As $s \rightarrow \infty$, the complex-temperature phase boundaries will approach this unit circle, and in this limit, one will be left with only the FM phase for $|u_\infty| < 1$ and the AFM phase for $|u_\infty| > 1$.

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