A Connection Between Complex-Temperature Properties of the 1D and 2D Spin $s$ Ising Model

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Abstract

Although the physical properties of the 2D and 1D Ising models are quite different, we point out an interesting connection between their complex-temperature phase diagrams. We carry out an exact determination of the complex-temperature phase diagram for the 1D Ising model for arbitrary spin $s$ and show that in the $u_s = e^{-K/s^2}$ plane (i) it consists of $N_{c,1D} = 4s^2$ infinite regions separated by an equal number of boundary curves where the free energy is non-analytic; (ii) these curves extend from the origin to complex infinity, and in both limits are oriented along the angles $\theta_n = (1 + 2n)\pi/(4s^2)$, for $n = 0, ..., 4s^2 - 1$; (iii) of these curves, there are $N_{c,NE,1D} = N_{c,NW,1D} = \lfloor s^2 \rfloor$ in the first and second (NE and NW) quadrants; and (iv) there is a boundary curve (line) along the negative real $u_s$ axis if and only if $s$ is half-integral. We note a close relation between these results and the number of arcs of zeros protruding into the FM phase in our recent calculation of partition function zeros for the 2D spin $s$ Ising model.

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Recently, we presented calculations of the complex-temperature (CT) zeros of the partition functions for square-lattice Ising models with several higher values of spin, $s = 1$, $3/2$, and $2$ [1]. In the thermodynamic limit, these zeros merge to form curves across which the free energy is non-analytic, and thus calculations for reasonably large finite lattices give insight into the complex-temperature phase diagrams of these models. These phase diagrams consist of the complex-temperature extensions of the $Z_2$-symmetric, paramagnetic (PM) phase; of the two phases in which the $Z_2$ symmetry is spontaneously broken with long-range ferromagnetic (FM) and antiferromagnetic (AFM) order; and, in addition, certain phases which have no overlap with any physical phase (denoted “O” for other). Some of the zeros lie along curves which, in the thermodynamic limit, separate the various phases. In addition, there are zeros lying along various curves or arcs which terminate in the interiors of the FM and AFM phase. Physical and CT singularities of the magnetization, susceptibility, and specific heat obtained from analysis of low-temperature series have been discussed recently for the square lattice Ising model with the higher spin values $s = 1$ [2] and $s = 1$, $3/2$, $2$, $5/2$, and $3$ [3].

Here we give some further insight into the complex-temperature phase diagrams for higher-spin Ising models. We first report an exact determination of the CT phase diagrams of the 1D Ising model for arbitrary spin $s$. We then point out a very interesting connection between features of these 1D phase diagrams and certain properties of the phase diagrams of the Ising model on the square lattice inferred from our calculation of partition function zeros for higher spin values. This connection is useful because, unlike the 2D spin $1/2$ case, no exact closed-form solution has ever been found for the 2D Ising model with spin $s \geq 1$, and hence further elucidation of its properties is of continuing value, especially insofar as these constrain conjectures for such a solution. Of course, the physical properties of a spin model at its lower critical dimensionality (here $d_{\ell.c.d.} = 1$) are quite different from those for $d > d_{\ell.c.d.}$. However, as we shall discuss, some of the properties of the CT phase diagram for $d = 2$ exhibit simple relations with the $d = 1$ case.  

There are several reasons why CT properties of statistical mechanical models are of interest. First, one can understand more deeply the behavior of various thermodynamic quantities by seeing how they behave as analytic functions of complex temperature. Second, one can see how the physical phases of a given model generalize to regions in appropriate CT variables. Third, a knowledge of the CT singularities of quantities which have not been calculated exactly helps in the search for exact expressions for these quantities. Fourth, one can see how CT singularities in functions such as the magnetization and susceptibility are

\[ ^1 \text{Indeed, from the } d = 1 + \epsilon \text{ and } d = 2 + \epsilon \text{ expansions for the Ising and O(N) models [4], one knows that expansions above } d_{\ell.c.d.} \text{ can even give useful information about physical critical behavior.} \]
associated with the boundaries of the phases and with other points where the free energy is non-analytic. Such CT properties were first considered (for the 2D, \( s = 1/2 \) square-lattice Ising model) in Ref. [5] and for higher-spin (2D and 3D) Ising models in Ref. [6].

The spin \( s \) (nearest-neighbor) Ising model is defined, for temperature \( T \) and external magnetic field \( H \), by the partition function \( Z = \sum_{n} e^{-\beta H} \) where, in a commonly used normalization,

\[
H = -(J/s^2) \sum_{<nn'>} S_n S_{n'} - (H/s) \sum_n S_n
\]

where \( S_n \in \{ -s, -s+1, \ldots, s-1, s \} \) and \( \beta = (k_B T)^{-1} \). \( H = 0 \) unless otherwise indicated. We define \( K = \beta J \) and \( u_s = e^{-K/s^2} \). \( Z \) is then a generalized (i.e. with negative as well as positive powers) polynomial in \( u_s \). The (reduced) free energy is \( f = -\beta F = \lim_{N_s \to \infty} N_s^{-1} \ln Z \) in the thermodynamic limit.

For \( d = 1 \), one can solve this model by transfer matrix methods. One has

\[
Z = \text{Tr}(\mathcal{T}^N) = \sum_{j=1}^{2s+1} \lambda_{s,j}^N
\]

where the \( \lambda_{s,j}, j = 1, \ldots, 2s + 1 \) denote the eigenvalues of the transfer matrix \( \mathcal{T} \) defined by \( \mathcal{T}_{nn'} = \lan n \mid \exp((K/s^2)S_n S_{n'}) \mid n' \ran \) (we assume periodic boundary conditions for definiteness). It is convenient to analyze the phase diagram in the \( u_s \) plane. For physical temperature, phase transitions are associated with degeneracy of leading eigenvalues [7]. There is an obvious generalization of this to the case of complex temperature: in a given region of \( u_s \), the eigenvalue of \( \mathcal{T} \) which has maximal magnitude, \( \lambda_{\text{max}} \), gives the dominant contribution to \( Z \) and hence, in the thermodynamic limit, \( f \) receives a contribution only from \( \lambda_{\text{max}} \): \( f = \ln(\lambda_{\text{max}}) \). For complex \( K \), \( f \) is, in general, also complex. The CT phase boundaries are determined by the degeneracy, in magnitude, of leading eigenvalues of \( \mathcal{T} \). As will be evident in our 1D case, as one moves from a region with one dominant eigenvalue \( \lambda_{\text{max}} \) to a region in which a different eigenvalue \( \lambda'_{\text{max}} \) dominates, there is a non-analyticity in \( f \) as it switches from \( f = \ln(\lambda_{\text{max}}) \) to \( f = \ln(\lambda'_{\text{max}}) \). The boundaries of these regions are defined by the degeneracy condition \( |\lambda_{\text{max}}| = |\lambda'_{\text{max}}| \). These form curves in the \( u_s \) plane.

Of course, a 1D spin model with finite-range interactions has no non-analyticities for any (finite) value of \( K \), so that, in particular, the 1D spin \( s \) Ising model is analytic along the positive real \( u_s \) axis. For a bipartite lattice, \( Z \) and \( f \) are invariant under \( K \to -K \), i.e., \( u_s \to 1/u_s \). It follows that the CT phase diagram also has this symmetry, i.e., is invariant under inversion about the unit circle in the \( u_s \) plane. This symmetry also holds for a finite bipartite lattice; for \( d = 1 \), the lattice is bipartite iff \( N \) is even, and for our comments

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2By “curves” we include also the special case of a line segment.
about finite-lattice results, we thus make this restriction. Further, since the $\lambda_{s,j}$ are analytic functions of $u_s$, whence $\lambda_{s,j}(u_s^*) = \lambda_{s,j}(u_s)^*$, it follows that the solutions to the degeneracy equations defining the boundaries between different phases, $|\lambda_{s,j}| = |\lambda_{s,\ell}|$, are invariant under $u_s \to u_s^*$. Hence, the complex-temperature phase diagram is invariant under $u_s \to u_s^*$.

We shall present results for a few $s$ values explicitly. For $s = 1/2$, one has $(u_{1/2})^{1/2} = 1\pm (u_{1/2})^{1/2}$. $f$ is an analytic function of $u_{1/2}$ except at points which constitute the solution to $|\lambda_{1/2,1}| = |\lambda_{1/2,2}|$; these comprise the negative real axis, $-\infty \leq u_{1/2} \leq 0$. Apart from this line, the dominant eigenvalue of $\mathcal{T}$ is $\lambda_{1/2,1}$. For $s = 1$, the eigenvalues of $T_s$ are $\lambda_{1,1} = u_1^{-1} - u_1$ and

$$\lambda_{1,j=2,3} = (1/2)\left[u_1^{-1} + 1 + u_1 \pm (u_1^{-2} - 2u_1^{-1} + 11 - 2u_1 + u_1^2)^{1/2}\right]$$

(3)

As shown in Fig. 1(a), the phase diagram consists of four phases, the complex-temperature extension of the PM phase, together with three O phases. The curves separating these phases are the solutions of $|\lambda_{1,1}| = |\lambda_{1,2}|$. The third eigenvalue, $\lambda_{1,3}$, is always subdominant. In the two phases containing the real $u_s$ axis, $\lambda_{1,2}$ has maximal magnitude, while in the two containing the imaginary $u_s$ axis, $\lambda_{1,1}$ is dominant. The CT zeros of $Z$ calculated for finite lattices lie on or close to these curves, starting a finite distance from the origin and being distributed in a manner symmetric under the inversion $u_s \to 1/u_s$. As the lattice size increases, the zeros spread out, the one with smallest (largest) magnitude moving closer to (farther from) the origin. For $s = 3/2$, the eigenvalues are given by

$$2u^{9/4}\lambda_{3/2,j} = (1 + u)^2(1 + \eta u^{5/2})$$

$$\zeta\left[(1 - 2u^2 + 4u^3 + u^4 + u^5 + 4u^6 - 2u^7 + u^9) - 2\eta u^{5/2}(1 - 6u^2 + u^4)\right]^{1/2}$$

(4)

where here $u \equiv u_{3/2}$ and $(\eta, \zeta) = (+, +), (-, +), (+, -), (-, -)$ for $j = 1, 2, 3, 4$. The phase diagram is shown in Fig. 1(b) and consists of nine regions separated by the curves where $|\lambda_{3/2,1}| = |\lambda_{3/2,2}|$. In the region containing the positive real $u_s$ axis, $\lambda_{3/2,1}$ is dominant, and as one makes a circle around the origin, each of the nine times that one crosses a boundary, there is an alternation between $\lambda_{3/2,1}$ and $\lambda_{3/2,2}$ as the dominant eigenvalue.

We find the following results for general $s$: (i) the complex-temperature phase diagram consists of

$$N_{c,1D} = 4s^2$$

(5)

(infinite) regions separated by an equal number of boundary curves where the free energy is non-analytic; (ii) these curves extend from the origin to complex infinity, and in both limits are oriented along the angles

$$\theta_n = \frac{(1 + 2n)\pi}{4s^2}$$

(6)
for \( n = 0, \ldots, 4s^2 - 1 \); (iii) of these curves, there are

\[ N_{c,NE,1D} = N_{c,NW,1D} = [s^2] \quad (7) \]

in the first and second (NE and NW) quadrants, where \([x]\) denotes the integral part of \(x\); and (iv) there is a boundary curve (which in this case is a straight line) along the negative real \(u_s\) axis if and only if \(s\) is half-integral. \((N_{c,SE,1D} = N_{c,NE,1D} \text{ and } N_{c,SW,1D} = N_{c,NW,1D} \text{ by the } u \to u^* \text{ symmetry.})\) To derive these results, we carry out a Taylor series expansion of the \(\lambda_{s,j}\) in the vicinity of \(u_s = 0\). The dominant eigenvalues have the form

\[ u_s^{s^2} \lambda_{s,j} = 1 + \ldots + a_{s,j} u_s^{2s^2} + \ldots \quad (8) \]

where the first \(\ldots\) dots denote terms which are independent of \(j\) and the second \(\ldots\) dots represent higher order terms which are dependent upon \(j\). Setting \(u_s = re^{i\theta}\) and solving the equation \(|\lambda_{s,j}| = |\lambda_{s,\ell}|\) yields \(\cos(2s^2\theta) = 0\), whence

\[ 2s^2\theta = \frac{\pi}{2} + n\pi, \quad n = 0, \ldots, 4s^2 - 1 \quad (9) \]

Each of these solutions yields a curve across which \(f\) is non-analytic, corresponding to a switching of dominant eigenvalue. These curves cannot terminate since if they did, one could analytically continue from a region where the expression for \(f\) depends on a given dominant eigenvalue, to a region where it depends on a different eigenvalue. Owing to the \(u_s \to 1/u_s\) symmetry of the model, a given curve labelled by \(n\) approaches complex infinity in the same direction \(\theta_n\) as it approaches the origin. This yields (i) and (ii). From (6), it follows that

\[ 0 < \theta_n < \pi/2 \quad \text{for } 0 \leq n < [s^2 - 1/2] \quad (10) \]

which comprises \([s^2]\) values, and similarly,

\[ \pi/2 < \theta_n < \pi \quad \text{for } [s^2 - 1/2] < n < [2s^2 - 1/2] \quad (11) \]

which again comprises \([s^2]\) values. Finally, if and only if \(s\) is half-integral, then the equation \(\theta_n = \pi\) has a solution (for integral \(n\), viz., \(n = (2s + 1)(2s - 1)/2\). From the \(u_s \to u_s^*\) symmetry of the phase diagram, the curve corresponding to this solution must lie on the negative real axis for all \(r\), not just \(r \to 0\) and \(r \to \infty\). This yields (iii)-(iv). \(\Box\).

We note that from (6), the angular size of each region near the origin (or infinity) is

\[ \Delta\theta = \frac{\pi}{2s^2} \quad (12) \]

Also, from the \(u_s \to u_s^*\) symmetry of the phase diagram, it follows in particular, that for each curve starting out from the origin at \(\theta_n\), there is a complex conjugate curve at \(-\theta_n\). As
is true of any theory at its lower critical dimensionality, the model is singular at $K = \infty$, i.e., $u_s = 0$. If and only if $s$ is integral, the $n'$th curve has another, $m'$th curve which is related to it by $\theta_m = \theta_n + \pi$ (whence $m = n + 2s^2$), so that as one travels through the origin on the $n'$th curve, one emerges on the other side on the $m'$th curve.

As one can see from Fig. 1, as the boundary curves approach the unit circle $|u_s| = 1$, some of them twist in $s$-dependent ways. Interestingly, several of the points where they cross the unit circle coincide with points which we inferred to be likely multiple (=intersection) points of the boundary curves of the complex-temperature phase diagrams for the corresponding spin $s$ 2D Ising model. For example, for the 1D $s = 1$ model, the $n = 0$ and $n = 1$ curves cross the unit circle at $u_1 = i$ and $u_1 = e^{2\pi i/3}$, respectively, and hence the complex-conjugate curves ($n = 3$ and $n = 2$) cross this circle at $u_1 = -i$ and $u_1 = e^{-2\pi i/3}$. The points $u_1 = e^{\pm 2\pi i/3}$ are precisely the values which we inferred for the intersection points of boundary curves in the second (“northwest”=NW) and third (SW) quadrants of the 2D $s = 1$ phase diagram from our calculation of partition function zeros [1]. For the 1D $s = 3/2$ case, the $n = 0, 1, 2$ and 3 curves cross the unit circle at the respective points $u_{3/2} = e^{i\pi/3}$, $e^{2i\pi/5}$, $i$, and $e^{4i\pi/5}$, and so forth for the complex conjugate curves. Among these, the points $\pm i$ and $e^{\pm 4i\pi/5}$ are points inferred as likely intersection points of phase boundaries in the NW and SW quadrants of the $u_{3/2}$ plane for the 2D $s = 3/2$ model [1]. Similar correspondences hold for $s = 2$. These are intriguing results.

The spin 1/2 Ising model is equivalent to the two-state Potts model. While determining the CT phase diagram of the 1D spin $s$ Ising model, it is thus also of interest to compare this with that of the 1D $q$-state Potts model, defined by $Z_P = \sum_{\sigma_n} e^{-\beta \mathcal{H}_P}$ with $\mathcal{H}_P = -J_P \sum_{\langle mn \rangle} \delta_{\sigma_m \sigma_n}$, where $\sigma_n \in \{1, \ldots, q\}$. We define $K_P = \beta J_P$ and $u_P = e^{-K_P}$. The eigenvalues of the transfer matrix are $\lambda = u_P^{-1} - 1$ ($q - 1$ times) and $\lambda' = u_P^{-1} + (q - 1)$. Setting $u_P = re^{i\theta}$, the equation for $|\lambda| = |\lambda'|$ is

$$q \left( (q - 2)r + 2 \cos \theta \right) = 0$$

(13)

For $q = 2$, the solution is the imaginary axis, $u_P = \pm ir$, equivalent to the negative real axis in the $u_{1/2}$ variable. For $q \neq 2$ (and $q \neq 0$), the solution is $\cos \theta = -(q - 2)r/2$ for $0 \leq r \leq 2/(q - 2)$, i.e.,

$$u_P = \frac{-1 + e^{i\omega}}{q - 2}$$

(14)

for $0 \leq \omega < 2\pi$, viz., a circle centered at $u_P = -1/(q - 2)$ with radius $1/(q - 2)$. Thus, for all $q > 2$, the complex-temperature phase diagram is qualitatively the same, consisting of a

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3Recall that the equivalence of $\mathcal{H}_P$ for $q = 2$ to [1] for $s = 1/2$ entails $K_P = 2K$. 
PM phase containing the positive real \( u \) axis, and an O phase inside the circle. This is quite different from the 1D spin \( s \) Ising phase diagram, for which the number of phases does depend on \( s \). This difference can be traced to the fact that the structure of the transfer matrix is qualitatively the same for different \( q \) in the Potts model (all diagonal entries equal to \( u^{-1} \) and all off-diagonal entries equal to 1), whereas it depends on \( s \) in the Ising model.

In addition to the correspondences already above, we have found a further very interesting connection between the features of the 1D spin \( s \) Ising model and certain properties which we have observed from our calculations of partition function zeros for the 2D (square-lattice) Ising model with \( s = 1, \frac{3}{2}, \) and 2 \(^4\). One of the interesting features which we found in the 2D case was a certain number of finite arcs which protrude into the FM phase. (By the \( u_s \to \frac{1}{u_s} \) symmetry, there are also corresponding arcs protruding into the AFM phase). By combining our results with low-temperature series analyses in Refs. \(^2\) \(^3\), we observed that the divergences of the spontaneous magnetization \( M \) (which also imply divergences in the susceptibility \(^10\)) occur at the endpoints of these arcs. The arc endpoints are thus of considerable interest for the study of CT singularities.

For the cases \( s = 1, \frac{3}{2}, \) and 2, the numbers of arcs protruding into and terminating in the first and second (NE and NW) quadrants of the (complex-temperature extension of the) FM phase are given in terms of the numbers of boundary curves of the corresponding 1D spin \( s \) model as

\[
N_{e,NE,2D} = N_{c,NE,1D} - 1 = [s^2] - 1
\]  \hspace{1cm} (15)

and

\[
N_{e,NW,2D} = N_{c,NW,1D} = [s^2]
\]  \hspace{1cm} (16)

so that the total number of arcs protruding into the FM (equivalently, AFM) phase is \( 4[s^2] - 2 \). Our derivations in the present paper thus provide the explanation underlying our conjecture \(^4\) that the total number of arcs protruding into the FM (equivalently AFM) phase for the Ising model on the square lattice with arbitrary spin \( s \) is

\[
N_{e,FM} = N_{e,AFM} = \max\{0, 4[s^2] - 2\}
\]  \hspace{1cm} (17)

where we have incorporated also the exact result that \( N_{e,FM} = N_{e,AFM} = 0 \) for \( s = 1/2 \).

One can qualitatively describe how the complex-temperature phase diagram changes as one goes from \( d = 1 \) to \( d = 2 \) as follows. For \( d > 1 \), the model is analytic in the vicinity of \( u_s = 0 \) (equivalently, it has a low-temperature series expansion with finite radius of convergence), so one knows that all of the \( 4s^2 \) curves which emanate from \( u_s = 0 \) must move

\(^4\)One may also formally consider other values of \( q \), as in the 2D Potts model. In particular, for \( q = 0 \), all eigenvalues are identically equal, and the phase diagram is trivial.
away from the origin. Evidently, the inner branches of the \( n = 0 \) curve and its complex conjugate \( (n = 4s^2 - 1) \) curve move to the right and join at the point \( (u_s)_c = e^{-K_c/s^2} \) which constitutes the critical point between the FM and PM phases; given the \( u_s \to 1/u_s \) symmetry, this means that the outer branches no longer run separately to complex infinity but join each other at the critical point \( 1/(u_s)_c \) separating the PM and AFM phases of the 2D model. This leaves \([s^2] - 1\) curves in the first (NE) quadrant, which form finite arcs; the inner and outer branches of these arcs protrude into and terminate in the FM and AFM phases respectively (these branches and phases are interchanged by the \( u_s \to 1/u_s \) mapping). The situation in the complex conjugate fourth (SE) quadrant is the same, by the \( u_s \to u_s^* \) symmetry of the phase diagram. In the second (NW) quadrant, the \([s^2]\) curves in 1D correspond to the \([s^2]\) arcs in 2D, which again have inner and outer branches terminating in the FM and AFM phases. The symmetry under complex conjugation implies the same for the third (SW) quadrant.

In summary, we have found an intriguing connection between the complex-temperature phase diagrams, as calculated exactly for 1D and inferred from partition function zeros for 2D, of the Ising model with higher spin. Our derivations here explain the basis for the conjecture that we made in Ref. [1] on the total number of arc endpoints in the FM phase and hence complex-temperature divergences in the magnetization for the square–lattice Ising model with arbitrary spin.

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Figure Captions

Fig. 1. Complex-temperature phase diagrams in the $u_s$ plane for the 1D Ising model with (a) $s = 1$ (with $u \equiv u_1$) and (b) $s = 3/2$ (with $u \equiv u_{3/2}$). The phase boundaries are shown as the dark curves (including the line along the negative $u_s$ axis for $s = 3/2$). The unit circle is drawn in lightly for reference.
