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LETTER TO THE EDITOR

On the boundaries and density of partition function temperature zeros for the two-dimensional Ising model

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Abstract. Explicit expressions, which determine the boundaries of the regions containing temperature zeros of the partition function of the two-dimensional Ising model on an anisotropic triangular lattice, are obtained, along with a general formula for the density of zeros valid everywhere in regions containing zeros.

Recent numerical and algebraic studies by several authors (Stephenson and Couzens 1984, Stephenson and van Aalst 1986, van Saarloos and Kurtze 1984, Wood 1985) of the temperature zeros of the partition function of the two-dimensional Ising model on quadratic and triangular lattices have revealed that these zeros are generally confined to finite regions of the complex plane of the Boltzmann factor for the interaction energy.

From the mathematical point of view, the occurrence and location of the boundaries of these regions is of some interest. It is easy to see, although proof seems to be lacking, in the cases of the quadratic and partially anisotropic triangular lattices, that the relevant boundaries are determined by giving special values to the angles in the polynomial factors whose roots yield the partition function zeros. However, on a general anisotropic triangular lattice, the boundary problem cannot be resolved by such elementary observations and a more systematic approach is required.

In this letter, I show first quite generally how the boundaries of a region containing zeros of any two-parameter family of functions of a complex variable can be located in the complex plane. Then I derive the explicit 'boundary equation' for the zeros of the Ising model partition function on a general anisotropic triangular lattice. The known results for the quadratic and partially anisotropic triangular lattices are included, and are now derived, as special cases of the more general result.

Furthermore, I have rearranged the defining expression for the (two-dimensional) density of zeros into a form which permits its numerical evaluation everywhere in the regions of the complex plane which contain zeros. Moreover, from this new expression one sees that the density of zeros is infinite on the boundary.

Details of the numerical calculations of boundaries and densities of zeros will be presented elsewhere.

The polynomial factors which determine the zeros of the partition function of the Ising model on an anisotropic $m \times n$ two-dimensional triangular lattice have the form

$$\begin{aligned} f(z; \phi_r, \phi_s) &\equiv g + \mathrm{i}h \\ &= A + B\cos\phi_r + C\cos\phi_s + D\cos(\phi_r + \phi_s) \end{aligned} \tag{1}$$

where

$$\phi_r = (2r-1)\pi/m \qquad r = 1, \ldots, m$$
$$\phi_s = (2s-1)\pi/n \qquad s = 1, \ldots, n.$$

If the three interactions on the triangular lattice are J_1, J_2, J_3 along the horizontal, vertical and diagonal axes, respectively, and J is their greatest common factor, then one has $J_1 = aJ$, $J_2 = bJ$, $J_3 = cJ$, for integer a, b, c, and the Boltzmann factor is

$$z \equiv x + \mathrm{i}y = \exp(-J/k_{\mathrm{B}}T). \tag{2}$$

In (1) A, B, C, D, are polynomials in z:

$$\begin{aligned} A &= 1 + z^{2(a+b)} + z^{2(b+c)} + z^{2(c+a)} = 1 + z^{2d} + z^{2e} + z^{2f} \\ B &= 2z^{b+c}(z^{2a}-1) = 2(z^{d+e} - z^f) \\ C &= 2z^{c+a}(z^{2b}-1) = 2(z^{f+d} - z^e) \\ D &= 2z^{a+b}(z^{2c}-1) = 2(z^{e+f} - z^d) \end{aligned} \tag{3}$$

where

$$d = a + b \qquad e = c + a \qquad f = b + c. \tag{4}$$

Thus we have a two-parameter set of zeros, determined by

$$f = 0 \qquad \text{so } g(x, y; \phi_r, \phi_s) = 0 \qquad \text{and} \qquad h(x, y; \phi_r, \phi_s) = 0. \tag{5}$$

Now suppose in the complex plane $z = x + \mathrm{i}y$ we change x while keeping y fixed within a region containing zeros where $f = 0$, thereby inducing corresponding changes in the values of ϕ_r and ϕ_s. These changes are related through the partial derivatives of g and h with respect to x:

$$\frac{\partial g}{\partial x} = -\left[\frac{\partial g}{\partial \phi_r}\frac{\partial \phi_r}{\partial x} + \frac{\partial g}{\partial \phi_s}\frac{\partial \phi_s}{\partial x}\right] \qquad \frac{\partial h}{\partial x} = -\left[\frac{\partial h}{\partial \phi_r}\frac{\partial \phi_r}{\partial x} + \frac{\partial g}{\partial \phi_s}\frac{\partial \phi_s}{\partial x}\right] \tag{6}$$

or in a more compact notation, denoting derivatives of g and h with respect to ϕ_r and ϕ_s by subscripts r and s:

$$g_x = -[g_r\phi_{rx} + g_s\phi_{sx}] \qquad h_x = -[h_r\phi_{rx} + h_s\phi_{sx}]. \tag{7}$$

Thus we have a pair of simultaneous linear equations for ϕ_{rx} and ϕ_{sx}. These equations fail to have a solution on a boundary where the determinant of the coefficients vanishes:

$$g_r h_s - g_s h_r = 0. \tag{8}$$

Similarly, if one keeps x fixed and changes y instead, one obtains two equations for ϕ_{ry} and ϕ_{sy}:

$$g_y = -[g_r\phi_{ry} + g_s\phi_{sy}] \qquad h_y = -[h_r\phi_{ry} + h_s\phi_{sy}] \tag{9}$$

which have no solution for ϕ_{ry} and ϕ_{sy} when the *same* equation (8) holds. So equation (8) becomes our 'boundary equation'.

The boundary equation can also be derived by the following alternative method. We consider the case when both parameters vary along a boundary. Following the method described by Piaggio (1965, ch 6) in his treatise on differential equations, we solve the equation $h = 0$ in (5) for ϕ_s in terms of ϕ_r, x and y, and substitute in g, so

$$g(x, y; \phi_r, \phi_s(x, y; \phi_r)) = 0. \tag{10}$$

The above equation $g=0$ represents a one-parameter (ϕ_r) family of curves in the x, y plane. The envelope of this set of curves is, following Piaggio, obtained by differentiating with respect to the parameter, to obtain

$$\frac{\partial g}{\partial \phi_r}+\frac{\partial g}{\partial \phi_s}\left(\frac{\partial \phi_s}{\partial \phi_r}\right)_{x,y}=0 \tag{11}$$

and similarly for h:

$$\frac{\partial h}{\partial \phi_r}+\frac{\partial h}{\partial \phi_s}\left(\frac{\partial \phi_s}{\partial \phi_r}\right)_{x,y}=0. \tag{12}$$

Assuming that these two envelopes are identical, and form the boundary of the zero distribution, we obtain the same 'boundary equation' as before in (8):

$$\frac{\partial g}{\partial \phi_r}\frac{\partial h}{\partial \phi_s}-\frac{\partial g}{\partial \phi_s}\frac{\partial h}{\partial \phi_r}=0.$$

The LHS of (8) is just the Jacobian of g, h with respect to x, y.

To see why the same derivative $(\partial\phi_s/\partial\phi_r)_{xy}$ is present in both envelope equations (11) and (12), consider two solution curves to (10) corresponding to fixed values ϕ_{r1}, ϕ_{r2}, of the parameter differing by a small increment $\delta\phi_r$. Let these adjacent curves intersect at a point x, y lying on the boundary. Along these curves the corresponding values ϕ_{s1}, ϕ_{s2}, of the other parameter are obtained by solving the equation $h=0$, and differ by $\delta\phi_s$. So at the point of intersection (x, y) both the conditions $g=0$ and $h=0$ are satisfied. Consequently the increments $\delta\phi_r$, $\delta\phi_s$, and the associated derivative, are common to both envelopes.

Now applying (8) to the function $f=g+\mathrm{i}h$ in (1) for the Ising model, we obtain the 'boundary equation'

$$\begin{aligned}(B'C''-B''C')&\sin\phi_r\sin\phi_s\\&+\sin(\phi_r+\phi_s)[(B'D''-B''D')\sin\phi_r-(C'D''-C''D')\sin\phi_s]\\&\equiv\frac{\partial(g,h)}{\partial(\phi_r,\phi_s)}=0\end{aligned} \tag{13}$$

where we have written $B=B'+\mathrm{i}B''$, etc.

In order to determine the boundary, one has to solve the boundary equation (13) simultaneously with equation (1) for the zeros.

For the quadratic lattice, $J_3=0$ so $D=0$, and the boundary values of the angles ϕ_r and ϕ_s are 0 or π, as expected. For the partially anisotropic triangular lattice, $J_1=J_2$ so $B=C$, and now $\phi_r=\pm\phi_s$. In general there is no simple relation between the angles along the boundary and it is necessary to solve the boundary equation (13) numerically in conjunction with equation (1) for the zeros. The smallest values of (a, b, c) which yield a non-trivial triangular lattice are (3, 2, 1). The variation of the angles around the various segments of the boundary can most easily be displayed by plotting ϕ_s against ϕ_r as in figure 1. The complete boundary is shown as full curves in figure 2, where 'interior' zeros for a 16×16 lattice have also been plotted.

On the quadratic lattice with $D=0$ there is substantial simplification in (1), which becomes

$$\begin{aligned}g&=A'+B'\cos\phi_r+C'\cos\phi_s=0\\h&=A''+B''\cos\phi_r+C''\cos\phi_s=0.\end{aligned} \tag{14}$$

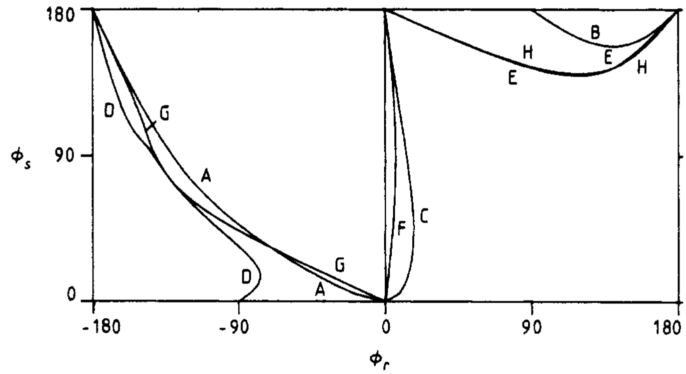

Figure 1. Graphs of ϕ_s plotted against ϕ_r, showing the variation in the angles along the various segments of the boundary (as in figure 2) for a (3, 2, 1) anisotropic triangular lattice. For convenience we have altered the range of the angles. The complete diagram is obtained by reversing the signs of both ϕ_r and ϕ_s.

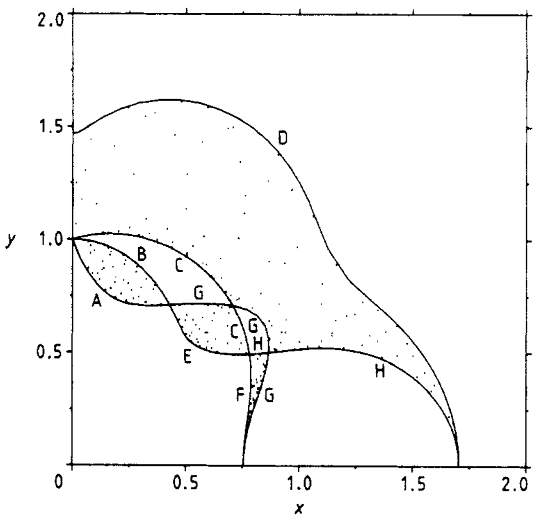

Figure 2. The complex z plane showing the boundary lines (full curves) for a (3, 2, 1) anisotropic triangular lattice. The various segments are labelled A-H. 'Interior' zeros for a 16×16 lattice have also been plotted. The complete distribution of zeros is symmetrical on reflection in both axes.

These are two simultaneous linear equations for the cosines, with solution

$$\begin{aligned}\cos\phi_r &= [A'C''-A''C']/[B'C''-B''C'] \equiv E\\ \cos\phi_s &= [A'B''-A''B']/[C'B''-C''B'] \equiv F.\end{aligned} \tag{15}$$

Now differentiating with respect to x and y in turn:

$$\begin{aligned} -\sin\phi_r\frac{\partial\phi_r}{\partial x} &= E_x \qquad & -\sin\phi_r\frac{\partial\phi_r}{\partial y} &= E_y\\ -\sin\phi_s\frac{\partial\phi_s}{\partial x} &= F_x \qquad & -\sin\phi_s\frac{\partial\phi_s}{\partial y} &= F_y.\end{aligned} \tag{16}$$

Taking the derivatives of ϕ_r and ϕ_s from (16), one can in this case construct the density of zeros directly from the basic formula (Stephenson and Couzens 1984), obtaining

$$2\pi^2 G(x, y) = \left|\frac{\partial(\phi_r, \phi_s)}{\partial(x, y)}\right| = |(E_x F_y - E_y F_x)|/(\sin\phi_r \sin\phi_s). \tag{17}$$

However, the calculation of the derivatives of E and F is extremely awkward and it is easier to use the formula (22) derived below.

A similar direct calculation can be made for the partially anisotropic triangular lattice, for which $B = C$. The resulting formula for the density of zeros resembles (17) and is equally inconvenient for calculation.

The density of zeros per lattice site is given by

$$2\pi^2 G(x, y) = \left|\frac{\partial(\phi_r, \phi_s)}{\partial(x, y)}\right| = \left|\frac{\partial(x, y)}{\partial(\phi_r, \phi_s)}\right|^{-1}. \tag{18}$$

But

$$\frac{\partial(g, h)}{\partial(\phi_r, \phi_s)} = -\frac{\partial(g, h)}{\partial(x, y)}\frac{\partial(x, y)}{\partial(\phi_r, \phi_s)} \tag{19}$$

where the minus sign is essential since the variables are interrelated by (1). This apparently little known result may be proved by writing equations (7) and (9) in matrix form:

$$\begin{pmatrix} g_x & g_y \\ h_x & h_y \end{pmatrix} = -\begin{pmatrix} g_r & g_s \\ h_r & h_s \end{pmatrix}\begin{pmatrix} \phi_{rx} & \phi_{ry} \\ \phi_{sx} & \phi_{sy} \end{pmatrix} \tag{20}$$

and taking the determinants of both sides. Moreover, using the Cauchy-Riemann conditions, the Jacobian of g, h with respect to x, y is

$$\frac{\partial(g, h)}{\partial(x, y)} = |f'(z)|^2. \tag{21}$$

So we obtain

$$2\pi^2 G(x, y) = |f'(z)|^2 \left|\frac{\partial(g, h)}{\partial(\phi_r, \phi_s)}\right|^{-1}. \tag{22}$$

For the Ising model the remaining Jacobian, in the denominator of (22), is given explicitly as in (13). All the quantities in this form for the density of zeros can be calculated directly, using (1) and (13).

Finally we observe, on applying the 'boundary equation' (8) to the denominator in (22), that the density of zeros is infinite on the boundary, provided $f'(z) \neq 0$, which is generally the case except at critical points, where (1) is a perfect square.

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